

Homogenisation of Periodic Quantum Graphs

an MSc. Mathematical Modelling Dissertation

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Abstract

This dissertation analyses the asymptotic behaviour of the solution of problems on periodic quantum graphs as the period tends to zero. We consider variants of periodic quantum graphs with periodicity in one and two directions. Variants analysed include contrasts and stretching, and the question of existence of spectral gaps is addressed for the case of a contrasting graph with periodicity in one direction.

September 2017

1. Introduction

A quantum graph is a metric graph equipped with an operator that acts as the negative second order derivative along edges and is accompanied by “appropriate” vertex conditions [E]. A common vertex condition, and the one we will be using in this dissertation, is that the functions acted on by the operator are continuous at each vertex (and on the whole graph, for that matter), and the sum of all their “outgoing” first derivatives at each vertex is equal to zero. Here “outgoing” derivatives refer to derivatives on edges incident to a vertex, taken in the directions away from the vertex.

Quantum graphs find applications mainly as simplified models in fields related to mesoscopic physics and nanotechnology, where they are used to model systems such as photonic crystals, quantum wires, conjugated molecules, and carbon allotropes related to graphene [B, E, F].

We consider a quantum graph to be periodic if its underlying graph has a repeating geometrical structure with translational symmetry along one or more axes when embedded in a Euclidean space.

Homogenisation is an asymptotic method applied to partial differential equation systems on domains that possess some kind of inhomogeneous periodic “micro-structure” that gives rise to rapidly oscillating coefficients. By considering the averaged behaviour of the system over a much larger length scale than the characteristic length of the “micro-structure”, it allows us to analyse a simplified version of the problem where the periodicity is “smoothed-out”.

In this dissertation we will be applying homogenisation to periodic quantum graphs, and analysing the averaged “macro-scale” behaviour of solutions of a periodic operator problem on them.

2. Problem Statement

We will be analysing the behaviour of a periodic operator problem of the form

$$\Delta_{\Gamma_\epsilon} u - \lambda u = f$$

on variants of two types of planar periodic quantum graphs, where Δ_{Γ_ϵ} is a Laplacian operator on each graph Γ_ϵ with period ϵ . Here $\lambda \in \mathbb{R}$, u is an unknown vector in some function space to be defined later, and f is a given vector in the space L^2 of square integrable functions (and, for the problems that require it, in the space C^2 of continuous functions with continuous first and second derivatives). This can be seen as a simplified version of operators commonly used in electromagnetism, solid-state physics, and quantum mechanics, and where analysis of the spectrum and its gaps has led to useful applications such as semiconductors and so-called “meta-materials”.

We will be using the Method of Multiple Scales, where we will assume our unknown functions have two distinct behaviours, one at a “short” scale, and another at a “long” scale. We represent this by using ansatzes consisting of power series expansions in ϵ of functions of the two variables y (for the “short” scale) and $x = \epsilon y$ (for the “long” scale), where we will treat the variables as if they were effectively independent. The scaling parameter ϵ is to be considered a small parameter such that $0 < \epsilon \ll 1$. We will also assume that some of the unknown functions, as well as their first derivatives, are periodic in the “short” scale on unit-cells to be defined for each problem type. Based on this, we will look for the homogenised behaviour of the unknown functions on the “long” scale, which will be our main objective.

In order to simplify calculations, instead of working directly on Γ_ϵ we will be working on re-scaled graphs Γ with period 1. The price to pay for this approach is the appearance of large coefficients in front of the differential operator after re-scaling.

3. Homogenisation of Quantum Graphs Exhibiting Periodicity in One Direction

In this section we will analyse the behaviour of our periodic operator on a thin, infinite-length planar “ladder” quantum graph which presents periodicity in the infinite length direction when embedded in the plane (y_1, y_2) and aligned to its coordinate basis, as illustrated in figure 3.1:

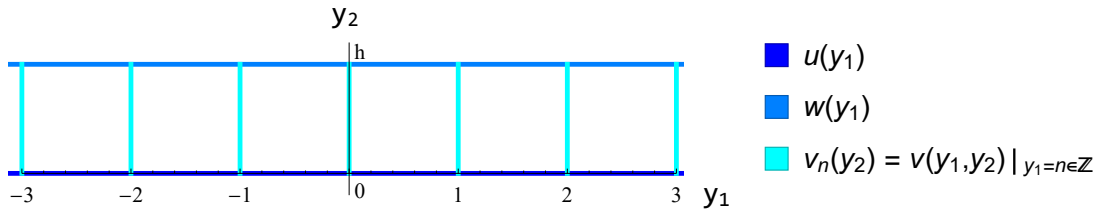


Figure 3.1: Close-up of the quantum graph embedded in the plane, displaying the six “horizontal”-periodicity cells closest to the origin

The graph has height $h = \gamma$ for the “simple” and “contrasting” cases, and $h = \frac{\gamma}{\epsilon}$ for the “stretched” case, for positive γ of $O(1)$.

We define unknown functions $u(y_1)$ and $w(y_1)$ in the Sobolev space $H^1(\mathbb{R})$ acting on the “horizontal” paths at $y_2 = 0$ and $y_2 = \gamma$ respectively, and a family of unknown functions $v_n(y_2)$ in $H^1(0, h)$ acting on each “vertical” edge at $y_1 = n \in \mathbb{Z}$. We define $f_0(\epsilon y_1)$ and $f_1(\epsilon y_1)$ as known functions in $L^2(\mathbb{R})$ acting on the “horizontal” paths at $y_2 = 0$ and $y_2 = h$ respectively. In this context, our periodic operator takes the form:

$$\alpha v_n''(y_2) - \lambda v_n(y_2) = 0, \quad n \in \mathbb{Z}, y_2 \in (0, h) \quad (\text{E1})$$

$$\epsilon^{-2} u''(y_1) - \lambda u(y_1) = f_0(\epsilon y_1), \quad y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E2})$$

$$\epsilon^{-2} w''(y_1) - \lambda w(y_1) = f_1(\epsilon y_1), \quad y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E3})$$

where $\alpha = \epsilon^{-2}$ for the “simple” and “stretched” cases, and $\alpha = 1$ for the “contrasting” case. These terms appear as coefficients of the periodic operator because of the rescaling of the graph.

Since the unknown functions on the graph must be continuous at any vertex, we have the following continuity conditions:

$$u(n) = v_n(0), \quad \forall n \in \mathbb{Z} \quad (\text{C1})$$

$$w(n) = v_n(h), \quad \forall n \in \mathbb{Z} \quad (\text{C2})$$

As the sum of the appropriately scaled outgoing derivatives of the unknown functions on each vertex must be 0, we have the following derivative sum conditions:

$$\lim_{\sigma \rightarrow 0} \epsilon^{-2} u'(n + \sigma) - \epsilon^{-2} u'(n - \sigma) + \alpha v_n'(\sigma) = 0 \quad (\text{D1})$$

$$\lim_{\sigma \rightarrow 0} \epsilon^{-2} w'(n + \sigma) - \epsilon^{-2} w'(n - \sigma) - \alpha v_n'(h - \sigma) = 0 \quad (\text{D2})$$

Existence and Uniqueness

Existence and uniqueness of the unknown functions can be established by means of the Lax-Milgram Theorem for $\lambda > 0$. We consider a Hilbert space

$$V = \left\{ u \in H^1(\mathbb{R}), w \in H^1(\mathbb{R}), v_n \in H^1(0, h) : \sum_n \|v_n\|_{H^1}^2 < +\infty, v_n(0) = u(n), v_n(h) = w(n), n \in \mathbb{Z} \right\}$$

with the norm defined by

$$\|U\|_V^2 = \|u\|_{H^1}^2 + \|w\|_{H^1}^2 + \sum_n \|v_n\|_{H^1}^2$$

and noting that the conditions on the derivatives are not included in the definition of V since they are automatically satisfied by the solution of the variational problem.

