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HOMOGENIZATION OF BOUNDARY LAYERS IN THE BOLTZMANN–POISSON SYSTEM*

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Abstract. We homogenize the Boltzmann–Poisson system where the background medium is given by a periodic permittivity and a periodic charge concentration. The domain is the half-space with a periodic charge concentration on the boundary. Hence the domain consists of cells in $\mathbb{R}^3$ that are periodically repeated in two dimensions and unbounded in the third dimension. We obtain formal results for this homogenization problem. We prove the existence and uniqueness of the solution of the Laplace and Poisson problems in the fast variables with periodic and surface charge boundary conditions generating an electric field at infinity, obtaining formal solutions for the potential in terms of Magnus expansions for the case where the diagonal permittivity matrix depends on the vertical fast variable. Further on, splitting the potential into a stationary part and a self-consistent part, performing the two-scale homogenization expansions for the Poisson and the Boltzmann equations, and applying a solvability condition, we arrive at the drift-diffusion equations for the boundary-layer problem.

Key words. homogenization, Boltzmann–Poisson system, nanowire sensors

AMS subject classifications. 82C05, 82C10, 82C40

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1. Introduction.

In this work, the Boltzmann–Poisson system describes charge transport in the general setting of the presence of a manifold that carries a periodic charge concentration. As the spatial period of the oscillations of the charge concentration goes to zero, a homogenization problem arises and effective equations are sought.

The Boltzmann–Poisson system considered here is general enough to describe various physical systems. One example is nanowire bio- and gas sensors [9, 10, 11, 12, 13, 14]; in [10], semiconducting nanowires were fabricated and characterized as highly sensitive and selective sensors for the label-free detection of low concentrations of many types of biomolecules. Such nanoscale devices are only one motivation for the model equations, which include the more general physical situation of phenomena at a surface due to a spatially fast oscillating electrostatic potential. Therefore, we study the homogenization of boundary layers in the Boltzmann–Poisson model for collisional electron transport described below.

We consider the Boltzmann–Poisson system in the form

$$-\nabla \cdot (A^\varepsilon \nabla u^\varepsilon) = \rho^\varepsilon + g^\varepsilon, \tag{1.1a}$$

$$\partial_t f^\varepsilon + \frac{1}{\varepsilon}\{E^\varepsilon, f^\varepsilon\}_{xv} = \frac{1}{\varepsilon^2} Q(f^\varepsilon) \tag{1.1b}$$

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in a diffusive scaling and on the whole space $\mathbb{R}^d$. In the Poisson equation, $A^\varepsilon(x) = A(x, x/\varepsilon)$ is a matrix and denotes the given permittivity, $u^\varepsilon(x) = u(x, x/\varepsilon)$ is the electric potential,

$$\rho^\varepsilon(t,x) = \rho(t,x,x/\varepsilon) := \int_{\mathbb{R}^d} f(t,x,x/\varepsilon,v)\mathrm{d}v$$

is the concentration of free charges, and $g^\varepsilon(x) = g(x, x/\varepsilon)$ is the given concentration of fixed charges. In the Boltzmann equation, $f^\varepsilon(t,x,v) = f(t,x,x/\varepsilon,v)$ denotes the distribution function of particles in the phase space (x,v) considering a velocity proportional to the momentum,

$$\{E,f\}_{xv} := \nabla_v E \cdot \nabla_x f - \nabla_x E \cdot \nabla_v f$$

is the Poisson bracket,

$$E^\varepsilon := u^\varepsilon + \frac{|v|^2}{2}$$

is the particle energy, and Q is the collision operator modeling the scattering over the electrons.

We suppose that Q is a linear operator, which is a reasonable assumption under a low density of electrons (obtaining Boltzmann statistics), and that it has the form

$$Q(f) := \int_{\mathbb{R}^d} S(x,v,v')(Mf' - M(v')f)\mathrm{d}v' \tag{1.2}$$

with M being the normalized Maxwellian

$$M(v) := \frac{e^{-|v|^2/2}}{(\sqrt{2\pi})^d}, \tag{1.3}$$

$f' := f(t,x,x/\varepsilon,v')$, and $S(x,v,v') = S(x,v',v)$ the collision cross section. In our theoretical work we will assume as in [2] that the collision cross section is uniformly bounded; i.e., $0 < \underline{S} \leq S(x,v,v') \leq \overline{S}$ holds for two constants $\underline{S}$ and $\overline{S}$. (However, there are physical situations of interest where collision cross sections that do not satisfy this requirement become relevant. For example, for the case of electron-phonon collisions in a lattice, the collision cross section is $S(x,v,v') = M^{-1}(v)\sum_{l=-1}^{+1} c_l \delta(\varepsilon(v) - \varepsilon(v') + l\hbar w)$, accounting for the electron energy transitions due to inelastic and elastic interactions with the phonons.)

Previous work related to the diffusion approximation and homogenization of the Boltzmann–Poisson model for collisional electron transport has been developed in several papers. First, we consider [2], which deals with the diffusion approximation of the semiconductor Boltzmann equation in the presence of a spatially oscillating electrostatic potential. This work proved that if the oscillation period is of the same order as the mean free path, there is convergence to the drift-diffusion equation with a homogenized potential resulting in a diffusion matrix that contains the small-scale information. The convergence was rigorously proved under Boltzmann statistics, whereas for Fermi–Dirac statistics a formal analysis was performed.

Before this work, the same authors studied the diffusion limit of the initial-value problem for the Boltzmann–Poisson system in one dimension in [1], but homogenization was not considered at that point. L^p estimates were established for the solution of the Boltzmann–Poisson system with well-prepared initial and boundary conditions by analyzing entropy production terms due to the boundary. The convergence of the solution towards the solution of the drift-diffusion-Poisson system was proved using a hybrid Hilbert expansion obtaining a convergence rate. Later on, in [7], the diffusion and homogenization approximation of the Boltzmann–Poisson system with a spatially oscillating electrostatic potential was studied. A uniform energy estimate was proved for well-prepared boundary data by analyzing the relative entropy. The convergence of the scaled Boltzmann equation coupled to the Poisson equation to a homogenized drift-diffusion-Poisson system was proved using an averaging lemma and two-scale convergence techniques.

In previous work, a multiscale model for the electrostatics of planar and nanowire field-effect sensors was developed by homogenizing the Poisson equation in the biofunctionalized boundary layer [5]. This multiscale model can be coupled to any charge-transport model and hence makes the self-consistent quantitative investigation of the physics of field-effect sensors possible. Numerical verifications of the multiscale model were given, and a silicon-nanowire biosensor was simulated to find the influence of the surface charge density and the dipole-moment density on the conductance of the semiconductor transducer.

In [6], a system of diffusion-type equations for transport in 3D confined structures was derived from the Boltzmann transport equation for charged particles. The scaling in the derivation of the diffusion equation is chosen so that transport and scattering occur in the longitudinal direction and the particles are confined in the two transversal directions. Two diffusion-type equations for the concentration and fluxes as functions of position in the longitudinal direction and energy are obtained, and entropy estimates are given. An important feature in this work is that the coefficients in the resulting diffusion-type equations are calculated explicitly such that the six position and momentum dimensions of the original 3D Boltzmann equation are reduced to a 2D problem. The applications of this work are related to the simulation of charge transport in nanowires, nanopores, ion channels, and similar confined structures.

The work in [3] presents existence and local uniqueness theorems for a system of partial differential equations modeling field-effect nanosensors. The system consists of the Poisson–Boltzmann equation and the drift-diffusion equations coupled to a homogenized boundary layer. The existence proof is based on the Leray–Schauder fixed-point theorem. A maximum principle is used to obtain a priori estimates for the electric potential, the electron density, and the hole density. Local uniqueness around the equilibrium state is obtained from the implicit function theorem. Due to the multiscale problem inherent in field-effect biosensors, a homogenized equation for the potential with interface conditions at a surface is used. These interface conditions depend on the surface charge density and the dipole-moment density in the boundary layer and still admit existence and local uniqueness of the solution when certain conditions are satisfied.

In this work, we consider the theory of homogenization for the Boltzmann–Poisson system for electron transport focusing on problems related to fast oscillating charge concentrations at manifolds occurring, for example, in nanotechnological devices but including a general physical setting. Since the phenomena that occur at the surface of these devices is of particular interest for the prediction of observable quantities, the geometry of the problem considered here is the half-space with its boundary representing the surface of the device and with periodic cells along the manifold. We will study in this work the boundary-layer effects along the unbounded direction normal to this manifold.

2. Formal result for periodic media. We define

$$y := \frac{x}{\varepsilon}$$

and use the ansatz

$$u^\varepsilon(x) = u_0(x,y) + \varepsilon u_1(x,y) + \varepsilon^2 u_2(x,y) + \cdots,$$
$$f^\varepsilon(t,x,v) = f_0(t,x,y,v) + \varepsilon f_1(t,x,y,v) + \varepsilon^2 f_2(t,x,y,v) + \cdots.$$

Substituting this ansatz into the Boltzmann equation (1.1b), noting that $\nabla = \nabla_x + (1/\varepsilon)\nabla_y$, and comparing the coefficients of ε^{-2}, ε^{-1}, ε^0, and ε^{i-2}, $i \geq 0$, respectively, we obtain the equations

$$v \cdot \nabla_y f_0 - \nabla_y u_0 \cdot \nabla_v f_0 = Q(f_0), \tag{2.1a}$$

$$v \cdot \nabla_x f_0 - \nabla_x u_0 \cdot \nabla_v f_0 + v \cdot \nabla_y f_1 - \nabla_y u_1 \cdot \nabla_v f_0 - \nabla_y u_0 \cdot \nabla_v f_1 = Q(f_1), \tag{2.1b}$$

$$\begin{aligned} &\partial_t f_0 + v \cdot \nabla_x f_1 - \nabla_x u_1 \cdot \nabla_v f_0 - \nabla_x u_0 \cdot \nabla_v f_1 \\ &+ v \cdot \nabla_y f_2 - \nabla_y u_2 \cdot \nabla_v f_0 - \nabla_y u_1 \cdot \nabla_v f_1 - \nabla_y u_0 \cdot \nabla_v f_2 = Q(f_2), \end{aligned} \tag{2.1c}$$

$$\begin{aligned} &\partial_t f_{i-2} + v \cdot \nabla_x f_{i-1} - \sum_{k=0}^{i-1} \nabla_x u_{i-1-k} \cdot \nabla_v f_k \\ &+ v \cdot \nabla_y f_i - \nabla_y u_0 \cdot \nabla_v f_i - \sum_{k=0}^{i-1} \nabla_y u_{i-k} \cdot \nabla_v f_k = Q(f_i) \quad \forall i \geq 2. \end{aligned} \tag{2.1d}$$

We define the linear operator

$$L := -v \cdot \nabla_y + \nabla_y u_0 \cdot \nabla_v + Q.$$

Regarding the first equation, (2.1a), which can now be written as $Lf_0 = 0$, we find that f_0 must be of the form

$$f_0 = N(t,x,y)M(v), \quad N(t,x,y) = \rho(t,x)\frac{e^{-u_0(t,x,y)}}{\int_Y e^{-u_0(t,x,y)}\,dy},$$

according to [2, Proposition 3.1], where $M(v)$ denotes the normalized Maxwellian distribution (1.3). The second equation, (2.1b), becomes

$$\begin{aligned} Lf_1 &= v \cdot \nabla_x f_0 - \nabla_x u_0 \cdot \nabla_v f_0 - \nabla_y u_1 \cdot \nabla_v f_0 \\ &= Mv \cdot \nabla_x N + NMv \cdot \nabla_x u_0 + NMv \cdot \nabla_y u_1 \\ &= Mv \cdot (\nabla_x N + N\nabla_x u_0 + N\nabla_y \psi \nabla_x u_0). \end{aligned}$$

In the last equality in the last term, we have used the identity $u_1 = \psi(y) \cdot \nabla_x u_0$ that is well known from the homogenization of elliptic operators. (Note that $\psi(y)$, the first-order correction, is a vector field and that the gradient with respect to z of a vector a is a matrix with the entries $(\nabla_z a)_{ij} = \partial_{z_j} a_i$.) It is immediate to see that the solvability condition from [2, Proposition 3.1] is always satisfied for the last equation. After defining the vector

$$\chi(y,v) := L^{-1}(Mv)^T,$$

where L^{-1} is applied componentwise, we can write

$$f_1 = (\nabla_x N + N\nabla_x u_0)\cdot\chi + NL^{-1}(Mv^T\nabla_y\psi)\cdot\nabla_x u_0.$$

Furthermore, we define the vector

$$\theta(y,v) := L^{-1}(Mv^T\nabla_y\psi)^T \tag{2.2}$$

to have

$$f_1 = (\nabla_x N + N\nabla_x u_0)\cdot\chi + N\nabla_x u_0\cdot\theta. \tag{2.3}$$

We now consider the third equation, (2.1c), i.e.,

$$Lf_2 = \partial_t f_0 + v\cdot\nabla_x f_1 - \nabla_x u_1\cdot\nabla_v f_0 - \nabla_x u_0\cdot\nabla_v f_1 - \nabla_y u_2\cdot\nabla_v f_0 - \nabla_y u_1\cdot\nabla_v f_1.$$

We have to check the solvability condition from [2, Proposition 3.1] again to ensure that now a solution f_2 exists. Therefore, we consider the condition

$$\iint(\partial_t f_0 + v\cdot\nabla_x f_1 - \nabla_x u_1\cdot\nabla_v f_0 - \nabla_x u_0\cdot\nabla_v f_1 - \nabla_y u_2\cdot\nabla_v f_0 - \nabla_y u_1\cdot\nabla_v f_1)\mathrm{d}y\mathrm{d}v = 0,$$

which simplifies, by using (2.3) and the divergence theorem with respect to v for the terms containing ∇_v, to

$$\begin{aligned}
0 &= \iint M(v)\partial_t N(t,x,y)dydv + \iint v\cdot\nabla_x\big((\nabla_x N + N\nabla_x u_0)\cdot\chi + N\nabla_x u_0\cdot\theta\big)\mathrm{d}y\mathrm{d}v\\
&= \partial_t\int_Y \rho(t,x)\frac{e^{-u_0(t,x,y)}}{\int_Y e^{-u_0(t,x,y')}\,dy'}dy + \nabla_x\cdot\iint\big((\nabla_x N + N\nabla_x u_0)\cdot\chi + N\nabla_x u_0\cdot\theta\big)v\mathrm{d}y\mathrm{d}v\\
&= \partial_t\rho + \nabla_x\cdot\left(\iint v\otimes\chi(y,v)\nabla_x N(t,x,y)\mathrm{d}y\mathrm{d}v - \frac{\rho(t,x)\iint v\otimes(\theta+\chi)\nabla_x e^{-u_0(t,x,y)}\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}\,dy'}\right)\\
&= \partial_t\rho + \nabla_x\cdot\left(\iint v\otimes\chi\left(\frac{e^{-u_0(t,x,y)}\nabla_x\rho}{\int_Y e^{-u_0(t,x,y')}\,dy'} + \rho(t,x)\nabla_x\frac{e^{-u_0(t,x,y)}}{\int_Y e^{-u_0(t,x,y')}\,dy'}\right)\mathrm{d}y\mathrm{d}v\right.\\
&\quad\left. - \frac{\rho\iint v\otimes(\theta+\chi)\nabla_x e^{-u_0(t,x,y)}\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}\,dy'}\right)\\
&= \partial_t\rho + \nabla_x\cdot\left(\nabla_x\rho\frac{\iint v\otimes\chi e^{-u_0(t,x,y)}\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}\,dy'} + \rho\iint v\otimes\chi\nabla_x\frac{e^{-u_0(t,x,y)}}{\int_Y e^{-u_0(t,x,y')}\,dy'}\mathrm{d}y\mathrm{d}v\right.\\
&\quad\left. - \frac{\rho\iint v\otimes(\theta+\chi)\nabla_x e^{-u_0(t,x,y)}\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}\,dy'}\right)\\
&= \partial_t\rho + \nabla_x\cdot\left(\frac{\iint \mathrm{d}y\mathrm{d}v e^{-u_0(t,x,y)}v\chi}{\int_Y e^{-u_0(t,x,y')}\,dy'}\cdot\nabla_x\rho + \rho\left(\iint v\nabla_x\cdot\frac{\chi e^{-u_0(t,x,y)}}{\int_Y e^{-u_0(t,x,y')}\,dy'}\mathrm{d}y\mathrm{d}v\right.\right.\\
&\quad\left.\left. - \frac{\iint v\nabla_x\cdot\left[(\theta+\chi)e^{-u_0(t,x,y)}\right]\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}\,dy'}\right)\right).
\end{aligned}$$

The tensor product is defined as $(v\otimes\chi)\varphi := (\chi\cdot\varphi)v$. Therefore, the solvability condition becomes the drift-diffusion-type transport equation

$$\begin{aligned}
0 &= \partial_t\rho + \nabla_x\\
&\cdot\left(\frac{1}{\int_Y e^{-u_0}dy}\left\{\iint \mathrm{d}y\mathrm{d}v e^{-u_0}v\chi\cdot\nabla_x\rho + \rho\left[\int_Y e^{-u_0}dy'\,\nabla_x\cdot\iint\frac{v\chi e^{-u_0(t,x,y)}\mathrm{d}y\mathrm{d}v}{\int_Y e^{-u_0(t,x,y')}dy'}\right.\right.\right.\\
&\quad\left.\left.\left. -\nabla_x\cdot\iint v(\theta+\chi)e^{-u_0}\mathrm{d}y\mathrm{d}v\right]\right\}\right).
\end{aligned}$$

3. Formal result for boundary layers. We consider the domain $\Omega := \{x = (\xi_1, \xi_2, z) \in \mathbb{R}^3 \mid z \geq 0\} \subset \mathbb{R}^3$ and set $\partial\Omega_0 := \{x = (\xi_1, \xi_2, z) \in \mathbb{R}^3 \mid z = 0\}$. We split the domain into cells and define a cell as $\mathcal{C} := Y \times (0, \infty)$, where Y is the square $Y := (0,1)^2$, and we set $\partial\mathcal{C}_0 := \{y = (y_1, y_2, y_3) \in \mathcal{C} \mid y_3 = 0\}$.

We consider again the Boltzmann–Poisson system

$$-\nabla_x \cdot (A\nabla_x u) = n_D + n, \tag{3.1a}$$

$$\partial_t f + v \cdot \nabla_x f - \nabla_x u \cdot \nabla_v f = Q(f), \tag{3.1b}$$

where $n_D(x)$ is a given charge concentration (the doping density) and $n(t,x) := \int f(t,x,v)\mathrm{d}v$.

We introduce the notation $x = (\xi, z)$ for the position, where $\xi = (\xi_1, \xi_2) \in \mathbb{R}^2$ and $z \in \mathbb{R}$, and $v = (w, \zeta)$ for the velocity, where $w = (w_1, w_2) \in \mathbb{R}^2$ and $\zeta \in \mathbb{R}$, and we define $y := \xi/\varepsilon$ and $\omega := z/\varepsilon$.

The boundary condition for the Boltzmann equation at $\partial\Omega_0$ is specular reflection, and the boundary condition for the Poisson equation as $z \to \infty$ is $\lim_{z\to\infty} u = F \in \mathbb{R}$. On the boundary $\partial\Omega_0$, there is a surface charge density

$$\sigma^\varepsilon(\xi) := \sigma(\xi, \xi/\varepsilon) = \sigma(\xi, y) = \sigma_0(y) + \varepsilon\sigma_1(\xi, y) + \varepsilon^2\sigma_2(\xi, y) + \cdots$$

with $\sigma_0(y)$ such that in the limit σ_0 "looks" constant from far away, and only the small-scale structure of the surface charge becomes visible as one zooms in. In the following, we split the electrostatic potential u into the stationary potential $\varphi(\xi, z)$ due to the surface charge density σ and the fixed charges n_D and the self-consistent potential $\psi(t, \xi, z)$ due to the charges n; i.e., we write

$$u(t, \xi, z) = \varphi(\xi, z) + \psi(t, \xi, z).$$

The scaling of n_D^ε and σ^ε is chosen so that the stationary potential $\varphi(\xi, \xi/\varepsilon, z, z/\varepsilon) = \varphi^\varepsilon(\xi, z)$ is the solution of the problem (denoting as ν the normal to the boundary)

$$\begin{aligned} -\nabla_x \cdot (A\nabla_x \varphi^\varepsilon) &= n_D^\varepsilon \quad && \text{in } \Omega, \\ \nu \cdot A\nabla_x \varphi^\varepsilon &= \sigma^\varepsilon && \text{on } \partial\Omega_0, \\ \nu \cdot A\nabla_x \varphi^\varepsilon &\to F && \text{as } z \to \infty. \end{aligned}$$

We specify Neumann boundary conditions since they are consistent with the physical situation of an infinite charged plate. It is well known that an infinite charged plate gives rise to a constant force normal to the plate; we call it $F \in \mathbb{R}$ here.

The self-consistent potential $\psi(t, \xi, \xi/\varepsilon, z, z/\varepsilon) = \psi^\varepsilon(t, \xi, z)$ solves the problem

$$\begin{aligned} -\nabla_x \cdot (A\nabla_x \psi^\varepsilon) &= n^\varepsilon \quad && \text{in } \Omega, \\ \nu \cdot A\nabla_x \psi^\varepsilon &= 0 && \text{on } \partial\Omega_0, \\ \nu \cdot A\nabla_x \psi^\varepsilon &\to 0 && \text{as } z \to \infty. \end{aligned}$$

Due to the fast variations, the ansatz for the particle-density function f is

$$f^\varepsilon(t, \xi, z, w, \zeta) = f(t, \xi, z, \xi/\varepsilon, z/\varepsilon, w, \zeta) = f(t, \xi, z, y, \omega, w, \zeta).$$

We rescale to a diffusive scaling in the Boltzmann equation by changing variables so that $\tau := t\varepsilon$ and $Q \mapsto (1/\varepsilon)Q$, remembering that $\omega = z/\varepsilon$. Recalling

$$\nabla_x = \begin{pmatrix}\nabla_\xi \\ \partial_z\end{pmatrix} + \frac{1}{\varepsilon}\begin{pmatrix}\nabla_y \\ \partial_\omega\end{pmatrix},$$
$$\nabla_v = \begin{pmatrix}\nabla_w \\ \partial_\zeta\end{pmatrix},$$

the Boltzmann equation becomes

$$\varepsilon\partial_\tau f^\varepsilon + (w\cdot\nabla_\xi f^\varepsilon + \zeta\partial_z f^\varepsilon - \nabla_\xi u^\varepsilon\cdot\nabla_w f^\varepsilon - \partial_z u^\varepsilon\partial_\zeta f^\varepsilon) + \frac{1}{\varepsilon}\big(w\cdot\nabla_y f^\varepsilon + \zeta\partial_\omega f^\varepsilon - \nabla_y u^\varepsilon\cdot\nabla_w f^\varepsilon - \partial_\omega u^\varepsilon\partial_\zeta f^\varepsilon - Q(f^\varepsilon)\big) = 0, \tag{3.2}$$

and the Poisson equation for the stationary potential φ^ε becomes

$$\begin{aligned}
\frac{1}{\varepsilon^2}\mathcal{A}_0\varphi^\varepsilon + \frac{1}{\varepsilon}\mathcal{A}_1\varphi^\varepsilon + \mathcal{A}_2\varphi^\varepsilon &= n_D^\varepsilon \quad &&\text{in } \Omega,\\
\nu\cdot A\bigg(\nabla_{(\xi,z)} + \frac{1}{\varepsilon}\nabla_{(y,\omega)}\bigg)\varphi^\varepsilon &= \sigma^\varepsilon \quad &&\text{on } \partial\Omega_0,\\
\nu\cdot A\bigg(\nabla_{(\xi,z)} + \frac{1}{\varepsilon}\nabla_{(y,\omega)}\bigg)\varphi^\varepsilon &\to F \quad &&\text{as } \omega\to\infty,
\end{aligned}$$

where we have defined the three operators

$$\begin{aligned}
\mathcal{A}_0 &:= -\begin{pmatrix}\nabla_y \\ \partial_\omega\end{pmatrix}\cdot\left(A\begin{pmatrix}\nabla_y \\ \partial_\omega\end{pmatrix}\right),\\
\mathcal{A}_1 &:= -\begin{pmatrix}\nabla_y \\ \partial_\omega\end{pmatrix}\cdot\left(A\begin{pmatrix}\nabla_\xi \\ \partial_z\end{pmatrix}\right) - \begin{pmatrix}\nabla_\xi \\ \partial_z\end{pmatrix}\cdot\left(A\begin{pmatrix}\nabla_y \\ \partial_\omega\end{pmatrix}\right),\\
\mathcal{A}_2 &:= -\begin{pmatrix}\nabla_\xi \\ \partial_z\end{pmatrix}\cdot\left(A\begin{pmatrix}\nabla_\xi \\ \partial_z\end{pmatrix}\right)
\end{aligned}$$

to simplify notation. The equations for the self-consistent potential ψ^ε are analogous, but the right-hand sides are n^ε, 0, and 0, respectively.

We make the multiscale ansatz

$$\begin{aligned}
f^\varepsilon(t,\xi,z,w,\zeta) &= f_0(t,\xi,z,y,\omega,w,\zeta) + \varepsilon f_1(t,\xi,z,y,\omega,w,\zeta) + \cdots,\\
\varphi^\varepsilon(\xi,z) &= \varphi_0(\xi,z,y,\omega) + \varepsilon\varphi_1(\xi,z,y,\omega) + \cdots,\\
n_D^\varepsilon(\xi,z) &= n_{D0}(\xi,z,y,\omega) + \varepsilon n_{D1}(\xi,z,y,\omega) + \cdots,\\
\psi^\varepsilon(t,\xi,z) &= \psi_0(t,\xi,z,y,\omega) + \varepsilon\psi_1(t,\xi,z,y,\omega) + \cdots,\\
n^\varepsilon(t,\xi,z) &= n_0(t,\xi,z,y,\omega) + \varepsilon n_1(t,\xi,z,y,\omega) + \cdots.
\end{aligned}$$

Comparing the coefficients in the Poisson equation yields the three problems for φ_0, φ_1, and φ_2. We will discuss the problem for φ_0 in the following, returning in a later section to the respective problems for φ_1 and φ_2.