We define the following sesquilinear form based on the left hand side of the weak formulation of the above system of equations:

$$\begin{aligned} a(U, \tilde{U}) &= a(u, w, v_n, \tilde{u}, \tilde{w}, \tilde{v}_n) \\ &= \epsilon^{-2} \left(\int_{-\infty}^{\infty} u' \tilde{u}' dy_1 + \int_{-\infty}^{\infty} w' \tilde{w}' dy_1 \right) + \\ &+ \alpha \left(\sum_{n \in \mathbb{Z}} \int_{-\infty}^{\infty} v_n' \tilde{v}_n' dy_2 \right) + \lambda \left(\int_{-\infty}^{\infty} u \tilde{u} dy_1 + \int_{-\infty}^{\infty} w \tilde{w} dy_1 + \left(\sum_{n \in \mathbb{Z}} \int_0^h v_n \tilde{v}_n dy_2 \right) \right) \end{aligned}$$

for all test functions $\tilde{u}, \tilde{w}, \tilde{v}_n \in V$. This form is continuous since

$$\begin{aligned} |a(U, \tilde{U})| &\leq \epsilon^{-2} \left(\int_{-\infty}^{\infty} (u')^2 dy_1 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} (\tilde{u}')^2 dy_1 \right)^{\frac{1}{2}} + \\ &+ \epsilon^{-2} \left(\int_{-\infty}^{\infty} (w')^2 dy_1 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} (\tilde{w}')^2 dy_1 \right)^{\frac{1}{2}} + \alpha \left(\sum_{n \in \mathbb{Z}} \left(\int_{-\infty}^{\infty} (v_n')^2 dy_2 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} (\tilde{v}_n')^2 dy_2 \right)^{\frac{1}{2}} \right) + \\ &+ \lambda \left(\int_{-\infty}^{\infty} u^2 dy_1 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} \tilde{u}^2 dy_1 \right)^{\frac{1}{2}} + \lambda \left(\int_{-\infty}^{\infty} w^2 dy_1 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} \tilde{w}^2 dy_1 \right)^{\frac{1}{2}} + \\ &+ \lambda \left(\sum_{n \in \mathbb{Z}} \left(\int_{-\infty}^{\infty} v_n^2 dy_2 \right)^{\frac{1}{2}} \left(\int_{-\infty}^{\infty} \tilde{v}_n^2 dy_2 \right)^{\frac{1}{2}} \right) \\ &\leq \max \{ \epsilon^{-2}, \alpha, \lambda \} \|U\|_V^2 \|\tilde{U}\|_V^2 \end{aligned}$$

and it's coercive for $\lambda > 0$ since

$$\begin{aligned} |a(\tilde{U}, \tilde{U})| &= \epsilon^{-2} \left(\int_{-\infty}^{\infty} (\tilde{u}')^2 dy_1 + \int_{-\infty}^{\infty} (\tilde{w}')^2 dy_1 \right) + \\ &+ \alpha \left(\sum_{n \in \mathbb{Z}} \int_{-\infty}^{\infty} (\tilde{v}_n')^2 dy_2 \right) + \lambda \left(\int_{-\infty}^{\infty} \tilde{u}^2 dy_1 + \int_{-\infty}^{\infty} \tilde{w}^2 dy_1 + \left(\sum_{n \in \mathbb{Z}} \int_0^h \tilde{v}_n^2 dy_2 \right) \right) \\ &\geq \min \{ \epsilon^{-2}, \alpha, \lambda \} \|\tilde{U}\|_V^2 \end{aligned}$$

Thus by the Lax-Milgram Theorem, there exists a unique vector (u, w, v_n) in V such that

$$a(u, w, v_n, \tilde{u}, \tilde{w}, \tilde{v}_n) = - \int_{-\infty}^{\infty} f_0 \tilde{u} dx_1 - \int_{-\infty}^{\infty} f_1 \tilde{w} dx_1, \quad \forall (\tilde{u}, \tilde{w}, \tilde{v}_n) \in V$$

which is the weak formulation of the aforementioned system of equations.

3.1. Homogenisation of a “Simple Ladder” Periodic Quantum Graph

This is the “simple” case where the height $h = \gamma$ and $\alpha = \epsilon^{-2}$. Thus our system of equations looks like this

$$\epsilon^{-2} v_n''(y_2) - \lambda v_n(y_2) = 0 \quad , n \in \mathbb{Z}, y_2 \in (0, \gamma) \quad (\text{E1})$$

$$\epsilon^{-2} u''(y_1) - \lambda u(y_1) = f_0(\epsilon y_1) \quad , y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E2})$$

$$\epsilon^{-2} w''(y_1) - \lambda w(y_1) = f_1(\epsilon y_1) \quad , y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E3})$$

From the quantum graph continuity condition at each vertex we get the following condition equations:

$$u(n) = v_n(0) \quad , \forall n \in \mathbb{Z} \quad (\text{C1})$$

$$w(n) = v_n(\gamma) \quad , \forall n \in \mathbb{Z} \quad (\text{C2})$$

From the quantum graph condition of the sum of all outgoing first derivatives being equal to zero at each vertex we get the following condition equations:

$$\lim_{\sigma \rightarrow 0} u'(n + \sigma) - u'(n - \sigma) + v_n'(\sigma) = 0 \quad (\text{D1})$$

$$\lim_{\sigma \rightarrow 0} w'(n + \sigma) - w'(n - \sigma) - v_n'(\gamma - \sigma) = 0 \quad (\text{D2})$$

Per the Method of Multiple Scales, we assign to each unknown function a two-scale ansatz as follows:

$$v_n(y_2) = \left[v_0(x_1, y_2) + \epsilon v_1(x_1, y_2) + \epsilon^2 v_2(x_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n}$$

$$u(y_1) = \left[u_0(x_1) + \epsilon u_1(x_1, y_1) + \epsilon^2 u_2(x_1, y_1) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w(y_1) = \left[w_0(x_1) + \epsilon w_1(x_1, y_1) + \epsilon^2 w_2(x_1, y_1) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

Their first derivatives become:

$$v_n'(y_2) = \left[\frac{\partial v_0}{\partial y_2}(x_1, y_2) + \epsilon \frac{\partial v_1}{\partial y_2}(x_1, y_2) + \epsilon^2 \frac{\partial v_2}{\partial y_2}(x_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n}$$

$$u'(y_1) = \left[\epsilon \left(\frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial u_1}{\partial x_1}(x_1, y_1) + \frac{\partial u_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w'(y_1) = \left[\epsilon \left(\frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial w_1}{\partial x_1}(x_1, y_1) + \frac{\partial w_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

and their second derivatives become:

$$v_n''(y_2) = \left[\frac{\partial^2 v_0}{\partial y_2^2}(x_1, y_2) + \epsilon \frac{\partial^2 v_1}{\partial y_2^2}(x_1, y_2) + \epsilon^2 \frac{\partial^2 v_2}{\partial y_2^2}(x_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n}$$

$$u''(y_1) = \left[\epsilon \left(\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w''(y_1) = \left[\epsilon \left(\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

We will assume that functions u_m, w_m (for $m = 1, 2, \dots$), as well as their first derivatives, are 1-periodic in y_1 .