For φ_0, the boundary value problem is

$$\mathcal{A}_0\varphi_0 = 0 \quad \text{in } \mathcal{C}, \tag{3.3a}$$
$$\varphi_0(\xi,z,\_,\omega) \quad \text{is 1-periodic}, \tag{3.3b}$$
$$\nu\cdot A\nabla_{(y,\omega)}\varphi_0 = 0 \quad \text{on } \partial\mathcal{C}_0, \tag{3.3c}$$
$$\nu\cdot A\nabla_{(y,\omega)}\varphi_0 \to 0 \quad \text{as } \omega\to\infty. \tag{3.3d}$$

According to Proposition 3.1, which will be proved in the next subsection, this boundary value problem determines φ_0 up to an additive constant and implies that φ_0 does not depend on the fast variables y and ω, i.e., $\varphi_0 = \varphi_0(\xi, z)$.

3.1. $\mathcal{A}_0$ boundary value problems. We will prove the existence and uniqueness of solutions to the $\mathcal{A}_0$-Laplace (homogeneous) and $\mathcal{A}_0$-Poisson (inhomogeneous) boundary value problems for 1-periodic functions across Y-cells with Neumann boundary conditions at zero and infinity. These results will be useful in the following to treat with the different elliptic problems arising from the appearance of the operators $\mathcal{A}_0$, $\mathcal{A}_1$, $\mathcal{A}_2$ in the homogenization problem.

We start with the homogeneous $\mathcal{A}_0$-Laplace problem as it is related to the boundary value problem for φ_0.

PROPOSITION 3.1. *Suppose $F \in \mathbb{R}$ and $\sigma\colon Y \mapsto \mathbb{R}$ are given. Suppose further that the 3×3 matrix A is coercive and bounded and that it has the diagonal form*

$$A(\omega) = \begin{pmatrix} a_{11}(\omega) & 0 & 0 \\ 0 & a_{22}(\omega) & 0 \\ 0 & 0 & a_{33}(\omega) \end{pmatrix}.$$

The diagonal entries a_{ii} may depend on ω but not on y. If $\int_Y \sigma(y)\mathrm{d}y = F$ holds, then the solution $u(y, \omega)$ of the boundary value problem

$$\begin{aligned} \mathcal{A}_0 u = 0 \qquad & \text{in } \mathcal{C}, \\ u(\_, \omega) \qquad & \text{is 1-periodic}, \\ \nu \cdot A\nabla_{(y,\omega)} u(y, 0) = \sigma(y) \qquad & \text{on } \partial\mathcal{C}_0, \\ \nu \cdot A\nabla_{(y,\omega)} u(y, \omega) \to F \qquad & \text{as } \omega \to \infty \end{aligned}$$

is unique up to an additive constant and, as $\omega \to \infty$, the solution u converges exponentially quickly to a function of ω only (which is linear if a_{33} is constant). Otherwise, if $\int_Y \sigma(y)\mathrm{d}y \neq F$, the problem has no solution.

Proof. First, we consider the case

$$A = \begin{pmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{pmatrix}$$

with constant $a_{ii} > 0$. The Fourier modes are the basis

$$\psi_{nm}(y) := \exp(i2\pi(ny_1 + my_2)), \quad (n, m) \in \mathbb{Z}^2,$$

and of course the equation $\mathcal{A}_0\psi_{nm} = (2\pi)^2(a_{11}n^2 + a_{22}m^2)\psi_{nm}$ holds. We write the solution u as the sum

$$u(y, \omega) = \sum_{(n,m)\in\mathbb{Z}^2} c_{nm}(\omega)\psi_{nm}(y),$$

and the coefficient functions $c_{nm}(\omega)$ are to be determined, keeping in mind the boundary conditions

$$a_{33}\partial_\omega u|_{\omega=0} = \sigma(y) = \sum_{(n,m)\in\mathbb{Z}^2} \sigma_{nm}\psi_{nm}(y) \quad \text{on } \partial\Omega_0$$

(taking the normal at $\omega = 0$ as $+\hat{e}_\omega$ when restricting our domain to the half-space) and

$$a_{33}\partial_\omega u|_{\omega\to\infty} = F = F + \sum_{(n,m)\neq(0,0)\in\mathbb{Z}^2} 0\cdot\psi_{nm}(y).$$

After substitution, the equation becomes

$$\sum_{(n,m)\in\mathbb{Z}^2} \big((2\pi)^2(a_{11}n^2 + a_{22}m^2)c_{nm}(\omega) - \partial_\omega(a_{33}\partial_\omega c_{nm}(\omega))\big)\psi_{nm}(y) = 0.$$

Therefore, the coefficients $c_{nm}(\omega)$ have to solve the problem

$$\partial_\omega(a_{33}\partial_\omega c_{nm}(\omega)) - (2\pi)^2(a_{11}n^2 + a_{22}m^2)c_{nm}(\omega) = 0 \qquad \forall\omega > 0, \tag{3.4}$$

$$a_{33}\partial_\omega c_{nm}|_{\omega=0} = \sigma_{nm}, \tag{3.5}$$

$$a_{33}\partial_\omega c_{00}|_{\omega=\infty} = F, \tag{3.6}$$

$$a_{33}\partial_\omega c_{nm}|_{\omega=\infty} = 0, \quad n+m>0. \tag{3.7}$$

We discern two cases. In the case $(n,m)\neq(0,0)$, we find—given that a_{11}, a_{22}, a_{33} are independent of ω (and also of y)—that

$$c_{nm}(\omega) = \alpha_{nm}\exp\left(2\pi\sqrt{\frac{a_{11}n^2 + a_{22}m^2}{a_{33}}}\omega\right) + \beta_{nm}\exp\left(-2\pi\sqrt{\frac{a_{11}n^2 + a_{22}m^2}{a_{33}}}\omega\right),$$

and this implies $\alpha_{nm} = 0$ due to the boundary condition (3.7) for $\omega\to\infty$. In the case $n = 0 = m$, the equation is $-\partial_\omega(a_{33}\partial_\omega c_{00}) = 0$, and hence $c_{00}(\omega) = a_{00} + b_{00}\omega/a_{33}$. The boundary condition (3.6) for $\omega\to\infty$ yields $c_{00}(\omega) = a_{00} + F\omega/a_{33}$.

Therefore, the solution is of the form

$$u(y,\omega) = a_{00} + \frac{F\omega}{a_{33}} + \sum_{(n,m)\in\mathbb{Z}^2\setminus(0,0)} \beta_{nm}\exp\left(-2\pi\sqrt{\frac{a_{11}n^2 + a_{22}m^2}{a_{33}}}\omega\right)\psi_{nm}(y), \tag{3.8}$$

and hence the kernel consists of linear functions in ω and the solutions decay exponentially to these linear functions as $\omega\to\infty$.

Comparing the boundary conditions (3.5)–(3.7) with (3.8) for u implies $F = \sigma_{00}$ and $\sigma_{nm}/a_{33} = -\beta_{nm}2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}$. Therefore, the solution is

$$u(y,\omega) = a_{00} + \frac{F\omega}{a_{33}} - \sum_{(n,m)\in\mathbb{Z}^2\setminus(0,0)} \frac{\exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2\pi\sqrt{a_{33}(a_{11}n^2 + a_{22}m^2)}}\sigma_{nm}\psi_{nm}(y).$$

This concludes the proof for the first case, since $\sigma_{00} = \int_Y \sigma(y)\mathrm{d}y$.

The second case is

$$A(\omega) = \begin{pmatrix} a_{11}(\omega) & 0 & 0 \\ 0 & a_{22}(\omega) & 0 \\ 0 & 0 & a_{33}(\omega)\end{pmatrix}$$

with $a_{ii}(\omega) > 0$ assumed to have no y-dependence.

We express the solution u as the sum

$$u(y,\omega) = \sum_{(n,m)\in\mathbb{Z}^2} c_{nm}(\omega)\psi_{nm}(y),$$

since for this second case the equation $\mathcal{A}_0\psi_{nm} = (2\pi)^2(a_{11}(\omega)n^2 + a_{22}(\omega)m^2)\psi_{nm}$ also holds and the coefficient functions $c_{nm}(\omega)$ must then satisfy the boundary conditions

$$\begin{aligned} a_{33}\partial_\omega u|_{\omega=0} &= \sigma(y) = \sum_{(n,m)\in\mathbb{Z}^2} \sigma_{nm}\psi_{nm}(y) \quad \text{on } \partial\Omega_0, \\ a_{33}\partial_\omega u|_{\omega\to\infty} &= F = F + \sum_{(n,m)\neq(0,0)\in\mathbb{Z}^2} 0\cdot\psi_{nm}(y) \quad \text{as } \omega\to\infty. \end{aligned}$$

The equation after substitution is again

$$\sum_{(n,m)\in\mathbb{Z}^2} \big((2\pi)^2(a_{11}n^2 + a_{22}m^2)c_{nm}(\omega) - \partial_\omega(a_{33}\partial_\omega c_{nm}(\omega))\big)\psi_{nm}(y) = 0.$$

Also, in this case, the coefficients $c_{nm}(\omega)$ must solve the problem

$$\partial_\omega(a_{33}\partial_\omega c_{nm}(\omega)) = (2\pi)^2(a_{11}n^2 + a_{22}m^2)c_{nm}(\omega) \quad \forall\omega > 0, \tag{3.9}$$

$$a_{33}\partial_\omega c_{nm}|_{\omega=0} = \sigma_{nm}, \tag{3.10}$$

$$a_{33}\partial_\omega c_{00} \to F \qquad \text{as } \omega\to\infty, \tag{3.11}$$

$$a_{33}\partial_\omega c_{nm} \to 0 \qquad \text{as } \omega\to\infty, \quad n+m>0, \tag{3.12}$$

which can be rewritten as the system

$$\partial_\omega \begin{pmatrix} b_{nm} \\ c_{nm} \end{pmatrix}(\omega) = \begin{pmatrix} 0 & (2\pi)^2(a_{11}n^2 + a_{22}m^2) \\ a_{33}(\omega)^{-1} & 0 \end{pmatrix} \begin{pmatrix} b_{nm} \\ c_{nm} \end{pmatrix}(\omega) \tag{3.13}$$

of ODEs, or equivalently as

$$\partial_\omega \vec{c}_{nm} = B_{nm}(\omega)\vec{c}_{nm}(\omega) \tag{3.14}$$

by defining

$$\vec{c}_{nm}(\omega) := \begin{pmatrix} b_{nm} \\ c_{nm} \end{pmatrix}, \quad B_{nm}(\omega) := \begin{pmatrix} 0 & (2\pi)^2(a_{11}n^2 + a_{22}m^2) \\ a_{33}^{-1}(\omega) & 0 \end{pmatrix}. \tag{3.15}$$

This is a family of first-order general ODE systems. The case $n = 0 = m$ has the solution of a constant b_{00} and

$$c_{00}(\omega) = c_{00}(\omega_0) + b_{00}\int_{\omega_0}^{\omega} \frac{d\tilde{\omega}}{a_{33}(\tilde{\omega})}, \quad a_{33}(\omega)\partial_\omega c_{00} = b_{00} = F = \sigma_{00}, \tag{3.16}$$

where the last equalities are due to the boundary conditions. Therefore, it follows that the force due to the electric field is the result of the average of the surface charge over the periodic cell.

The systems with $(m,n) \neq (0,0)$ have positive definite matrices and can be solved by the Magnus expansion method [4], where we express the solution by an exponential of a matrix given by an expansion of

$$\vec{c}_{nm}(\omega) = \exp(\Omega(\omega))\,\vec{c^0}_{nm}, \quad \omega_0 = 0, \quad \Omega(\omega) = \sum_{k=1}^{\infty}\Omega_k(\omega). \tag{3.17}$$

The first terms of the expansion have the form

$$\Omega_1(\omega) = \int_0^\omega B_{nm} d\tilde{\omega} = \begin{pmatrix} 0 & (2\pi)^2 \left(n^2 \int_0^\omega a_{11} d\tilde{\omega} + m^2 \int_0^\omega a_{22} d\tilde{\omega}\right) \\ \int_0^\omega a_{33}^{-1} d\tilde{\omega} & 0 \end{pmatrix},$$

$$\Omega_2(\omega) = \frac{1}{2} \int_0^\omega \int_0^{\omega_1} \left[B_{nm}(\omega_1), B_{nm}(\omega_2)\right] d\omega_2 d\omega_1,$$

$$\Omega_3(\omega) = \frac{1}{6} \int_0^\omega \int_0^{\omega_1} \int_0^{\omega_2} \left([B_{nm}(\omega_1), [B_{nm}(\omega_2), B_{nm}(\omega_3)]] d\omega_3 d\omega_2 d\omega_1 \right.$$
$$\left. + [B_{nm}(\omega_3), [B_{nm}(\omega_2), B_{nm}(\omega_1)]]\right)$$

with the commutator $[B,C] := BC - CB$. The recursive relation for the terms in the expansion can be found in [4]. The Magnus series is known to converge for $\omega \in [0, W)$ such that B_{nm} is a bounded operator on a Hilbert space, and this operator satisfies the condition $\int_0^W \|B_{nm}(\omega)\| \mathrm{d}\omega < \pi$. This yields

$$\begin{pmatrix} b_{nm}(\omega) \\ c_{nm}(\omega) \end{pmatrix} = \exp\left(\Omega(\omega)\right) \begin{pmatrix} b_{nm}^0 \\ c_{nm}^0 \end{pmatrix} = \begin{pmatrix} a_{33}(\omega)\partial_\omega c_{nm}(\omega) \\ c_{nm} \end{pmatrix}. \tag{3.18}$$