We substitute the ansatz into equations (E1) through (E3) and consider independently the terms corresponding to each order of ϵ . At order ϵ^{-2} we get:

$$\frac{\partial^2 v_0}{\partial y_2^2}(x_1, y_2) = 0 \quad (\text{E1,-2})$$

At order ϵ^{-1} we get:

$$\frac{\partial^2 v_1}{\partial y_2^2}(x_1, y_2) = 0 \quad (\text{E1,-1})$$

$$\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E2,-1})$$

$$\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E3,-1})$$

At order ϵ^0 we get:

$$\frac{\partial^2 v_2}{\partial y_2^2}(x_1, y_2) - \lambda v_0(x_1, y_2) = 0 \quad (\text{E1,0})$$

$$\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) - \lambda u_0(x_1) = f_0(x_1) \quad (\text{E2,0})$$

$$\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) - \lambda w_0(x_1) = f_1(x_1) \quad (\text{E3,0})$$

We do the same for condition equations (C1), (C2), (D1), and (D2), noting that for any function argument we can take $\epsilon n = x_1$ since ϵn can take any value in \mathbb{R} . Also, by periodicity on the unit-cell we can take $n = 0$ on any periodic function of y_1 evaluated at n . Thus, at order ϵ^0 we get:

$$u_0(x_1) = v_0(x_1, 0) \quad (\text{C1,0})$$

$$w_0(x_1) = v_0(x_1, \gamma) \quad (\text{C2,0})$$

$$\frac{\partial v_0}{\partial y_2}(x_1, 0) = 0 \quad (\text{D1,0})$$

$$\frac{\partial v_0}{\partial y_2}(x_1, \gamma) = 0 \quad (\text{D2,0})$$

At order ϵ^1 we get:

$$u_1(x_1, 0) = v_1(x_1, 0) \quad (\text{C1,1})$$

$$w_1(x_1, 0) = v_1(x_1, \gamma) \quad (\text{C2,1})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, \sigma) - \frac{\partial u_0}{\partial x_1}(x_1) - \frac{\partial u_1}{\partial y_1}(x_1, -\sigma) + \frac{\partial v_1}{\partial y_2}(x_1, \sigma) = 0 \quad (\text{D1,1})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, \sigma) - \frac{\partial w_0}{\partial x_1}(x_1) - \frac{\partial w_1}{\partial y_1}(x_1, -\sigma) - \frac{\partial v_1}{\partial y_2}(x_1, \gamma - \sigma) = 0 \quad (\text{D2,1})$$

At order ϵ^2 we get:

$$u_2(x_1, 0) = v_2(x_1, 0) \quad (C1,2)$$

$$w_2(x_1, 0) = v_2(x_1, \gamma) \quad (C2,2)$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, \sigma) + \frac{\partial u_2}{\partial y_1}(x_1, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) + \frac{\partial v_2}{\partial y_2}(x_1, \sigma) = 0 \quad (D1,2)$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_1}{\partial x_1}(x_1, \sigma) + \frac{\partial w_2}{\partial y_1}(x_1, \sigma) - \frac{\partial w_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial v_2}{\partial y_2}(x_1, \gamma - \sigma) = 0 \quad (D2,2)$$

Determination of v_0

From equations (E1,-2) and (D1,0) we find that v_0 is only a function of x_1 , and using equations (C1,0) and (C2,0) we get

$$v_0(x_1, y_2) = w_0(x_1) = u_0(x_1)$$

Determination of v_1

From equation (E2,-1) we know that on the interval $(-\frac{1}{2}, \frac{1}{2})$, u_1 should have the form

$$u_1(x_1, y_1) = \begin{cases} \alpha_1^-(x_1)y_1 + \beta_1^-(x_1) & , -\frac{1}{2} \leq y_1 < 0 \\ \alpha_1^+(x_1)y_1 + \beta_1^+(x_1) & , 0 < y_1 \leq \frac{1}{2} \end{cases}$$

where $\alpha_1^-, \alpha_1^+, \beta_1^-, \beta_1^+$ are all functions of x_1 . Testing at the limit $y_1 = 0$ and by continuity, functions β_1^- and β_1^+ must be equal. Using this fact and periodicity on y_1 we have

$$\begin{aligned} u_1\left(x_1, -\frac{1}{2}\right) &= u_1\left(x_1, \frac{1}{2}\right) \\ \Rightarrow -\frac{1}{2}\alpha_1^-(x_1) + \beta_1^-(x_1) &= \frac{1}{2}\alpha_1^+(x_1) + \beta_1^+(x_1) \\ &\Rightarrow -\alpha_1^-(x_1) = \alpha_1^+(x_1) \end{aligned}$$

and evaluating the partial derivative with respect to y_1 at the same points we have

$$\begin{aligned} \frac{\partial u_1}{\partial y_1}\left(x_1, -\frac{1}{2}\right) &= \frac{\partial u_1}{\partial y_1}\left(x_1, \frac{1}{2}\right) \\ &\Rightarrow \alpha_1^-(x_1) = \alpha_1^+(x_1) \end{aligned}$$

which combined with the previous result shows that u_1 is just a function of x_1 . The exact same argument applied to equation (E3,-1) proves that w_1 is also just a function of x_1 . Then equations (D1,1) and (D2,1) give

$$\frac{\partial v_1}{\partial y_2}(x_1, 0) = \frac{\partial v_1}{\partial y_2}(x_1, \gamma) = 0$$

and with equations (E1,-1), (C1,1), and (C2,1) we find that

$$v_1(x_1, y_2) = w_1(x_1) = u_1(x_1)$$

Homogenisation

Now from equation (E1,0) and our result for v_0 we know that

$$\frac{\partial^2 v_2}{\partial y_2^2}(x_1, y_2) = \lambda u_0(x_1)$$

and applying our results for v_0 and v_1 , equations (E2,0) and (E3,0) can be rewritten as

$$\begin{aligned} \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) &= f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \\ \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) &= f_1(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \end{aligned}$$

Integrating these three equations on a representative unit cell, for example on y_2 on the open interval $(0, \gamma)$, and y_1 on $(-\frac{1}{2}, 0) \cup (0, \frac{1}{2})$, and taking their sum we have

$$\begin{aligned} &\lim_{\sigma \rightarrow 0} \frac{\partial v_2}{\partial y_2}(x_1, \sigma) - \frac{\partial v_2}{\partial y_2}(x_1, \gamma - \sigma) + \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial u_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) + \\ &\quad - \frac{\partial u_2}{\partial y_1}(x_1, \sigma) + \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial w_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) - \frac{\partial w_2}{\partial y_1}(x_1, \sigma) \\ &= \int_0^\gamma \lambda u_0(x_1) dy_2 + \int_{-1/2}^{1/2} \left(f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \right) dy_1 + \\ &\quad + \int_{-1/2}^{1/2} \left(f_1(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \right) dy_1 \end{aligned}$$

where from applying our result for v_1 to equations (D1,2) and (D2,2), and using the periodicity conditions on $\frac{\partial u_2}{\partial y_1}$, $\frac{\partial w_2}{\partial y_1}$, $\frac{\partial u_1}{\partial y_1}$, and $\frac{\partial w_1}{\partial y_1}$, the left hand side cancels out and becomes 0, and the right hand side after rearranging gives the single homogenised equation:

$$2 \frac{d^2 u_0}{dx_1^2}(x_1) - (2 + \gamma) \lambda u_0(x_1) = f_0(x_1) + f_1(x_1)$$

3.2. Homogenisation of a ‘‘Vertically-Stretched Ladder’’ Periodic Quantum Graph

This can be considered a modification of the ‘‘simple’’ case, equivalent to stretching the graph vertically by an order of magnitude of ϵ^{-1} , giving us a system that after scaling converges geometrically to a 2D strip in the ‘‘long’’ scale, as opposed to the ‘‘simple ladder’’ which converges to a line. Here the height $h = \frac{\gamma}{\epsilon}$ and $\alpha = \epsilon^{-2}$. Thus our system of equations now looks like this:

$$\epsilon^{-2} v_n''(y_2) - \lambda v_n(y_2) = 0 \quad , n \in \mathbb{Z} , y_2 \in \left(0, \frac{\gamma}{\epsilon}\right) \quad (\text{E1})$$

$$\epsilon^{-2} u''(y_1) - \lambda u(y_1) = f_0(\epsilon y_1) \quad , y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E2})$$

$$\epsilon^{-2} w''(y_1) - \lambda w(y_1) = f_1(\epsilon y_1) \quad , y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E3})$$

and our continuity and outgoing derivative sum conditions become:

$$u(n) = v_n(0) \quad , \quad \forall n \in \mathbb{Z} \quad (\text{C1})$$

$$w(n) = v_n\left(\frac{\gamma}{\epsilon}\right) \quad , \quad \forall n \in \mathbb{Z} \quad (\text{C2})$$

$$\lim_{\sigma \rightarrow 0} u'(n + \sigma) - u'(n - \sigma) + v_n'(\epsilon\sigma) = 0 \quad (\text{D1})$$

$$\lim_{\sigma \rightarrow 0} w'(n + \sigma) - w'(n - \sigma) - v_n'(\gamma - \epsilon\sigma) = 0 \quad (\text{D2})$$