The matrix exponential of a 2×2 matrix B is given by

$$\exp(B) = \exp\left(\frac{\operatorname{tr} B}{2}\right)\left(\left(\cosh(q) - \frac{\operatorname{tr} B}{2}\frac{\sinh(q)}{q}\right) I + \frac{\sinh(q)}{q} B\right),$$

$$q = \pm\sqrt{-\det\left(B - \frac{\operatorname{tr} B}{2} I\right)}.$$

Both the positive and negative values of q give the same result for $\exp(B)$ as $\cosh(q)$ and $\sinh(q)/q$ are even functions of q. Therefore, the exponential matrix $e^{\Omega(\omega)}$ and the associated solution of the coefficients c_{nm} are

$$\exp \Omega(\omega) = \exp\left(\frac{\operatorname{tr} \Omega(\omega)}{2}\right)\left[\left(\cosh(q) - \frac{\operatorname{tr} \Omega(\omega)}{2}\frac{\sinh(q)}{q}\right) I + \frac{\sinh(q)}{q}\Omega(\omega)\right],$$

$$q(\omega) = \sqrt{\left(\frac{\Omega_{11}(\omega) - \Omega_{22}(\omega)}{2}\right)^2 + \Omega_{12}(\omega)\Omega_{21}(\omega)} \quad \Longrightarrow$$

$$c_{nm}(\omega) = \exp\left(\frac{\operatorname{tr} \Omega(\omega)}{2}\right)\left(a_{33}(0)\partial_\omega c_{nm}(0)\frac{\sinh(q)}{q}\Omega_{21}(\omega)\right.$$
$$\left. + c_{nm}(0)\left[\frac{\sinh(q)}{q}\Omega_{22}(\omega) + \left(\cosh(q) - \frac{\operatorname{tr} \Omega(\omega)}{2}\frac{\sinh(q)}{q}\right)\right]\right).$$

Taking into account the boundary condition (3.10) at $\omega = 0$, the solution has the form

$$c_{nm}(\omega) = e^{\frac{\operatorname{tr} \Omega(\omega)}{2}}\left(\sigma_{nm}\frac{\sinh q(\omega)}{q(\omega)}\Omega_{21}(\omega) + c_{nm}(0)\left(\frac{\sinh q(\omega)}{q(\omega)}\Omega_{22}(\omega)\right.\right.$$
$$\left.\left. + \left(\cosh q(\omega) - \frac{\operatorname{tr} \Omega(\omega)}{2}\frac{\sinh q(\omega)}{q(\omega)}\right)\right)\right).$$

To apply the second boundary condition, we consider the coefficients

$$b_{nm}(\omega) = e^{\frac{\operatorname{tr} \Omega(\omega)}{2}}\left(\sigma_{nm}\left(\frac{\sinh q(\omega)}{q(\omega)}\Omega_{11}(\omega) + \cosh q(\omega) - \frac{\operatorname{tr} \Omega(\omega)}{2}\frac{\sinh q(\omega)}{q(\omega)}\right)\right.$$
$$\left. + c_{nm}(0)\frac{\sinh q(\omega)}{q(\omega)}\Omega_{12}(\omega)\right).$$

Since it must hold that $b_{nm}(\omega) = a_{33}\partial_\omega c_{nm} \to 0$ as $\omega \to \infty$, we have

$$0 = e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\sigma_{nm}\left(\frac{\sinh q(\omega)}{q(\omega)}\Omega_{11}(\omega) + \cosh q(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\frac{\sinh q(\omega)}{q(\omega)}\right)\right.$$
$$\left.\left. + c_{nm}(0)\frac{\sinh q(\omega)}{q(\omega)}\Omega_{12}(\omega)\right)\right|_{\omega\to\infty},$$

which implies

$$e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\sigma_{nm}\left(\Omega_{11}(\omega) + q(\omega)\coth q(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\right) + c_{nm}(0)\Omega_{12}(\omega)\right) \to 0.$$

Although the decay of $e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}$ to zero would satisfy this condition, in order to guarantee the latter we can require that for $c_{nm}(0)$ the condition

$$c_{nm}(0) = \sigma_{nm}\left(\frac{\frac{1}{2}\operatorname{tr}\Omega(\omega) - \Omega_{11}(\omega) - q(\omega)}{\Omega_{12}(\omega)}\right)\Bigg|_{\omega\to\infty},$$
$$c_{nm}(0) = \sigma_{nm}\left(\frac{\Omega_{22}(\omega) - \Omega_{11}(\omega)}{2\Omega_{12}(\omega)} - \sqrt{\left(\frac{\Omega_{11}(\omega) - \Omega_{22}(\omega)}{2\Omega_{12}(\omega)}\right)^2 + \frac{\Omega_{21}(\omega)}{\Omega_{12}(\omega)}}\right)\Bigg|_{\omega\to\infty}$$

with a speed of convergence faster than $e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}$ holds in case this last term blows up so that we satisfy the condition

$$e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\sigma_{nm}\left(\Omega_{11}(\omega) + q(\omega)\coth q(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\right) + c_{nm}(0)\Omega_{12}(\omega)\right)\Bigg|_{\omega\to\infty} = 0.$$

Therefore, the solution of our original problem has the expression

$$u(y,\omega) = c_{00}(0) + F\int_0^\omega \frac{d\tilde{\omega}}{a_{33}(\tilde{\omega})} + \sum_{(n,m)\neq(0,0)} \psi_{nm}(y)\sigma_{nm}e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\frac{\sinh q(\omega)}{q(\omega)}\Omega_{21}(\omega)\right.$$
$$\left. + \left(\frac{\frac{1}{2}\operatorname{tr}\Omega(\omega) - \Omega_{11}(\omega) - q(\omega)}{\Omega_{12}(\omega)}\right)\Bigg|_{\omega\to\infty}\left(\frac{\sinh q(\omega)}{q(\omega)}\left(\Omega_{22}(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\right) + \cosh q(\omega)\right)\right)$$

with $F = \sigma_{00}$.

However, in order to arrive at more explicit, though approximate, formulas for the coefficients $c_{nm}(\omega)$, we have to resort to truncated Magnus expansions, obtaining approximations of $\Omega = \sum_{k=1}^{\infty}\Omega_k$ up to a given order of k.

We will compute the first two matrices of the Magnus expansion and their associated solution for $c_{nm}(\omega)$ up to first and second order in the expansion.

The exponential matrix and associated solution up to the first term of the expansion are

$$\exp(\Omega_1(\omega)) = \left(\cosh(q)I + \frac{\sinh(q)}{q}\begin{pmatrix} 0 & (2\pi)^2\left[n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right) \\ \int_0^\omega \frac{d\tilde{\omega}}{a_{33}} & 0\end{pmatrix}\right],$$
$$q = \sqrt{-\det\Omega_1(\omega)} = 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega\frac{d\tilde{\omega}}{a_{33}}}.$$

This matrix simplifies to

$$\exp\Omega_1(\omega) = \begin{pmatrix} \cosh(q) & \frac{\sinh(q)}{q}(2\pi)^2\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right) \\ \frac{\sinh(q)}{q}\int_0^\omega\frac{d\tilde{\omega}}{a_{33}} & \cosh(q)\end{pmatrix}. \tag{3.19}$$

Moreover, after writing the $q(\omega)$ term explicitly in the matrix above, it has the form

$$e^{\Omega_1(\omega)} = \begin{pmatrix} \cosh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}} & \frac{\sinh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}}{\frac{\sqrt{\int_0^\omega a_{33}^{-1}d\tilde{\omega}}}{2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)}}} \\ \frac{\sinh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}}{\frac{2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)}}{\sqrt{\int_0^\omega a_{33}^{-1}d\tilde{\omega}}}} & \cosh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}} \end{pmatrix}.$$

Therefore, the solution for the coefficients up to first order in the Magnus expansion is

$$c_{nm}(\omega) = \sigma_{nm}\frac{\sinh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}}{\frac{2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)}}{\sqrt{\int_0^\omega a_{33}^{-1}d\tilde{\omega}}}} + c_{nm}(0)\cosh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}},$$

for which the boundary condition (3.10), $\sigma_{nm} = a_{33}(0)\partial_\omega c_{nm}(0)$, holds at zero, keeping in mind that

$$\left.\frac{\sinh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}}{\frac{2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega}+m^2\int_0^\omega a_{22}d\tilde{\omega}\right)}}{\sqrt{\int_0^\omega a_{33}^{-1}d\tilde{\omega}}}}\right|_{\omega=0} = \lim_{q\to 0}\frac{\sinh(q)}{q}\int_0^0 a_{33}^{-1}d\tilde{\omega} = 0.$$

The coefficient $c_{nm}(0)$ is determined from the boundary condition by the formula

$$c_{nm}(0) = -\sigma_{nm}\left.\sqrt{\frac{\Omega_{21}(\omega)}{\Omega_{12}(\omega)}}\right|_{\omega\to\infty} = \frac{-\sigma_{nm}}{2\pi}\left.\sqrt{\frac{\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}{n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}}}\right|_{\omega\to\infty}.$$

The solution of our original problem up to first order of the Magnus expansion is

$$\begin{aligned} u(y,\omega) = {} & c_{00}(0) + F\int_0^\omega \frac{d\tilde{\omega}}{a_{33}(\tilde{\omega})} + \sum_{(n,m)\neq(0,0)} \psi_{nm}(y)\sigma_{nm} \\ & \cdot\Bigg(\sqrt{\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}\,\frac{\sinh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}}{2\pi\sqrt{n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}}} \\ & - \frac{1}{2\pi}\left.\sqrt{\frac{\int_0^\omega a_{33}^{-1}d\tilde{\omega}}{n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}}}\right|_{\omega\to\infty} \\ & \cdot\cosh 2\pi\sqrt{\left(n^2\int_0^\omega a_{11}d\tilde{\omega} + m^2\int_0^\omega a_{22}d\tilde{\omega}\right)\int_0^\omega \frac{d\tilde{\omega}}{a_{33}}}\Bigg). \end{aligned}$$

The solution up to second order of the Magnus expansion is given by

$$\exp\left(\sum_{k=1}^{2}\Omega_k(\omega)\right) = e^{\frac{\operatorname{tr}\sum_{k=1}^{2}\Omega_k(\omega)}{2}}\left(\left(\cosh(q) - \frac{\operatorname{tr}\sum_{k=1}^{2}\Omega_k(\omega)}{2}\frac{\sinh(q)}{q}\right)I + \frac{\sinh(q)}{q}\sum_{k=1}^{2}\Omega_k(\omega)\right),$$

$$q = \sqrt{-\det\left(\sum_{k=1}^{2}\Omega_k(\omega) - \frac{\operatorname{tr}\sum_{k=1}^{2}\Omega_k(\omega)}{2}I\right)},$$

so we have to compute the second matrix term of the Magnus expansion by calculating

$$\Omega_2(\omega) = \frac{1}{2}\int_0^{\omega} d\omega_1 \int_0^{\omega_1} d\omega_2\,(B_{nm}(\omega_1)B_{nm}(\omega_2) - B_{nm}(\omega_2)B_{nm}(\omega_1)) = I(\omega)M,$$

$$M = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$I(\omega) = \int_0^{\omega}\int_0^{\omega_1} \frac{d\omega_1 d\omega_2}{2}(2\pi)^2\left(\frac{a_{11}(\omega_1)n^2 + a_{22}(\omega_1)m^2}{a_{33}(\omega_2)} - \frac{a_{11}(\omega_2)n^2 + a_{22}(\omega_2)m^2}{a_{33}(\omega_1)}\right).$$

Therefore, the Magnus expansion up to the second-order term adds up to

$$(\Omega_1 + \Omega_2)(\omega) = \begin{pmatrix} I(\omega) & (2\pi)^2\left(n^2\int_0^{\omega} a_{11}d\tilde{\omega} + m^2\int_0^{\omega} a_{22}d\tilde{\omega}\right) \\ \int_0^{\omega} a_{33}^{-1}d\tilde{\omega} & -I(\omega) \end{pmatrix}, \tag{3.20}$$

for which we have that $\operatorname{tr}\sum_{k=1}^{2}\Omega_k(\omega) = 0$. Then

$$q(\omega) = \sqrt{-\det\sum_{k=1}^{2}\Omega_k(\omega)} = \sqrt{I^2(\omega) + (2\pi)^2\left(n^2\int_0^{\omega} a_{11}d\tilde{\omega} + m^2\int_0^{\omega} a_{22}d\tilde{\omega}\right)\int_0^{\omega}\frac{d\tilde{\omega}}{a_{33}}},$$

$$\exp\left(\sum_{k=1}^{2}\Omega_k\right) = \cosh q(\omega) I + \frac{\sinh q(\omega)}{q(\omega)}\begin{pmatrix} I(\omega) & (2\pi)^2\left(n^2\int_0^{\omega} a_{11}d\tilde{\omega} + m^2\int_0^{\omega} a_{22}d\tilde{\omega}\right) \\ \int_0^{\omega} a_{33}^{-1}d\tilde{\omega} & -I(\omega) \end{pmatrix},$$

$$c_{nm}(\omega) = \left(\sigma_{nm}\frac{\sinh q(\omega)}{q(\omega)}\int_0^{\omega}\frac{d\tilde{\omega}}{a_{33}} + c_{nm}(0)\left(\cosh q(\omega) - I(\omega)\frac{\sinh q(\omega)}{q(\omega)}\right)\right)$$

is the solution up to second order of the Magnus expansion, recalling that $\sigma_{nm} = a_{33}(0)\partial_\omega c_{nm}(0)$ due to the boundary condition (3.10) at zero. To determine $c_{nm}(0)$, we recall that

$$c_{nm}(0) = \sigma_{nm}\left(\frac{\Omega_{22}(\omega) - \Omega_{11}(\omega)}{2\Omega_{12}(\omega)} - \sqrt{\left(\frac{\Omega_{11}(\omega) - \Omega_{22}(\omega)}{2\Omega_{12}(\omega)}\right)^2 + \frac{\Omega_{21}(\omega)}{\Omega_{12}(\omega)}}\right)\Bigg|_{\omega\to\infty}$$

$$= -\frac{\sigma_{nm}}{(2\pi)^2}\left.\frac{I(\omega) + q(\omega)}{n^2\int_0^{\omega} a_{11}d\tilde{\omega} + m^2\int_0^{\omega} a_{22}d\tilde{\omega}}\right|_{\omega\to\infty}.$$

The solution of our original problem with coefficients approximate up to the second order of the Magnus expansion is

$$u(y,\omega) = c_{00}(0) + F\int_0^{\omega}\frac{d\tilde{\omega}}{a_{33}} + \sum_{n,m\neq 0,0}\psi_{nm}(y)\sigma_{nm}\left(\frac{\sinh q(\omega)}{q(\omega)}\int_0^{\omega}\frac{d\tilde{\omega}}{a_{33}} - \frac{\cosh q(\omega) - I(\omega)\frac{\sinh q(\omega)}{q(\omega)}}{\left.\frac{(2\pi)^2\left(n^2\int_0^{\omega} a_{11}d\tilde{\omega} + m^2\int_0^{\omega} a_{22}d\tilde{\omega}\right)}{I(\omega)+q(\omega)}\right|_{\omega\to\infty}}\right).$$

We notice that for the particular case of all a_{ii} being constant, the formulas for the first and second orders in the Magnus expansion yield

$$c_{nm}^{(1)}(\omega) = \partial_\omega c_{nm}(0)\frac{\sinh\left(2\pi\sqrt{\frac{n^2a_{11}+m^2a_{22}}{a_{33}}}\,\omega\right)}{2\pi\sqrt{\frac{n^2a_{11}+m^2a_{22}}{a_{33}}}} + c_{nm}(0)\cosh\left(2\pi\sqrt{\frac{n^2a_{11}+m^2a_{22}}{a_{33}}}\,\omega\right),$$

$$c_{nm}^{(2)}(\omega) = \partial_\omega c_{nm}(0)\frac{\sinh q(\omega)}{q(\omega)}\omega + c_{nm}(0)\cosh q(\omega) = c_{nm}^{(1)}(\omega), \quad q(\omega) = 2\pi\sqrt{\frac{n^2a_{11}+m^2a_{22}}{a_{33}}}\,\omega$$

($I(\omega) = 0$ in this case), which is just the same expansion in terms of exponentials of $\pm 2\pi\sqrt{\frac{n^2a_{11}+m^2a_{22}}{a_{33}}}\omega$. For this case of constant a_{ii}, it is known that all the solutions $c_{nm}^{(N)}$ will give the exact solution, since in this case the commutator $[B_{nm}(\omega_1), B_{nm}(\omega_2)] = [B_{nm}, B_{nm}] = 0$ vanishes (which is why $I(\omega) = 0$ holds in the second-order case).

As a final check, we compare the last equations with the previous formulas

$$c_{nm}^{(1)}(0) = -\frac{\sigma_{nm}}{2\pi}\lim_{\omega\to\infty}\sqrt{\frac{\int_0^\omega \frac{d\tilde\omega}{a_{33}}}{\int_0^\omega (n^2a_{11}+m^2a_{22})d\tilde\omega}} = \frac{-\sigma_{nm}}{2\pi\sqrt{a_{33}\,(n^2a_{11}+m^2a_{22})}},$$

$$c_{nm}^{(2)}(0) = -\frac{\sigma_{nm}}{2\pi}\lim_{\omega\to\infty}\sqrt{\frac{\int_0^\omega a_{33}^{-1}d\tilde\omega}{\int_0^\omega (n^2a_{11}+m^2a_{22})d\tilde\omega}} = \frac{-\sigma_{nm}}{2\pi\sqrt{a_{33}\,(n^2a_{11}+m^2a_{22})}}$$

for the constants $c_{nm}(0)$ for the first- and second-order truncations of the Magnus expansion with all a_{ii} constant, which are in agreement with the coefficients obtained in the first part of the proof for the case of constant a_{ii}. ∎

Having solved the $\mathcal{A}_0$-Laplace homogeneous problem, we consider the Poisson inhomogeneous problem $\mathcal{A}_0 u = g$ next. This will be useful for handling boundary value problems such as those associated to the self-consistent potential ψ^ε, for example.

PROPOSITION 3.2. *Suppose F, $\sigma : Y \mapsto \mathbb{R}$ are given, and the 3×3 matrix $A = \operatorname{diag}(a_{11}, a_{22}, a_{33})$ is coercive and bounded, where the terms $a_{ii} > 0$ may depend on ω but not on y. For g satisfying the solvability condition $0 = (g, 1)$ of Proposition* A.1, *if $F = \int_Y \sigma(y)dy$ holds, then the solution $u(y,\omega)$ of the boundary value problem*

$$\begin{aligned} \mathcal{A}_0 u(y,\omega) &= g(y,\omega) && \text{in } \Omega,\\ u(\_,\omega) & && \text{is 1-periodic},\\ a_{33}\partial_\omega u(y,0) &= \sigma(y) && \text{on } \partial\Omega_0,\\ a_{33}\partial_\omega u(y,\omega) &\to F && \text{as } \omega\to\infty \end{aligned}$$

is unique up to an additive constant. If $F \neq \int_Y \sigma(y)dy$, the problem has no solution.

Proof. For the case of constant A we proceed as in the first part of the proof of Proposition 3.1, and we expand

$$g(y,\omega) = \sum_{(n,m)\in\mathbb{Z}^2} g_{nm}(\omega)\psi_{nm}(y).$$

The equation for the coefficient functions c_{nm} becomes

$$a_{33}\partial_\omega^2 c_{nm}(\omega) - (2\pi)^2(a_{11}n^2 + a_{22}m^2)c_{nm}(\omega) + g_{nm}(\omega) = 0,$$

and we discern two cases. In the case $n^2+m^2\neq 0$, the general solution is

$$\begin{aligned} c_{nm}(\omega) &= \alpha_{nm}\exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)+\beta_{nm}\exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)\\ &\quad-\frac{\exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2\cdot 2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}}\int_0^\omega \exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta/a_{33}\\ &\quad+\frac{\exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2\cdot 2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}}\int_0^\omega \exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta/a_{33}.\end{aligned}$$

The derivative of this function is

$$\begin{aligned}\partial_\omega c_{nm} &= 2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\left(\alpha_{nm}e^{2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega}-\beta_{nm}e^{-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega}\right)\\ &\quad-\frac{\exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2a_{33}}\int_0^\omega \exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta\\ &\quad-\frac{\exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2a_{33}}\int_0^\omega \exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta.\end{aligned}$$

To use the boundary conditions (3.10)–(3.12), we calculate

$$\sigma_{nm}=a_{33}\partial_\omega c_{nm}(0)=2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}\,(\alpha_{nm}-\beta_{nm})$$

and

$$\begin{aligned}F_{nm}=0=a_{33}\partial_\omega c_{nm}(\infty) &= 2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}\;\alpha_{nm}e^{2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega}\Big|_{\omega=\infty}\\ &\quad-\frac{\exp\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right)}{2}\Bigg|_{\omega=\infty}\int_0^\infty \exp\left(-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta.\end{aligned}$$

We deduce then that

$$\alpha_{nm}=\frac{\int_0^\infty \exp\left(-2\pi\sqrt{\frac{(a_{11}n^2+a_{22}m^2)}{a_{33}}}\zeta\right)g_{nm}(\zeta)\mathrm{d}\zeta}{2\cdot 2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}},\quad \beta_{nm}=\alpha_{nm}-\frac{\sigma_{nm}}{2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}}.$$

In the case $n=m=0$, the equation is

$$a_{33}\partial_\omega^2 c_{00}(\omega)+g_{00}(\omega)=0,$$

for which we have

$$a_{33}\partial_\omega c_{00}(\omega)=K_{00}-\int_0^\omega g_{00}(\omega')d\omega',\quad a_{33}c_{00}(\omega)=K'_{00}+K_{00}\omega-\int_0^\omega\int_0^\zeta g_{00}(\omega')d\omega' d\zeta,$$

and the imposition of boundary conditions renders as

$$\sigma_{00} = a_{33}\partial_\omega c_{00}(0) = K_{00}, \quad F_{00} = a_{33}\partial_\omega c_{00}(\infty) = \sigma_{00} - \int_0^\infty g_{00}(\omega')d\omega',$$

and so, remembering that $(1, g) = 0$, this gives the condition

$$F = \int_Y \sigma(y)dy - \int_0^\infty \int_Y g(y,\omega)dyd\omega = \int_Y \sigma(y)dy.$$

The solution is then

$$u = K'_{00} + \frac{F\omega}{a_{33}} - \int_0^\omega \int_0^\zeta \frac{g_{00}(\omega')}{a_{33}} d\omega' d\zeta - \sum_{(n,m)\neq\bar{0}\in\mathbb{Z}^2} \psi_{nm}(y) \frac{e^{-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega}\sigma_{nm}}{2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}}$$

$$+ \sum_{(n,m)\neq\bar{0}\in\mathbb{Z}^2} \psi_{nm}(y) \frac{\int_0^\infty e^{-2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\zeta} g_{nm}(\zeta)\mathrm{d}\zeta}{2\pi\sqrt{(a_{11}n^2+a_{22}m^2)a_{33}}} \cosh\left(2\pi\sqrt{\frac{a_{11}n^2+a_{22}m^2}{a_{33}}}\omega\right).$$

For the case with diagonal A such that $a_{ii}(\omega) > 0$, we can obtain the solution to our nonhomogeneous system by using the method of variation of parameters over the solutions of the homogeneous system.

$$c^1_{nm} = e^{\frac{\operatorname{tr}\Omega(\omega)}{2}} \frac{\sinh q(\omega)}{q(\omega)} \Omega_{21}(\omega),\ c^2_{nm} = e^{\frac{\operatorname{tr}\Omega(\omega)}{2}} \left(\frac{\sinh q(\omega)}{q(\omega)}\left(\Omega_{22}(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\right) + \cosh q(\omega)\right)$$

(remembering Ω has an implicit n, m dependence) are two linearly independent solutions to the $(n,m) \neq \bar{0}$ homogeneous system, so a particular solution to the nonhomogenous problem is (with $W(c^1_{nm}, c^2_{nm})$ representing the Wronskian)

$$v_{nm}(\omega) = c^1_{nm}(\omega)\int_0^\omega \frac{c^2_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds - c^2_{nm}(\omega)\int_0^\omega \frac{c^1_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds$$

$$v_{nm}(\omega) = e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\frac{\sinh q(\omega)}{q(\omega)}\Omega_{21}(\omega)\right)\int_0^\omega \frac{e^{\frac{\operatorname{tr}\Omega(s)}{2}}\left(\frac{\sinh q(s)}{q(s)}\left(\Omega_{22}(s) - \frac{\operatorname{tr}\Omega(s)}{2}\right) + \cosh q(s)\right)\frac{g_{nm}(s)}{a_{33}(s)}}{W(c^1_{nm},c^2_{nm})(s)}ds$$

$$- e^{\frac{\operatorname{tr}\Omega(\omega)}{2}}\left(\frac{\sinh q(\omega)}{q(\omega)}\left(\Omega_{22}(\omega) - \frac{\operatorname{tr}\Omega(\omega)}{2}\right) + \cosh q(\omega)\right)\int_0^\omega \frac{e^{\frac{\operatorname{tr}\Omega(s)}{2}}\left(\frac{\sinh q(s)}{q(s)}\Omega_{21}(s)\right)\frac{g_{nm}(s)}{a_{33}(s)}}{W(c^1_{nm},c^2_{nm})(s)}ds.$$