Since we effectively altered the scale of the domain of $v_n(y_2)$, we adjust its ansatz to reflect its new scale:

$$v_n(y_2) = \left[v_0(x_1, x_2) + \epsilon v_1(x_1, x_2) + \epsilon^2 v_2(x_1, x_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2}$$

and its derivatives are now

$$v_n'(y_2) = \left[\epsilon \frac{\partial v_0}{\partial x_2}(x_1, x_2) + \epsilon^2 \frac{\partial v_1}{\partial x_2}(x_1, x_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2}$$

$$v_n''(y_2) = \left[\epsilon^2 \frac{\partial^2 v_0}{\partial x_2^2}(x_1, x_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2}$$

The other unknown function ansätze and their derivatives stay the same as in the “simple” case, i.e.

$$u(y_1) = \left[u_0(x_1) + \epsilon u_1(x_1, y_1) + \epsilon^2 u_2(x_1, y_1) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$u'(y_1) = \left[\epsilon \left(\frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial u_1}{\partial x_1}(x_1, y_1) + \frac{\partial u_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$u''(y_1) = \left[\epsilon \left(\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w(y_1) = \left[w_0(x_1) + \epsilon w_1(x_1, y_1) + \epsilon^2 w_2(x_1, y_1) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w'(y_1) = \left[\epsilon \left(\frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial w_1}{\partial x_1}(x_1, y_1) + \frac{\partial w_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w''(y_1) = \left[\epsilon \left(\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

We will again assume that functions u_m, w_m (for $m = 1, 2, \dots$), as well as their first derivatives, are 1-periodic in y_1 .

We substitute the ansätze into equations (E1) through (E3) and consider independently the terms corresponding to each order of ϵ . At order ϵ^{-1} we get:

$$\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E2,-1})$$

$$\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E3,-1})$$

At order ϵ^0 we get:

$$\frac{\partial^2 v_0}{\partial x_2^2}(x_1, x_2) - \lambda v_0(x_1, y_2) = 0 \quad (\text{E1,0})$$

$$\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) - \lambda u_0(x_1) = f_0(x_1) \quad (\text{E2,0})$$

$$\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) - \lambda w_0(x_1) = f_1(x_1) \quad (\text{E3,0})$$

At order ϵ^1 we only need equation (E1) for our purpose:

$$\frac{\partial^2 v_1}{\partial x_2^2}(x_1, x_2) - \lambda v_1(x_1, y_2) = 0 \quad (\text{E1,1})$$

Doing the same for the condition equations (C1), (C2), (D1), and (D2), with the same considerations for taking $\epsilon n = x_1$ and $n = 0$ as in the “simple” case, we get at order ϵ^0 :

$$u_0(x_1) = v_0(x_1, 0) \quad (\text{C1,0})$$

$$w_0(x_1) = v_0(x_1, \gamma) \quad (\text{C2,0})$$

At order ϵ^1 we get:

$$u_1(x_1, 0) = v_1(x_1, 0) \quad (\text{C1,1})$$

$$w_1(x_1, 0) = v_1(x_1, \gamma) \quad (\text{C2,1})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, \sigma) - \frac{\partial u_0}{\partial x_1}(x_1) - \frac{\partial u_1}{\partial y_1}(x_1, -\sigma) + \frac{\partial v_0}{\partial x_2}(x_1, \epsilon\sigma) = 0 \quad (\text{D1,1})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, \sigma) - \frac{\partial w_0}{\partial x_1}(x_1) - \frac{\partial w_1}{\partial y_1}(x_1, -\sigma) - \frac{\partial v_0}{\partial x_2}(x_1, \gamma - \epsilon\sigma) = 0 \quad (\text{D2,1})$$

At order ϵ^2 we get:

$$u_2(x_1, 0) = v_2(x_1, 0) \quad (\text{C1,2})$$

$$w_2(x_1, 0) = v_2(x_1, \gamma) \quad (\text{C2,2})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, \sigma) + \frac{\partial u_2}{\partial y_1}(x_1, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) + \frac{\partial v_1}{\partial x_2}(x_1, \epsilon\sigma) = 0 \quad (\text{D1,2})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_1}{\partial x_1}(x_1, \sigma) + \frac{\partial w_2}{\partial y_1}(x_1, \sigma) - \frac{\partial w_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial v_1}{\partial x_2}(x_1, \gamma - \epsilon\sigma) = 0 \quad (\text{D2,2})$$

Determination of v_0

From equation (E1,0), taking $\lambda > 0$ we have:

$$v_0(x_1, x_2) = \alpha_0(x_1) e^{\sqrt{\lambda} x_2} + \alpha_1(x_1) e^{-\sqrt{\lambda} x_2}$$

for unknown functions α_0 and α_1 of x_1 .

Using equations (C1,0) and (C2,0) we then get the system

$$\begin{aligned} u_0(x_1) &= v_0(x_1, 0) = \alpha_0(x_1) + \alpha_1(x_1) \\ w_0(x_1) &= v_0(x_1, \gamma) = \alpha_0(x_1) e^{\sqrt{\lambda} \gamma} + \alpha_1(x_1) e^{-\sqrt{\lambda} \gamma} \end{aligned}$$

and solving for α_0 and α_1 we get

$$\begin{aligned} \alpha_0(x_1) &= \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) \\ \alpha_1(x_1) &= \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) \end{aligned}$$

(where $\operatorname{csch}(x) = \frac{1}{\sinh(x)}$) and thus v_0 becomes

$$\begin{aligned} v_0(x_1, x_2) &= \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) e^{\sqrt{\lambda} x_2} + \\ &+ \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) e^{-\sqrt{\lambda} x_2} \end{aligned}$$

and its first partial derivative with respect to x_2 becomes

$$\begin{aligned} \frac{\partial v_0}{\partial x_2}(x_1, x_2) &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) e^{\sqrt{\lambda} x_2} + \\ &- \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) e^{-\sqrt{\lambda} x_2} \end{aligned}$$

Now using the same logic as in the “simple” case, equations (E2,-1) and (E3,-1) imply $u_1(x_1, y_1)$ and $w_1(x_1, y_1)$ are functions of x_1 only. Thus equation (D1,1) gives

$$\begin{aligned} \frac{\partial v_0}{\partial x_2}(x_1, 0) &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) + \\ &- \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) = 0 \\ \Rightarrow w_0(x_1) &= \cosh(\sqrt{\lambda} \gamma) u_0(x_1) \end{aligned}$$

and applying this to equation (D2,1), we get

$$\begin{aligned} \frac{\partial v_0}{\partial x_2}(x_1, \gamma) &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (\cosh(\sqrt{\lambda} \gamma) u_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) e^{\sqrt{\lambda} \gamma} + \\ &- \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - \cosh(\sqrt{\lambda} \gamma) u_0(x_1)) e^{-\sqrt{\lambda} \gamma} = 0 \\ \Rightarrow (\cosh(\sqrt{\lambda} \gamma) u_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) - (e^{\sqrt{\lambda} \gamma} u_0(x_1) - \cosh(\sqrt{\lambda} \gamma) u_0(x_1)) &= 0 \\ \Rightarrow \cosh(\sqrt{\lambda} \gamma) u_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1) &= 0 \\ \Rightarrow \sinh(\sqrt{\lambda} \gamma) u_0(x_1) &= 0 \end{aligned}$$

This implies that $u_0(x_1)$ must be 0 as long as $\lambda \neq -\gamma^{-2} \pi^2 m^2 : m \in \mathbb{Z}$. As $\gamma > 0$, it could act as a tuning parameter in a hypothetical physical system with $\lambda < 0$ displaying this behaviour, allowing to adjust the values of λ where these changes in the behaviour of the system would occur. We will not be considering such a system, though it might warrant further research.