We know $c_{nm}(\omega) = K_1 c^1_{nm}(\omega) + K_2 c^2_{nm}(\omega) + v_{nm}(\omega)$ with K_1, K_2 given by the boundary conditions $\sigma_{nm} = a_{33}(0)\partial_\omega c_{nm}(0)$, $F_{nm} = 0 = a_{33}(\infty)\partial_\omega c_{nm}(\infty)$. Since

$$a_{33}\partial_\omega c^1_{nm} = e^{\frac{\operatorname{tr}\Omega}{2}}\left[\frac{\sinh q}{q}\left(\Omega_{11} - \frac{\operatorname{tr}\Omega}{2}\right) + \cosh q\right],\ a_{33}\partial_\omega c^2_{nm} = \frac{\sinh q}{q}\Omega_{12}e^{\frac{\operatorname{tr}\Omega}{2}},$$

we have that $\sigma_{nm} = K_1 + a_{33}(0)\partial_\omega v_{nm}(0) = K_1$, and, unless $0 = a_{33}(\infty)$,

$$K_2 = \int_0^\infty \frac{c^1_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds - \frac{\partial_\omega c^1_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)}\left(\sigma_{nm} + \int_0^\infty \frac{c^2_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds\right).$$

The remaining case $n = 0 = m$ is $\partial_\omega(a_{33}(\omega)\partial_\omega c_{00}) = -g_{00}(\omega)$, with solution

$$c_{00}(\omega) = K'_{00} + K_{00}\int_0^\omega \frac{d\omega'}{a_{33}(\omega')} - \int_0^\omega \frac{d\xi}{a_{33}(\xi)}\int_0^\xi g_{00}(\omega')d\omega'. \tag{3.21}$$

The boundary conditions are $\sigma_{00} = a_{33}(0)\partial_\omega c_{00}(0) = K_{00}$ and

$$F = a_{33}(\infty)\partial_\omega c_{00}(\infty) = \sigma_{00} - \int_0^\infty g_{00}(\omega')d\omega' = \int_Y \sigma(y)dy$$

since $(g,1)=0$. The solution to the nonhomogeneous problem for $a_{ii}(\omega)$ is then

$$u = K'_{00} + \int_0^\omega \frac{F d\omega'}{a_{33}(\omega')} - \int_0^\omega \int_0^\xi \frac{g_{00}(\omega')d\omega' d\xi}{a_{33}(\xi)} + \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)[K_1 c^1_{nm}(\omega) + K_2 c^2_{nm}(\omega) + v_{nm}(\omega)]$$

$$u = K'_{00} + \int_0^\omega \frac{F d\omega'}{a_{33}(\omega')} - \int_0^\omega \int_0^\xi \frac{g_{00}(\omega')d\omega' d\xi}{a_{33}(\xi)} + \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\sigma_{nm}\left[c^1_{nm}(\omega) - \frac{\partial_\omega c^1_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)} c^2_{nm}(\omega)\right]$$
$$+ \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\Bigg(c^2_{nm}(\omega)\left[\int_0^\infty \frac{c^1_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds - \frac{\partial_\omega c^1_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)}\int_0^\infty \frac{c^2_{nm}(s)g_{nm}(s)/a_{33}(s)}{W(c^1_{nm},c^2_{nm})(s)}ds\right]$$
$$+ v_{nm}(\omega)\Bigg)$$

$$u = K'_{00} + \int_0^\omega \frac{F d\omega'}{a_{33}(\omega')} - \int_0^\omega \int_0^\xi \frac{g_{00}(\omega')d\omega' d\xi}{a_{33}(\xi)} + \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\sigma_{nm}\left[c^1_{nm}(\omega) - \frac{\partial_\omega c^1_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)} c^2_{nm}(\omega)\right]$$
$$+ \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\left(v_{nm}(\omega) - c^2_{nm}(\omega)\frac{\partial_\omega v_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)}\right)$$

$$u = K'_{00} + \int_0^\omega \frac{F d\omega'}{a_{33}(\omega')} - \int_0^\omega \int_0^\xi \frac{g_{00}(\omega')d\omega' d\xi}{a_{33}(\xi)}$$
$$+ \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\frac{\sigma_{nm}\left[\partial_\omega c^2_{nm}(\infty)c^1_{nm}(\omega) - \partial_\omega c^1_{nm}(\infty)c^2_{nm}(\omega)\right] + \partial_\omega c^2_{nm}(\infty)v_{nm}(\omega) - c^2_{nm}(\omega)\partial_\omega v_{nm}(\infty)}{\partial_\omega c^2_{nm}(\infty)}.$$

□

We remark that the condition $\int_Y \sigma(y)\mathrm{d}y = F$ codifies the physical intuition that we recall from the well-known example of the infinite charged plate. An infinite homogeneous 2D charged plate gives rise to an electric field that is constant everywhere in 3D space; this result is a nice exercise in integration and can be found, e.g., in Feynman's *Lectures on Physics*. The condition means that the charge density of the plate and the electric field at infinity must agree quantitatively. Furthermore, this proposition tells us that the potential due to oscillations in the charge of the plate decays exponentially as we move away from the plate. The field $-F$ far away from the plate is only determined by its average charge density. Finally, the solution is only determined up to an additive constant due to the combination of periodic and Neumann boundary conditions.

In general, boundary value problems of the kind of (3.3) in divergence form must satisfy a solvability condition because of the lack of Dirichlet boundary conditions. The solvability condition generally arises from integrating both the left-hand and right-hand sides over (y,ω) over a cell $\mathcal{C}$ and applying the divergence theorem. Physically speaking, this means that the fluxes under the divergence must balance the total charge in the domain. More precisely, the solvability condition is given in Proposition A.1. For the problem (3.3) at hand, the solvability condition means that $\int_0^\infty \int_Y \mathcal{A}_0\varphi_0 \mathrm{d}y\mathrm{d}\omega = 0$ must hold; here this condition is always satisfied due to the periodic and zero Neumann boundary conditions.

The equation for φ_1 is

(3.22a) $$\mathcal{A}_0\varphi_1 = -\mathcal{A}_1\varphi_0 \quad \text{in } \mathcal{C},$$

(3.22b) $$\varphi_1(\xi, z, \_, \omega) \quad \text{is 1-periodic},$$

(3.22c) $$\nu \cdot A(\nabla_{(\xi,z)}\varphi_0 + \nabla_{(y,\omega)}\varphi_1) = \sigma_0 \quad \text{on } \partial\mathcal{C}_0,$$

(3.22d) $$\nu \cdot A(\nabla_{(\xi,z)}\varphi_0 + \nabla_{(y,\omega)}\varphi_1) \to F \quad \text{as } \omega \to \infty.$$

For a nonconstant $A(\omega)$ this 1-periodic problem reduces to

$$\mathcal{A}_0\varphi_1 = \partial_\omega a_{33}(\omega)\partial_z\varphi_0(\xi,z) \quad \text{in } \mathcal{C}, \tag{3.23a}$$

$$\varphi_1(\xi,z,\_,\omega) \quad \text{is 1-periodic,} \tag{3.23b}$$

$$a_{33}(0)\partial_\omega\varphi_1|_{\omega=0} = \sigma_0 - a_{33}(0)\partial_z\varphi_0 \quad \text{on } \partial\mathcal{C}_0, \tag{3.23c}$$

$$a_{33}(\infty)\partial_\omega\varphi_1|_{\omega=\infty} \to F - a_{33}(\infty)\partial_z\varphi_0 \quad \text{as } \omega\to\infty. \tag{3.23d}$$

Our source function $g(\omega;\xi,z) = \partial_\omega a_{33}(\omega)\partial_z\varphi_0(\xi,z)$ has no y-dependence, so $g_{nm}(\omega) = 0$ for $(n,m) \neq \bar{0}$, and the problem is nonhomogeneous only for the case $(n,m) = \bar{0}$. For the problem to have a solution, it should hold that

$$F - a_{33}(\infty)\partial_z\varphi_0 = \int_Y dy\,[\sigma_0 - a_{33}(0)\partial_z\varphi_0] - \int_0^\infty d\omega\,\partial_\omega a_{33}(\omega)\partial_z\varphi_0(\xi,z), \tag{3.24}$$

which reduces to $F = \int_Y \sigma_0\,dy$. We apply the solvability condition in Proposition A.1,

$$0 = (1,\partial_\omega a_{33}(\omega))\partial_z\varphi_0(\xi,z) = (a_{33}(\infty) - a_{33}(0))\partial_z\varphi_0(\xi,z).$$

We can provide an explicit solution for this problem, which is

$$\varphi_1 = K'_{00} + \int_0^\omega \frac{(F - a_{33}(\infty)\partial_z\varphi_0)d\omega'}{a_{33}(\omega')} - \int_0^\omega \frac{d\beta}{a_{33}(\beta)}\int_0^\beta \partial_\omega a_{33}(\omega')\partial_z\varphi_0 d\omega'$$
$$+ \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)(K^1_{nm}c^1_{nm} + K^2_{nm}c^2_{nm}),$$

and which can be reduced to (since $\partial_z\varphi_0$ has no y-dependence)

$$\varphi_1 = K'_{00} + (F - a_{33}(\infty)\partial_z\varphi_0)\int_0^\omega \frac{d\omega'}{a_{33}(\omega')} - \partial_z\varphi_0\int_0^\omega \frac{(a_{33}(\beta) - a_{33}(0))d\beta}{a_{33}(\beta)}$$
$$+ \sum_{(n,m)\neq\bar{0}} \psi_{nm}\left[c^1_{nm} - \left.\frac{\partial_\omega c^1_{nm}}{\partial_\omega c^2_{nm}}\right|_\infty c^2_{nm}\right]\sigma_{0nm}.$$

Further simplification from the solvability condition in Proposition A.1 renders as

$$\varphi_1 = K'_{00} + F\int_0^\omega \frac{d\tilde{\omega}}{a_{33}(\tilde{\omega})} - \omega\partial_z\varphi_0(\xi,z) + \sum_{(n,m)\neq\bar{0}} \psi_{nm}(y)\sigma_{0nm}\left[c^1_{nm}(\omega) - \left.\frac{\partial_\omega c^1_{nm}}{\partial_\omega c^2_{nm}}\right|_\infty c^2_{nm}(\omega)\right].$$

We observe that we can divide φ_1 by linearity into two components, one satisfying a Laplace problem with Neumann boundary conditions associated to the surface charge σ_0 plus another part satisfying a Poisson equation where the source and the boundary conditions are related to $\partial_z\varphi_0$, that is, $\varphi_1 = \varphi_1^P + \varphi_1^L$, such that $\varphi_1^P = -\omega\partial_z\varphi_0(\xi,z)$ satisfies

$$\mathcal{A}_0\varphi_1^P = \partial_\omega a_{33}(\omega)\partial_z\varphi_0(\xi,z) \quad \text{in } \mathcal{C}, \tag{3.25a}$$

$$\varphi_1^P(\xi,z,\_,\omega) \quad \text{is 1-periodic,} \tag{3.25b}$$

$$a_{33}(0)\partial_\omega\varphi_1^P|_{\omega=0} = -a_{33}(0)\partial_z\varphi_0 \quad \text{on } \partial\mathcal{C}_0, \tag{3.25c}$$

$$a_{33}(\infty)\partial_\omega\varphi_1^P|_{\omega=\infty} \to -a_{33}(\infty)\partial_z\varphi_0 \quad \text{as } \omega\to\infty, \tag{3.25d}$$

$\varphi_1^L = K'_{00} + F\int_0^\omega \frac{d\tilde\omega}{a_{33}(\tilde\omega)} + \sum_{(n,m)\neq\bar 0}\psi_{nm}(y)\sigma_{0nm}\left(c^1_{nm}(\omega) - \frac{\partial_\omega c^1_{nm}}{\partial_\omega c^2_{nm}}\Big|_\infty c^2_{nm}(\omega)\right)$ s.t.

$$\mathcal{A}_0\varphi_1^L = 0 \quad \text{in } \mathcal{C}, \tag{3.26a}$$

$$\varphi_1^L(\xi, z, \_, \omega) \quad \text{is 1-periodic}, \tag{3.26b}$$

$$a_{33}(0)\partial_\omega\varphi_1^L|_{\omega=0} = \sigma_0 \quad \text{on } \partial\mathcal{C}_0, \tag{3.26c}$$

$$a_{33}(\infty)\partial_\omega\varphi_1^L|_{\omega=\infty} \to F \quad \text{as } \omega\to\infty. \tag{3.26d}$$

The Poisson component can be expressed as $\varphi_1^P = -\omega\partial_z\varphi_0(\xi, z) = \chi(\omega)\cdot\nabla_{(\xi,z)}\varphi_0$ with $\chi(\omega) = (0, 0, -\omega)$.