Assuming λ is such that $u_0(x_1) = 0$, this implies that

$$v_0(x_1, x_2) = w_0(x_1) = u_0(x_1) = 0$$

Determination of v_1

From equation (E1,1), assuming again $\lambda > 0$ and for unknown functions α_2 and α_3 of x_1 , we get

$$v_1(x_1, x_2) = \alpha_2(x_1) e^{\sqrt{\lambda} x_2} + \alpha_3(x_1) e^{-\sqrt{\lambda} x_2}$$

and using equations (C1,1) and (C2,1) we then get the system

$$u_1(x_1) = v_1(x_1, 0) = \alpha_2(x_1) + \alpha_3(x_1)$$

$$w_1(x_1) = v_1(x_1, \gamma) = \alpha_2(x_1) e^{\sqrt{\lambda} \gamma} + \alpha_3(x_1) e^{-\sqrt{\lambda} \gamma}$$

and solving for α_2 and α_3 we get

$$\alpha_2(x_1) = \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1) \right)$$

$$\alpha_3(x_1) = \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(e^{\sqrt{\lambda} \gamma} u_1(x_1) - w_1(x_1) \right)$$

and thus v_1 becomes

$$\begin{aligned} v_1(x_1, x_2) &= \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1) \right) e^{\sqrt{\lambda} x_2} + \\ &+ \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(e^{\sqrt{\lambda} \gamma} u_1(x_1) - w_1(x_1) \right) e^{-\sqrt{\lambda} x_2} \end{aligned}$$

and its first partial derivative with respect to x_2 becomes

$$\begin{aligned} \frac{\partial v_1}{\partial x_2}(x_1, x_2) &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1) \right) e^{\sqrt{\lambda} x_2} + \\ &- \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(e^{\sqrt{\lambda} \gamma} u_1(x_1) - w_1(x_1) \right) e^{-\sqrt{\lambda} x_2} \end{aligned}$$

Homogenisation

Applying those previous results to equations (E2,0) and (E3,0), we have

$$\frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) = f_0(x_1)$$

$$\frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) = f_1(x_1)$$

Integrating these two equations on a representative unit cell with respect to y_1 on $(-\frac{1}{2}, 0) \cup (0, \frac{1}{2})$, we have

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial u_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) - \frac{\partial u_2}{\partial y_1}(x_1, \sigma) = \int_{-1/2}^{1/2} (f_0(x_1)) dy_1 = f_0(x_1)$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial w_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) - \frac{\partial w_2}{\partial y_1}(x_1, \sigma) = \int_{-1/2}^{1/2} (f_1(x_1)) dy_1 = f_1(x_1)$$

Eliminating the terms that cancel out by periodicity, and using equations (D1,2) and (D2,2), we get

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, -\sigma) + \frac{\partial v_1}{\partial x_2}(x_1, \epsilon\sigma) = f_0(x_1)$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_1}{\partial x_1}(x_1, \sigma) - \frac{\partial w_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial v_1}{\partial x_2}(x_1, \gamma - \epsilon\sigma) = f_1(x_1)$$

and using the result that u_1 and w_1 are only functions of x_1 , as well as our result for $\frac{\partial v_1}{\partial x_2}$, we get from the first equation

$$\begin{aligned} f_0(x_1) &= \frac{\partial v_1}{\partial x_2}(x_1, 0) = \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1)) + \\ &\quad - \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_1(x_1) - w_1(x_1)) \\ &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1) - e^{\sqrt{\lambda} \gamma} u_1(x_1) + w_1(x_1)) \\ &= \sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_1(x_1) - \cosh(\sqrt{\lambda} \gamma) u_1(x_1)) \end{aligned}$$

and from the second equation

$$\begin{aligned} -f_1(x_1) &= \frac{\partial v_1}{\partial x_2}(x_1, \gamma) = \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_1(x_1) - e^{-\sqrt{\lambda} \gamma} u_1(x_1)) e^{\sqrt{\lambda} \gamma} + \\ &\quad - \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_1(x_1) - w_1(x_1)) e^{-\sqrt{\lambda} \gamma} \\ &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} w_1(x_1) - u_1(x_1) - u_1(x_1) + e^{-\sqrt{\lambda} \gamma} w_1(x_1)) \\ &= \sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) (\cosh(\sqrt{\lambda} \gamma) w_1(x_1) - u_1(x_1)) \end{aligned}$$

Thus we end up with the homogenised system

$$\begin{cases} w_1(x_1) - \cosh(\sqrt{\lambda} \gamma) u_1(x_1) = \lambda^{-1/2} \sinh(\sqrt{\lambda} \gamma) f_0(x_1) \\ u_1(x_1) - \cosh(\sqrt{\lambda} \gamma) w_1(x_1) = \lambda^{-1/2} \sinh(\sqrt{\lambda} \gamma) f_1(x_1) \end{cases}$$

with solution

$$\begin{aligned} u_1(x_1) &= -\lambda^{-1/2} (\coth(\sqrt{\lambda} \gamma) f_0(x_1) + \operatorname{csch}(\sqrt{\lambda} \gamma) f_1(x_1)) \\ w_1(x_1) &= -\lambda^{-1/2} (\operatorname{csch}(\sqrt{\lambda} \gamma) f_0(x_1) + \coth(\sqrt{\lambda} \gamma) f_1(x_1)) \end{aligned}$$

(where $\coth(x) = \frac{1}{\tanh(x)}$).

3.3. Homogenisation of a “Contrasting Ladder” Periodic Quantum Graph

This is another modification of the “simple” case, this time with a contrast of order $O(\epsilon^{-2})$ between the coefficients of the “vertical” and “horizontal” path equations. We have $h = \gamma$ and $\alpha = 1$, and our system of equations becomes:

$$v_n''(y_2) - \lambda v_n(y_2) = 0, \quad n \in \mathbb{Z}, y_2 \in (0, \gamma) \quad (\text{E1})$$

$$\epsilon^{-2} u''(y_1) - \lambda u(y_1) = f_0(\epsilon y_1), \quad y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E2})$$

$$\epsilon^{-2} w''(y_1) - \lambda w(y_1) = f_1(\epsilon y_1), \quad y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E3})$$

The continuity conditions at each vertex are the same as before:

$$u(n) = v_n(0), \quad \forall n \in \mathbb{Z} \quad (\text{C1})$$

$$w(n) = v_n(\gamma), \quad \forall n \in \mathbb{Z} \quad (\text{C2})$$

Now the conditions of the sum of the outgoing first derivatives also reflect the contrast between coefficients:

$$\lim_{\sigma \rightarrow 0} \epsilon^{-2} u'(n + \sigma) - \epsilon^{-2} u'(n - \sigma) + v_n'(\sigma) = 0 \quad (\text{D1})$$

$$\lim_{\sigma \rightarrow 0} \epsilon^{-2} w'(n + \sigma) - \epsilon^{-2} w'(n - \sigma) - v_n'(\gamma - \sigma) = 0 \quad (\text{D2})$$

We use the same ansatz as in the “simple” case (noting however that unlike in that case, the dependence of v_0 on y_2 will turn out to be non-trivial as we shall see):

$$v_n(y_2) = [v_0(x_1, y_2) + \epsilon v_1(x_1, y_2) + \epsilon^2 v_2(x_1, y_2) + O(\epsilon^3)]_{x_1 = \epsilon n}$$

$$u(y_1) = [u_0(x_1) + \epsilon u_1(x_1, y_1) + \epsilon^2 u_2(x_1, y_1) + O(\epsilon^3)]_{x_1 = \epsilon y_1}$$

$$w(y_1) = [w_0(x_1) + \epsilon w_1(x_1, y_1) + \epsilon^2 w_2(x_1, y_1) + O(\epsilon^3)]_{x_1 = \epsilon y_1}$$

with first derivatives

$$v_n'(y_2) = \left[\frac{\partial v_0}{\partial y_2}(x_1, y_2) + \epsilon \frac{\partial v_1}{\partial y_2}(x_1, y_2) + \epsilon^2 \frac{\partial v_2}{\partial y_2}(x_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n}$$

$$u'(y_1) = \left[\epsilon \left(\frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial u_1}{\partial x_1}(x_1, y_1) + \frac{\partial u_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w'(y_1) = \left[\epsilon \left(\frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial w_1}{\partial x_1}(x_1, y_1) + \frac{\partial w_2}{\partial y_1}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

and second derivatives

$$v_n''(y_2) = \left[\frac{\partial^2 v_0}{\partial y_2^2}(x_1, y_2) + \epsilon \frac{\partial^2 v_1}{\partial y_2^2}(x_1, y_2) + \epsilon^2 \frac{\partial^2 v_2}{\partial y_2^2}(x_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n}$$

$$u''(y_1) = \left[\epsilon \left(\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

$$w''(y_1) = \left[\epsilon \left(\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1}$$

We will again assume that functions u_m, w_m (for $m = 1, 2, \dots$), as well as their first derivatives, are 1-periodic in y_1 .

As before, we substitute the ansatz into equations (E1) through (E3) and consider independently the terms corresponding to each order of ϵ . At order ϵ^{-1} we get:

$$\frac{\partial^2 u_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E2,-1})$$

$$\frac{\partial^2 w_1}{\partial y_1^2}(x_1, y_1) = 0 \quad (\text{E3,-1})$$

At order ϵ^0 we get:

$$\frac{\partial^2 v_0}{\partial y_2^2}(x_1, y_2) - \lambda v_0(x_1, y_2) = 0 \quad (\text{E1,0})$$

$$\frac{\partial^2 u_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) - \lambda u_0(x_1) = f_0(x_1) \quad (\text{E2,0})$$

$$\frac{\partial^2 w_0}{\partial x_1^2}(x_1) + 2 \frac{\partial^2 w_1}{\partial x_1 \partial y_1}(x_1, y_1) + \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) - \lambda w_0(x_1) = f_1(x_1) \quad (\text{E3,0})$$

Doing the same for the condition equations (C1), (C2), (D1), and (D2), with the same considerations for taking $\epsilon n = x_1$ and $n = 0$ as in the ‘‘simple’’ case, we get at order ϵ^{-1} :

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_0}{\partial x_1}(x_1) + \frac{\partial u_1}{\partial y_1}(x_1, \sigma) - \frac{\partial u_0}{\partial x_1}(x_1) - \frac{\partial u_1}{\partial y_1}(x_1, -\sigma) = 0 \quad (\text{D1,-1})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_0}{\partial x_1}(x_1) + \frac{\partial w_1}{\partial y_1}(x_1, \sigma) - \frac{\partial w_0}{\partial x_1}(x_1) - \frac{\partial w_1}{\partial y_1}(x_1, -\sigma) = 0 \quad (\text{D2,-1})$$

At order ϵ^0 we get:

$$u_0(x_1) = v_0(x_1, 0) \quad (\text{C1,0})$$

$$w_0(x_1) = v_0(x_1, \gamma) \quad (\text{C2,0})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, \sigma) + \frac{\partial u_2}{\partial y_1}(x_1, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) + \frac{\partial v_0}{\partial y_2}(x_1, \sigma) = 0 \quad (\text{D1,0})$$

$$\lim_{\sigma \rightarrow 0} \frac{\partial w_1}{\partial x_1}(x_1, \sigma) + \frac{\partial w_2}{\partial y_1}(x_1, \sigma) - \frac{\partial w_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial v_0}{\partial y_2}(x_1, \gamma - \sigma) = 0 \quad (\text{D2,0})$$

At order ϵ^1 we only need the continuity conditions:

$$u_1(x_1, 0) = v_1(x_1, 0) \quad (\text{C1,1})$$

$$w_1(x_1, 0) = v_1(x_1, \gamma) \quad (\text{C2,1})$$

Determination of v_0

From equations (E1,0), (C1,0), and (C2,0), following the exact same steps as in the “vertically-stretched” case, we get

$$v_0(x_1, y_2) = \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1) \right) e^{\sqrt{\lambda} y_2} + \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1) \right) e^{-\sqrt{\lambda} y_2}$$

with first partial derivative with respect to y_2

$$\begin{aligned} \frac{\partial v_0}{\partial y_2}(x_1, y_2) &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1) \right) e^{\sqrt{\lambda} y_2} + \\ &\quad - \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) \left(e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1) \right) e^{-\sqrt{\lambda} y_2} \end{aligned}$$

Homogenisation

Using the same logic as in the “simple” case, u_1 and w_1 are only functions of x_1 . Hence equations (E2,0) and (E3,0) become

$$\begin{aligned} \frac{\partial^2 u_2}{\partial y_1^2}(x_1, y_1) &= f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \\ \frac{\partial^2 w_2}{\partial y_1^2}(x_1, y_1) &= f_1(x_1) - \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \lambda w_0(x_1) \end{aligned}$$

Integrating these two equations on a representative unit cell with respect to y_1 on $(-\frac{1}{2}, 0) \cup (0, \frac{1}{2})$, we have

$$\begin{aligned} &\lim_{\sigma \rightarrow 0} \frac{\partial u_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial u_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial u_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) - \frac{\partial u_2}{\partial y_1}(x_1, \sigma) \\ &= \int_{-1/2}^{1/2} \left(f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \right) dy_1 = f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \\ &\lim_{\sigma \rightarrow 0} \frac{\partial w_2}{\partial y_1}(x_1, -\sigma) - \frac{\partial w_2}{\partial y_1}\left(x_1, -\frac{1}{2}\right) + \frac{\partial w_2}{\partial y_1}\left(x_1, \frac{1}{2}\right) - \frac{\partial w_2}{\partial y_1}(x_1, \sigma) \\ &= \int_{-1/2}^{1/2} \left(f_1(x_1) - \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \lambda w_0(x_1) \right) dy_1 = f_1(x_1) - \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \lambda w_0(x_1) \end{aligned}$$

Eliminating the terms that cancel out by periodicity, and using equations (D1,0) and (D2,0), we get

$$\begin{aligned} \lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, -\sigma) + \frac{\partial v_0}{\partial y_2}(x_1, \sigma) &= f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) \\ \lim_{\sigma \rightarrow 0} \frac{\partial w_1}{\partial x_1}(x_1, \sigma) - \frac{\partial w_1}{\partial x_1}(x_1, -\sigma) - \frac{\partial v_0}{\partial y_2}(x_1, \gamma - \sigma) &= f_1(x_1) - \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \lambda w_0(x_1) \end{aligned}$$

and using the result that u_1 and w_1 are only functions of x_1 , as well as our result for $\frac{\partial v_0}{\partial y_2}$, we get from the first equation

$$\begin{aligned} f_0(x_1) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + \lambda u_0(x_1) &= \frac{\partial v_0}{\partial y_2}(x_1, 0) \\ &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) - \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) \\ &= \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1) - e^{\sqrt{\lambda} \gamma} u_0(x_1) + w_0(x_1)) \\ &= \sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - \cosh(\sqrt{\lambda} \gamma) u_0(x_1)) \end{aligned}$$

and from the second equation

$$\begin{aligned} f_1(x_1) - \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \lambda w_0(x_1) &= -\frac{\partial v_0}{\partial y_2}(x_1, \gamma) \\ &= -\sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (w_0(x_1) - e^{-\sqrt{\lambda} \gamma} u_0(x_1)) e^{\sqrt{\lambda} \gamma} + \\ &\quad + \sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} u_0(x_1) - w_0(x_1)) e^{-\sqrt{\lambda} \gamma} \\ &= -\sqrt{\lambda} \frac{1}{2} \operatorname{csch}(\sqrt{\lambda} \gamma) (e^{\sqrt{\lambda} \gamma} w_0(x_1) - u_0(x_1) - u_0(x_1) + e^{-\sqrt{\lambda} \gamma} w_0(x_1)) \\ &= -\sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) (\cosh(\sqrt{\lambda} \gamma) w_0(x_1) - u_0(x_1)) \end{aligned}$$