Again, we apply Proposition A.1 for elliptic problems and see that the solvability condition

$$\int_{\mathcal{C}} \mathcal{A}_0\varphi_1 \mathrm{d}y\mathrm{d}\omega = -\int_{\mathcal{C}} \mathcal{A}_1\varphi_0\mathrm{d}y\mathrm{d}\omega$$

must be satisfied. The left-hand side simplifies to (defining $\partial\mathcal{C}$ as the boundary of $\mathcal{C}$ in the ω direction)

$$\int_{\mathcal{C}} \mathcal{A}_0\varphi_1\mathrm{d}y\mathrm{d}\omega = -\int_{\partial\mathcal{C}} \nu\cdot A\nabla_{(y,\omega)}\varphi_1\mathrm{d}y\mathrm{d}\omega = -\int_Y \nu\cdot A\nabla_{(y,\omega)}\varphi_1\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty},$$

and the right-hand side becomes

$$\begin{aligned}\int_{\mathcal{C}} \mathcal{A}_1\varphi_0\mathrm{d}y\mathrm{d}\omega &= -\int_{\mathcal{C}} \nabla_{(y,\omega)}\cdot(A\nabla_{(\xi,z)}\varphi_0) + \nabla_{(\xi,z)}\cdot(A\nabla_{(y,\omega)}\varphi_0)\mathrm{d}y\mathrm{d}\omega\\ &= -\int_Y \nu\cdot A\nabla_{(\xi,z)}\varphi_0\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty} - \int_{\mathcal{C}}(\nabla_{(y,\omega)}\cdot A^T)\cdot\nabla_{(\xi,z)}\varphi_0\mathrm{d}y\mathrm{d}\omega\\ &= -\int_Y \nu\cdot A\nabla_{(\xi,z)}\varphi_0\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty} - \nabla_{(\xi,z)}\varphi_0\cdot\int_{\mathcal{C}}\nabla_{(y,\omega)}\cdot A^T\mathrm{d}y\mathrm{d}\omega\\ &= -\int_Y \nu\cdot A\nabla_{(\xi,z)}\varphi_0\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty} - \nabla_{(\xi,z)}\varphi_0\cdot\Big(\int_Y \nu\cdot A^T\mathrm{d}y\Big)\Big|_{\omega=0}^{\omega\to\infty},\end{aligned}$$

since A^T is periodic in y (trivially). Hence the solvability condition becomes

$$\int_Y \sigma_0(y) - F\mathrm{d}y = \nabla_{(\xi,z)}\varphi_0\cdot\Big(\int_Y \nu\cdot A^T\mathrm{d}y\Big)\Big|_{\omega=0}^{\omega\to\infty} = a_{33}(\omega)\Big|_0^\infty\partial_z\varphi_0 = 0, \tag{3.27}$$

so in the case when the two surface integrals on the right-hand side are identical, we recover

$$\int_Y \sigma_0(y)\mathrm{d}y = \int_Y F\mathrm{d}y = F,$$

meaning that the field at infinity and the average surface charge density of the infinite charge plate must correspond when they are prescribed as boundary conditions. The equation for φ_2 is

$$\begin{aligned} \mathcal{A}_0\varphi_2 = n_{D0} - \mathcal{A}_1\varphi_1 - \mathcal{A}_2\varphi_0 &\quad \text{in } \mathcal{C},\\ \varphi_2(\xi, z, \_, \omega) &\quad \text{is 1-periodic},\\ \nu\cdot A(\nabla_{(\xi,z)}\varphi_1 + \nabla_{(y,\omega)}\varphi_2) = \sigma_1 &\quad \text{on } \partial\mathcal{C}_0,\\ \nu\cdot A(\nabla_{(\xi,z)}\varphi_1 + \nabla_{(y,\omega)}\varphi_2) \to 0 &\quad \text{as } \omega\to\infty.\end{aligned}$$

The solvability condition for this problem is

$$\int_{\mathcal{C}} \mathcal{A}_0\varphi_2 \mathrm{d}y\mathrm{d}\omega = \int_{\mathcal{C}} n_{D0} - \mathcal{A}_1\varphi_1 - \mathcal{A}_2\varphi_0 \mathrm{d}y\mathrm{d}\omega.$$

Applying the divergence theorem to the left-hand side, we find

$$\int_{\mathcal{C}} \mathcal{A}_0\varphi_2 \mathrm{d}y\mathrm{d}\omega = -\int_Y \nu\cdot(A\nabla_{(y,\omega)}\varphi_2)\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty},$$

whereas the right-hand side simplifies to

$$\begin{aligned}
&\int_{\mathcal{C}} n_{D0} - \mathcal{A}_1\varphi_1 - \mathcal{A}_2\varphi_0 \mathrm{d}y\mathrm{d}\omega \\
&= \int_C n_{D0}\mathrm{d}y\mathrm{d}\omega + \int_{\mathcal{C}} \nabla_{(y,\omega)}\cdot(A\nabla_{(\xi,z)}\varphi_1) + \nabla_{(\xi,z)}\cdot(A\nabla_{(y,\omega)}\varphi_1)\mathrm{d}y\mathrm{d}\omega \\
&\quad + \nabla_{(\xi,z)}\cdot\left(\int_{\mathcal{C}} A\mathrm{d}y\mathrm{d}\omega\nabla_{(\xi,z)}\varphi_0\right) \\
&= \int_{\mathcal{C}} n_{D0}\mathrm{d}y\mathrm{d}\omega + \int_Y \nu\cdot A\nabla_{(\xi,z)}\varphi_1\mathrm{d}y\Big|_{\omega=0}^{\omega\to\infty} + \int_{\mathcal{C}} \nabla_{(\xi,z)}\cdot(A(\nabla_{(y,\omega)}\chi_1)^T\nabla_{(\xi,z)}\varphi_0)\mathrm{d}y\mathrm{d}\omega \\
&\quad + \nabla_{(\xi,z)}\cdot\left(\int_{\mathcal{C}} A\mathrm{d}y\mathrm{d}\omega\nabla_{(\xi,z)}\varphi_0\right).
\end{aligned}$$

The problem for φ_2 can be reexpressed as

$$\begin{aligned}
\mathcal{A}_0\varphi_2 &= n_{D0} + \partial_\omega a_{33}(\partial_z K'_{00} - \omega\partial_z^2\varphi_0) - a_{33}\partial_z^2\varphi_0 + a_{11}\partial_{\xi_1}^2\varphi_0 + a_{22}\partial_{\xi_2}^2\varphi_0 && \text{in } \mathcal{C},\\
&\varphi_2(\xi,z,_,\omega) && \text{is 1-periodic},\\
a_{33}(0)\partial_\omega\varphi_2 &= \sigma_1 - a_{33}(0)\ \partial_z\varphi_1|_{\omega=0} = \sigma_1 - a_{33}(0)\partial_z K'_{00} && \text{on } \partial\mathcal{C}_0,\\
a_{33}(\omega)\partial_\omega\varphi_2 &\to -a_{33}(\omega)\partial_z\varphi_1 = -a_{33}(\omega)(\partial_z K'_{00} - \omega\partial_z^2\varphi_0) && \text{as } \omega\to\infty.
\end{aligned}$$

If this Poisson problem is to have a solution, it must hold that

(3.28)

$$\begin{aligned}
&-a_{33}(\omega)(\partial_z K'_{00} - \omega\partial_z^2\varphi_0)\Big|_{\omega=\infty} = \int_Y \sigma_1 dy - a_{33}(0)\partial_z K'_{00} \\
&-\int_0^\infty d\omega\int_Y dy\left[n_{D0} + \partial_\omega a_{33}(\partial_z K'_{00} - \omega\partial_z^2\varphi_0) - a_{33}\partial_z^2\varphi_0 + a_{11}\partial_{\xi_1}^2\varphi_0 + a_{22}\partial_{\xi_2}^2\varphi_0\right],
\end{aligned}$$

which can be simplified to

$$\partial_{\xi_1}^2\varphi_0\int_0^\infty a_{11}d\omega + \partial_{\xi_2}^2\varphi_0\int_0^\infty a_{22}d\omega = \int_Y \sigma_1 dy - \int_0^\infty\int_Y n_{D0}d\omega dy.$$

The solvability condition from Proposition A.1 is

(3.29)

$$\begin{aligned}
0 &= (1, n_{D0} + \partial_\omega a_{33}\partial_z\varphi_1 - a_{33}\partial_z^2\varphi_0 + a_{11}\partial_{\xi_1}^2\varphi_0 + a_{22}\partial_{\xi_2}^2\varphi_0) \\
&= (1, n_{D0}) + a_{33}(\omega)\ |_0^\infty\ \partial_z K'_{00} - a_{33}(\omega)\ \omega|_\infty\ \partial_z^2\varphi_0 + (1,a_{11})\partial_{\xi_1}^2\varphi_0 + (1,a_{22})\partial_{\xi_2}^2\varphi_0.
\end{aligned}$$

Applying the Proposition A.1 solvability condition in the relation between the electric force and the (surface and volumetric) charges, we have

$$-a_{33}(\omega)(\partial_z K'_{00} - \omega\partial_z^2\varphi_0)\big|_{\omega=\infty} = \int_Y \sigma_1 dy - a_{33}(0)\partial_z K'_{00}; \tag{3.30}$$

therefore, the Proposition A.1 solvability condition can be reexpressed as

$$(1, a_{11})\partial^2_{\xi_1}\varphi_0 + (1, a_{22})\partial^2_{\xi_2}\varphi_0 = \int_Y \sigma_1 dy - (1, n_{D0}), \tag{3.31}$$

which renders again as a Poisson equation in the ξ-domain for φ_0 (as the a_{33} term has vanished), having as sources the surface charge σ_1 and the doping $n_{D0}(\xi, z, y, \omega)$, and having permittivities averaged over the (y, ω)-domain.

Next we consider the equations for ψ_0, ψ_1, and ψ_2 for the self-consistent potential ψ^ε. The equation for ψ_0 is the same as the one for φ_0. This yields $\psi_0(t, \xi, z)$ as a function of the slow variables only. The equation for ψ_1 is the same as the one for φ_1 but with zero boundary conditions; that is,

$$\mathcal{A}_0\psi_1 = \partial_\omega a_{33}(\omega)\partial_z\psi_0(\xi, z) \quad \text{in } \mathcal{C}, \tag{3.32a}$$

$$\psi_1(\xi, z, \_, \omega) \quad \text{is 1-periodic,} \tag{3.32b}$$

$$a_{33}(0)\partial_\omega\psi_1|_{\omega=0} = -a_{33}(0)\partial_z\psi_0 \quad \text{on } \partial\mathcal{C}_0, \tag{3.32c}$$

$$a_{33}(\infty)\partial_\omega\psi_1|_{\omega=\infty} \to -a_{33}(\infty)\partial_z\psi_0 \quad \text{as } \omega \to \infty. \tag{3.32d}$$

We already know that the solution is $\psi_1 = -\omega\partial_z\psi_0(\xi, z) + K(\xi, z)$, a constant with respect to (y, ω) that uniquely defines the problem. Defining it up to a constant, ψ_1 has the form of a separation ansatz,

$$\psi_1(\xi, z, y, \omega) = \chi_1(y, \omega) \cdot \nabla_{(\xi,z)}\psi_0(\xi, z), \tag{3.33}$$

with $\chi_1(y, \omega) = (0, 0, -\omega) = \chi_1(\omega)$, for which the change of variables renders as a so-called cell problem,

$$-\nabla_{(y,\omega)} \cdot (A\nabla_{(y,\omega)}\chi_1) = \nabla_{(y,\omega)} \cdot A^T \quad \text{in } \mathcal{C}.$$

We remember that the self-consistent charge concentration is given by the two-scale formulation as $n^\varepsilon(t, \xi, z, y, \omega) = n_0(t, \xi, z, y, \omega) + \varepsilon n_1(t, \xi, z, y, \omega) + \cdots$. After comparing coefficients of ε, the equation for ψ_2 is found to be

$$\begin{aligned}
\mathcal{A}_0\psi_2 = n_0 - \mathcal{A}_1\psi_1 - \mathcal{A}_2\psi_0 &\quad \text{in } \mathcal{C},\\
\psi_2(\xi, z, _, \omega) &\quad \text{is 1-periodic,}\\
\nu \cdot A(\nabla_{(\xi,z)}\psi_1 + \nabla_{(y,\omega)}\psi_2) = 0 &\quad \text{on } \partial\mathcal{C}_0,\\
\nu \cdot A(\nabla_{(\xi,z)}\psi_1 + \nabla_{(y,\omega)}\psi_2) \to 0 &\quad \text{as } \omega \to \infty.
\end{aligned}$$

The solvability condition for this problem is equivalent to the one considered for φ_2. Defining more explicitly the source and boundary conditions for ψ_2, we have

$$\begin{aligned}
&\mathcal{A}_0\psi_2 = n_0 + \partial_\omega a_{33}\partial_z K(\xi, z) - \partial_\omega(\omega a_{33})\partial^2_z\psi_0 + a_{22}\partial^2_{\xi_2}\psi_0 + a_{11}\partial^2_{\xi_1}\psi_0 && \text{in } \mathcal{C},\\
&\psi_2(\xi, z, _, \omega) && \text{is 1-periodic,}\\
&a_{33}(0)\partial_\omega\psi_2 = -a_{33}(0)\partial_z K(\xi, z) && \text{on } \partial\mathcal{C}_0,\\
&a_{33}(\omega)\partial_\omega\psi_2 = -a_{33}(\omega)\partial_z K(\xi, z) + \omega a_{33}(\omega)\partial^2_z\psi_0(\xi, z) && \text{as } \omega \to \infty.
\end{aligned}$$

If this problem has a solution, then it must hold that

$$\begin{aligned}
&- a_{33}\big|_\infty \partial_z K + \lim_{\omega\to\infty} \omega a_{33}(\omega)\partial^2_z\psi_0(\xi, z) = -a_{33}(0)\partial_z K\\
&- \int_0^\infty \int_Y dy d\omega \left(n_0 + \partial_\omega a_{33}\partial_z K - \partial_\omega(\omega a_{33}(\omega))\partial^2_z\psi_0 + a_{22}(\omega)\partial^2_{\xi_2}\psi_0 + a_{11}(\omega)\partial^2_{\xi_1}\psi_0\right),
\end{aligned}$$

which is equal to

$$-\partial_{\xi_2}^2\psi_0\int_0^\infty a_{22}(\omega)d\omega-\partial_{\xi_1}^2\psi_0\int_0^\infty a_{11}(\omega)d\omega=\int_0^\infty\int_Y n_0(t,\xi,z,y,\omega)dyd\omega.$$

The solvability condition for this problem is

$$0=(1,n_0)+a_{33}|_0^\infty\,\partial_z K-\omega a_{33}(\omega)|_\infty\,\partial_z^2\psi_0+(1,a_{11})\partial_{\xi_1}^2\psi_0+(1,a_{22})\partial_{\xi_2}^2\psi_0, \tag{3.34}$$

which would simply reduce the equality between the electric field and the surface charge to

$$\partial_z^2\psi_0(\xi,z)\lim_{\omega\to\infty}\omega a_{33}(\omega)=a_{33}|_0^\infty\,\partial_z K(\xi,z), \tag{3.35}$$

and using this in the solvability condition gives us again

$$-(1,a_{11})\partial_{\xi_1}^2\psi_0-(1,a_{22})\partial_{\xi_2}^2\psi_0=(1,n_0), \tag{3.36}$$

which is an effective Poisson equation in the ξ-variable for the potential ψ_0 having as source the charge n_0 and averaged permittivities $(1,a_{11})$ and $(1,a_{22})$. This problem links the Poisson equation with the Boltzmann equation via ψ_0 and n_0.