Thus we end up with the homogenised system

$$\begin{cases} \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + (-\lambda - \sqrt{\lambda} \coth(\sqrt{\lambda} \gamma)) u_0(x_1) + \sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) w_0(x_1) = f_0(x_1) \\ \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \sqrt{\lambda} \operatorname{csch}(\sqrt{\lambda} \gamma) u_0(x_1) + (-\lambda - \sqrt{\lambda} \coth(\sqrt{\lambda} \gamma)) w_0(x_1) = f_1(x_1) \end{cases}$$

Wave propagation restrictions in the homogenised system

We can analyse if there exist restrictions of wave propagation for specific frequencies on the homogenised system by looking for gaps in the spectrum of the operator for $\lambda < 0$. Changing the sign of λ the homogenised system becomes

$$\begin{cases} \frac{\partial^2 u_0}{\partial x_1^2}(x_1) + (\lambda - \sqrt{\lambda} \cot(\sqrt{\lambda} \gamma)) u_0(x_1) + \sqrt{\lambda} \operatorname{csc}(\sqrt{\lambda} \gamma) w_0(x_1) = f_0(x_1) \\ \frac{\partial^2 w_0}{\partial x_1^2}(x_1) + \sqrt{\lambda} \operatorname{csc}(\sqrt{\lambda} \gamma) u_0(x_1) + (\lambda - \sqrt{\lambda} \cot(\sqrt{\lambda} \gamma)) w_0(x_1) = f_1(x_1) \end{cases}$$

We can analyse this by looking instead at the problems derived by diagonalizing this system in terms of odd and even modes,

$$\begin{aligned} \eta_1''(x_1) + \beta_1(\lambda) \eta_1(x_1) &= f_0(x_1) + f_1(x_1) \\ \eta_2''(x_1) + \beta_2(\lambda) \eta_2(x_1) &= f_0(x_1) - f_1(x_1) \end{aligned}$$

where

$$\begin{aligned} \eta_1(x_1) &= u_0(x_1) + w_0(x_1) \\ \eta_2(x_1) &= u_0(x_1) - w_0(x_1) \end{aligned}$$

and functions $\beta_1(\lambda)$ and $\beta_2(\lambda)$ correspond to the $\beta(\lambda)$ function attributed to V. Zhikov [A, I], and are equal to the eigenvalues of the coefficient matrix of the zero-order part of the homogenised system, i.e.

$$\beta_1(\lambda) = \lambda - \sqrt{\lambda} \cot\left(\frac{\sqrt{\lambda} \gamma}{2}\right)$$

$$\beta_2(\lambda) = \lambda + \sqrt{\lambda} \tan\left(\frac{\sqrt{\lambda} \gamma}{2}\right)$$

To have a unique solution in $H^1(\mathbb{R})$ of the system for any $f_0, f_1 \in L^2$, we need $\beta(\lambda) < 0$; having both $\beta_1(\lambda) < 0$ and $\beta_2(\lambda) < 0$ on an interval would be equivalent to λ being in the resolvent set of the homogenised system, which would imply a gap in its spectrum.

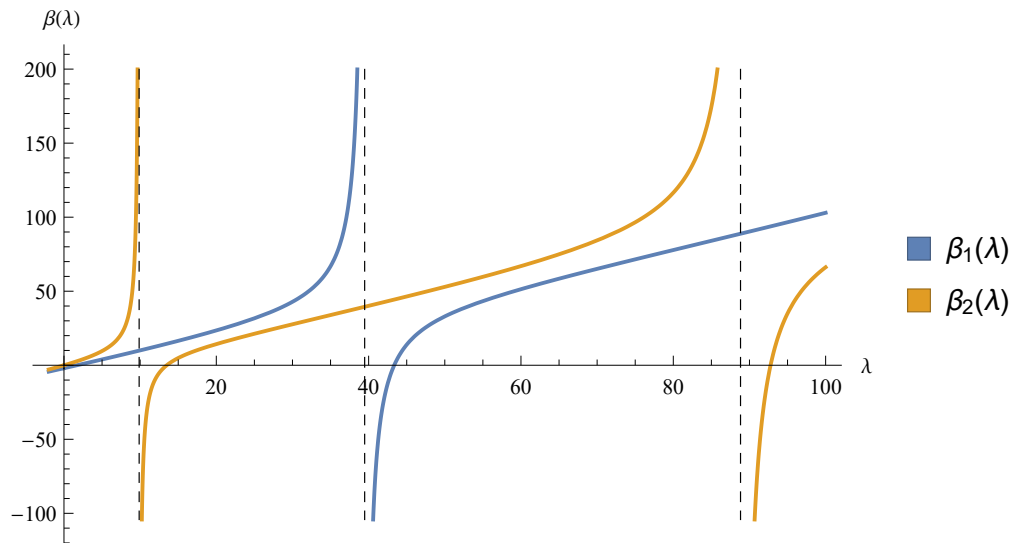


Figure 3.2: $\beta_1(\lambda)$ and $\beta_2(\lambda)$ plotted against λ , for $\gamma = 1$

The graphs for $\beta_1(\lambda)$ and $\beta_2(\lambda)$ present a clear pattern of the vertical asymptotes, with the asymptotes of $\beta_1(\lambda)$ at $\lambda = \frac{(2n)^2 \pi^2}{\gamma^2}$ and the ones for $\beta_2(\lambda)$ at $\lambda = \frac{(2n+1)^2 \pi^2}{\gamma^2}$. Looking at figure 3.2 and noting that modifying the height parameter γ only has the effect of moving the asymptotes closer together or further apart, which is akin to only compressing or stretching the horizontal scale, we can see that there do not seem to exist any spectral gaps. This can be proved by taking $t = \frac{\sqrt{\lambda} \gamma}{2}$ so that $\beta_1(\lambda) < 0$ and $\beta_2(\lambda) < 0$ become, after simplification:

$$\frac{2t}{\gamma} - \cot(t) < 0 \Leftrightarrow \frac{2t}{\gamma} < \cot(t)$$

$$\frac{2t}{\gamma} + \tan(t) < 0 \Leftrightarrow \frac{2t}{\gamma} < -\tan(t)$$

Since the asymptotes of $\cot(t)$ lie exactly at the zeroes of $-\tan(t)$, and vice-versa, and both functions are monotonically decreasing on each interval between their asymptotes, and since t must be greater than 0 there are no values of t where both inequalities hold.

While the system doesn't have spectrum gaps, $\beta_1(\lambda)$ and $\beta_2(\lambda)$ both oscillate between positive and negative values. This implies that for certain intervals of frequencies λ only even or odd modes can propagate, and the height parameter γ can be used to adjust the location of any one of these intervals.