3.2. Boltzmann problem. Having treated the elliptic problems arising from the Poisson equation, we now return to the Boltzmann equation (3.2). We now intend to obtain more information on the probability density function of our system and the equation that it obeys in the limit. We define

$$\eta:=\begin{pmatrix}y\\ \omega\end{pmatrix}.$$

By proceeding as in the derivation of (2.1), we find that the equation for f_0 at order ε^{-1} is

$$v\cdot\nabla_\eta f_0-\nabla_\eta u_0\cdot\nabla_v f_0-Q(f_0)=0.$$

By [2, Proposition 3.1], f_0 must have the form

$$f_0=\rho(t,x)\frac{\exp(-u_0(t,x,\eta))}{\int_Y dy\exp(-u_0(t,x,\eta))}M(v)=N_0(t,x,\eta)\mu(\xi,z,v), \tag{3.37}$$

where μ is the modulated Maxwellian

$$\mu(\xi,z,v):=M(v)\exp(-U(\xi,z)), \tag{3.38}$$

with $U(x)$ a time-independent potential of choice (for example, an ansatz for the equilibrium solution of the potential in terms of the slow variables only), and $N_0(t,x,\eta)$ the time-dependent density

$$N_0(t,x,\eta)=\rho(t,x)\frac{\exp(U(x)-u_0(t,x,\eta))}{\int_Y dy\exp(-u_0(t,x,\eta))}. \tag{3.39}$$

We will simply choose $U=0$, in which case $\mu=M(v)$, and $N_0(t,x,\eta)=\rho(t,x)e^{-u_0(t,x,\eta)}/\int_Y e^{-u_0(t,x,\eta)}dy$. The equation for f_1 obtained from (3.2) at the next order ε^0 is

$$Q(f_1)-v\cdot\nabla_\eta f_1+\nabla_\eta u_0\cdot\nabla_v f_1=(v\cdot\nabla_x-\nabla_x u_0\cdot\nabla_v-\nabla_\eta u_1\cdot\nabla_v)f_0. \tag{3.40}$$

We define $\mathcal{L}$ to be the operator on the left-hand side, i.e.,

$$\mathcal{L} := Q - v \cdot \nabla_\eta + \nabla_\eta u_0 \cdot \nabla_v.$$

Using (3.37) for f_0, we calculate the right-hand side of (3.40) as

$$\begin{aligned} R &:= (v \cdot \nabla_x - \nabla_x u_0 \cdot \nabla_v - \nabla_\eta u_1 \cdot \nabla_v) f_0 \\ &= \mu v \cdot \nabla_x N_0 + N_0 v \cdot \nabla_x \mu + N_0 \mu v \cdot \nabla_x u_0 + N_0 \mu v \cdot \nabla_\eta u_1 \\ &= \mu v \cdot (\nabla_x N_0 - N_0 \nabla_x U + N_0 \nabla_x u_0) + N_0 \mu v \cdot \nabla_\eta u_1 \\ &= \mu v \cdot \big(\nabla_x N_0 + N_0 \nabla_x u_0\big) + N_0 \mu v \cdot \nabla_\eta u_1, \end{aligned}$$

since $N_0 v \cdot \nabla_x \mu = -N_0 \mu v \cdot \nabla_x U = 0$.

The solvability condition for (3.40) according to [2, Proposition 3.1] is that the integral over the right-hand side vanishes, i.e.,

$$\lim_{L \to \infty} \int_0^L R \mathrm{d}v \mathrm{d}y \mathrm{d}z = 0.$$

This solvability condition is always satisfied. To see this, we note that the integrand has the form $\mu v \cdot T$, where T does not depend on v, and therefore it is an odd function with respect to v_i. Hence already the integrals over v_i vanish.

We now consider the last term of R. Recalling the separation ansatz (3.33) for ψ_1 and for part of the solution of φ_1, we have (up to a constant)

$$\begin{aligned} \varphi_1(x, \eta) &= \chi_1(\eta) \cdot \nabla_x \varphi_0(x) + \int_0^\omega \frac{F d\tilde{\omega}}{a_{33}(\tilde{\omega})} \\ &\quad + \sum_{(n,m) \neq \bar{0}} \sigma_{0nm} \psi_{nm}(y) \left[c^1_{nm}(\omega) - \left.\frac{\partial_\omega c^1_{nm}}{\partial_\omega c^2_{nm}}\right|_\infty c^2_{nm}(\omega) \right], \\ \psi_1(x, \eta) &= \chi_2(\eta) \cdot \nabla_x \psi_0(x), \end{aligned}$$

with $\chi_1(\omega) = (0, 0, -\omega) = \chi_2(\omega)$. Using these relationships for u_1, we find that the last term becomes

$$N_0 \mu v \cdot \nabla_\eta u_1 = N_0 \mu v \cdot (\nabla_\eta \chi_1 \nabla_x \varphi_0 + \nabla_\eta \chi_2 \nabla_x \psi_0 + \nabla_\eta \varphi_1^L),$$

with

$$\nabla_\eta \varphi_1^L = \frac{F \hat{e}_\omega}{a_{33}(\omega)} + \sum_{(n,m) \neq \bar{0}} \sigma_{0nm} \nabla_{(y,\omega)} \left(\psi_{nm}(y) \left[c^1_{nm}(\omega) - \left.\frac{\partial_\omega c^1_{nm}}{\partial_\omega c^2_{nm}}\right|_\infty c^2_{nm}(\omega) \right] \right).$$

We define

$$\begin{aligned} \theta_1 &:= \mathcal{L}^{-1}(\mu v), \\ \theta_{21} &:= \mathcal{L}^{-1}(\mu v \cdot \nabla_\eta \chi_1), \\ \theta_{22} &:= \mathcal{L}^{-1}(\mu v \cdot \nabla_\eta \chi_2), \\ \theta_L &:= \mathcal{L}^{-1}(\mu v \cdot \nabla_\eta \varphi_1^L), \end{aligned}$$

and using these new variables, (3.40) for f_1 becomes

$$f_1 = (\nabla_x N_0 + N_0 \nabla_x u_0) \cdot \theta_1 + N_0 \nabla_x \varphi_0 \cdot \theta_{21} + N_0 \nabla_x \psi_0 \cdot \theta_{22} + N_0 \theta_L.$$

The equation for f_2 obtained from (3.2) at the next order ε^1 is

$$\partial_\tau f_0 + v\cdot\nabla_x f_1 - \nabla_x u_0\cdot\nabla_v f_1 - \nabla_x u_1\cdot\nabla_v f_0 + v\cdot\nabla_\eta f_2 \\ - \nabla_\eta u_0\cdot\nabla_v f_2 - \nabla_\eta u_1\cdot\nabla_v f_1 - \nabla_\eta u_2\cdot\nabla_v f_0 = Q(f_2),$$

which can be rewritten as

$$\mathcal{L}f_2 = \partial_\tau f_0 + v\cdot\nabla_x f_1 - \nabla_x u_0\cdot\nabla_v f_1 - \nabla_x u_1\cdot\nabla_v f_0 - \nabla_\eta u_1\cdot\nabla_v f_1 - \nabla_\eta u_2\cdot\nabla_v f_0.$$

The solvability condition for this last equation is again that the integral over the right-hand side vanishes, i.e., that

$$\iint [\partial_\tau f_0 + v\cdot\nabla_x f_1 - \nabla_x u_0\cdot\nabla_v f_1 - \nabla_x u_1\cdot\nabla_v f_0 - \nabla_\eta u_1\cdot\nabla_v f_1 - \nabla_\eta u_2\cdot\nabla_v f_0]\,\mathrm{d}\eta\mathrm{d}v \\ = 0$$

holds. The first two terms are survivors. The last four terms vanish after partial integration with respect to v, since the u_i do not depend on v.

Therefore, the condition simplifies to

$$\lim_{L\to\infty}\Big(\partial_\tau N_0 \iint_0^L \mu\,\mathrm{d}\eta\mathrm{d}v \\ + \iint_0^L v\cdot\nabla_x\big((\nabla_x N_0 + N_0\nabla_x u_0)\cdot\theta_1 + N_0\nabla_x\varphi_0\cdot\theta_{21} + N_0\nabla_x\psi_0\cdot\theta_{22} + N_0\theta_L\big)\mathrm{d}\eta\mathrm{d}v\Big) = 0.$$

This can be rewritten as

$$\lim_{L\to\infty}\Big(\partial_\tau N_0 \iint_0^L \mu\,\mathrm{d}\eta\mathrm{d}v \\ + \nabla_x\cdot\iint_0^L \big((\nabla_x N_0 + N_0\nabla_x u_0)\cdot\theta_1 + N_0\nabla_x\varphi_0\cdot\theta_{21} + N_0\nabla_x\psi_0\cdot\theta_{22} + N_0\theta_L\big)v\,\mathrm{d}\eta\mathrm{d}v\Big) = 0$$

and furthermore as

$$\lim_{L\to\infty}\Big(\partial_\tau N_0 \iint_0^L \mu\,\mathrm{d}\eta\mathrm{d}v + \nabla_x\cdot\Big(\iint_0^L v\otimes\theta_1\,\mathrm{d}\eta\mathrm{d}v(\nabla_x N_0 + N_0\nabla_x u_0) \\ + \iint_0^L v\otimes\theta_{21}\,\mathrm{d}\eta\mathrm{d}v(N_0\nabla_x\varphi_0) + \iint_0^L v\otimes\theta_{22}\,\mathrm{d}\eta\mathrm{d}v(N_0\nabla_x\psi_0) + \iint_0^L v\theta_L\,\mathrm{d}\eta\mathrm{d}v N_0\Big)\Big) = 0.$$

Dividing by L and considering the limit $L\to\infty$, we obtain

$$\lim_{L\to\infty}\Big(\partial_\tau N_0 + \nabla_x\cdot\Big(\int\!\!\fint_0^L v\otimes\theta_1\,\mathrm{d}\eta\mathrm{d}v(\nabla_x N_0 + N_0\nabla_x u_0) \\ + \int\!\!\fint_0^L v\otimes\theta_{21}\,\mathrm{d}\eta\mathrm{d}v(N_0\nabla_x\varphi_0) + \int\!\!\fint_0^L v\otimes\theta_{22}\,\mathrm{d}\eta\mathrm{d}v(N_0\nabla_x\psi_0) + \int\!\!\fint_0^L v\theta_L\,\mathrm{d}\eta\mathrm{d}v N_0\Big)\Big) = 0.$$

This is a drift-diffusion equation with four different drift coefficients according to the kind of electric field and potential considered in the limit as $L\to\infty$, the last term being related to the contribution of the surface charge and the force generated by it.

4. Conclusion. We have homogenized the Boltzmann–Poisson system for surface problems under a periodic permittivity and periodic charge density conditions in the background medium. Formal results were obtained for this problem. Furthermore, we have shown the existence and uniqueness of the solutions of the Laplace and Poisson problems in the fast variables with periodic and surface charge boundary conditions generating an electric field at infinity. We have considered diagonal permittivity matrices which are functions of the fast variable orthogonal to the boundary, and we have obtained solutions for the potential in terms of Magnus expansions. We have also performed the two-scale homogenization expansion for the Boltzmann–Poisson system, considering the electric potential as the sum of a stationary part and a self-consistent one. A drift-diffusion-type equation is obtained for this problem by applying a solvability condition, which is characteristic of homogenization problems.

Appendix A. Solvability condition for elliptic problems.

PROPOSITION A.1 (Solvability condition). *Suppose that* $f \in L^2_{\#}(\mathbb{T}^d)$ *and* $A \in M_{\#}(\alpha, \beta, \mathbb{T}^d)$ *with* $A = A^\top$*. Then the Poisson equation*

$$-\nabla \cdot (A \nabla u) = f$$

has a unique (up to an additive constant a.e.) weak solution $u \in H$ *if and only if*

$$(f, 1) = 0.$$

Proof. See, for example, [8, section 7.2]. ∎

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