4. Homogenisation of Quantum Graphs Exhibiting Periodicity in Two Directions

In this section we will analyse the behaviour of our periodic operator on an infinite-length, infinite-height planar “mesh” quantum graph which presents periodicity in both orthogonal directions when embedded in the plane (y_1, y_2) and aligned to its coordinate basis, as illustrated in figure 4.1:

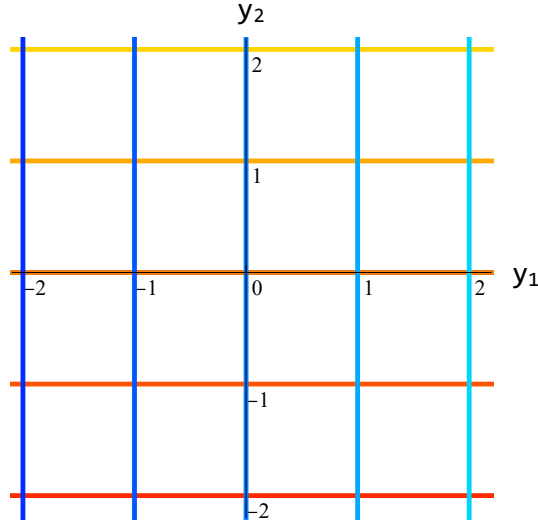


Figure 4.1: Close-up of the quantum graph embedded in the plane, displaying the sixteen periodicity cells closest to the origin

4.1 Homogenisation of a “Simple Mesh” Periodic Quantum Graph

We define an unknown function $u(y_1, y_2)$ in $H^1(\mathbb{R})$ acting on all “vertical” paths of the graph at $y_1 = m \in \mathbb{Z}$ and all “horizontal” paths at $y_2 = n \in \mathbb{Z}$. Taking $f(\epsilon y_1, \epsilon y_2)$ as a known function in $L^2(\mathbb{R})$, our periodic operator takes the form

$$\epsilon^{-2} \Delta_{\Gamma} u(y_1, y_2) - \lambda u(y_1, y_2) = f(\epsilon y_1, \epsilon y_2) \quad (\text{E1})$$

where Δ_{Γ} is the Laplacian operator on the graph. Existence and uniqueness of u can be proved for $\lambda > 0$ by the Lax Milgram Theorem in an analogous way to the “ladder” quantum graphs in Section 3.

From the quantum graph continuity condition at each vertex we get the following condition equations:

$$\lim_{\sigma \rightarrow 0} u(m + \sigma, n) - u(m - \sigma, n) = 0, \quad \forall m, n \in \mathbb{Z} \quad (\text{C1})$$

$$\lim_{\sigma \rightarrow 0} u(m, n + \sigma) - u(m, n - \sigma) = 0, \quad \forall m, n \in \mathbb{Z} \quad (\text{C2})$$

$$\lim_{\sigma \rightarrow 0} u(m + \sigma, n) - u(m, n - \sigma) = 0, \quad \forall m, n \in \mathbb{Z} \quad (\text{C3})$$

From the quantum graph condition of the sum of all outgoing first derivatives being equal to zero at each vertex we get the following condition equation:

$$\lim_{\sigma \rightarrow 0} u'(m + \sigma, n) - u'(m - \sigma, n) + u'(m, n + \sigma) - u'(m, n - \sigma) = 0, \quad \forall m, n \in \mathbb{Z} \quad (\text{D1})$$

Per the method of multiple scales, we assign to u the two-scale ansatz:

$$u(y_1, y_2) = \left[u_0(x_1, x_2) + \epsilon u_1(x_1, x_2, y_1, y_2) + \epsilon^2 u_2(x_1, x_2, y_1, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon y_2}$$

The first derivative becomes

$$u'(y_1, y_2) = \left[\epsilon(\nabla_x \cdot u_0(x_1, x_2) + \nabla_y \cdot u_1(x_1, x_2, y_1, y_2)) + \right. \\ \left. + \epsilon^2(\nabla_x \cdot u_1(x_1, x_2, y_1, y_2) + \nabla_y \cdot u_2(x_1, x_2, y_1, y_2)) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon y_2}$$

(where $\nabla_x = \left[\frac{d}{dx_1}, \frac{d}{dx_2} \right]$ and $\nabla_y = \left[\frac{d}{dy_1}, \frac{d}{dy_2} \right]$), and the Laplacian becomes

$$\nabla^2 u(y_1, y_2) = \left[\epsilon(\nabla_y \cdot \nabla_y u_1(x_1, x_2, y_1, y_2)) + \epsilon^2(\nabla_x \cdot \nabla_x u_0(x_1, x_2) + \right. \\ \left. + \nabla_y \cdot \nabla_x u_1(x_1, x_2, y_1, y_2) + \nabla_y \cdot \nabla_y u_2(x_1, x_2, y_1, y_2)) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon y_2}$$

We will assume that functions u_m (for $m = 1, 2, \dots$), as well as their first derivatives, are 1-periodic in both y_1 and y_2 .

We substitute the ansatz into equation (E1) and consider independently the terms corresponding to each order of ϵ . At order ϵ^{-1} we get:

$$\nabla_y \cdot \nabla_y u_1(x_1, x_2, y_1, y_2) = 0 \quad (\text{E1}, -1)$$

At order ϵ^0 we get:

$$\nabla_x \cdot \nabla_x u_0(x_1, x_2) + \nabla_y \cdot \nabla_x u_1(x_1, x_2, y_1, y_2) + \\ + \nabla_y \cdot \nabla_y u_2(x_1, x_2, y_1, y_2) - \lambda u_0(x_1, x_2) = f(x_1, x_2) \quad (\text{E1}, 0)$$

We do the same with the continuity and outgoing derivatives condition equations, taking $\epsilon n = x_1$ and $\epsilon m = x_2$ since they can take any value in \mathbb{R} , and taking $m = 0$ and $n = 0$ by periodicity on the unit-cell. We thus have at order ϵ^1 :

$$\lim_{\sigma \rightarrow 0} u_1(x_1, x_2, \sigma, 0) - u_1(x_1, x_2, -\sigma, 0) = 0 \quad (\text{C1}, 1)$$

$$\lim_{\sigma \rightarrow 0} u_1(x_1, x_2, 0, \sigma) - u_1(x_1, x_2, 0, -\sigma) = 0 \quad (\text{C2}, 1)$$

$$\lim_{\sigma \rightarrow 0} u_1(x_1, x_2, \sigma, 0) - u_1(x_1, x_2, 0, -\sigma) = 0 \quad (\text{C3}, 1)$$

$$\lim_{\sigma \rightarrow 0} \nabla_x \cdot u_0(x_1, x_2) + \nabla_y u_1(x_1, x_2, \sigma, 0) - \nabla_x \cdot u_0(x_1, x_2) - \nabla_y u_1(x_1, x_2, -\sigma, 0) + \\ + \nabla_x \cdot u_0(x_1, x_2) + \nabla_y u_1(x_1, x_2, 0, \sigma) - \nabla_x \cdot u_0(x_1, x_2) - \nabla_y u_1(x_1, x_2, 0, -\sigma) = 0 \quad (\text{D1}, 1)$$

For the outgoing derivatives condition equation, we have at order ϵ^2 :

$$\lim_{\sigma \rightarrow 0} \nabla_x \cdot u_1(x_1, x_2, \sigma, 0) + \nabla_y \cdot u_2(x_1, x_2, \sigma, 0) - \nabla_x \cdot u_1(x_1, x_2, -\sigma, 0) + \\ - \nabla_y \cdot u_2(x_1, x_2, -\sigma, 0) + \nabla_x \cdot u_1(x_1, x_2, 0, \sigma) + \nabla_y \cdot u_2(x_1, x_2, 0, \sigma) + \\ - \nabla_x \cdot u_1(x_1, x_2, 0, -\sigma) - \nabla_y \cdot u_2(x_1, x_2, 0, -\sigma) = 0 \quad (\text{D1}, 2)$$

Determination of u_1

From equation (E1,-1) we know that on the interval $y_1 \in \left(-\frac{1}{2}, \frac{1}{2}\right)$ for $y_2 = 0$, u_1 should have the “horizontal” form

$$u_1^{(h)}(x_1, x_2, y_1) = \begin{cases} \alpha_h^-(x_1, x_2)y_1 + \beta_h^-(x_1, x_2) & , -\frac{1}{2} \leq y_1 < 0 \\ \alpha_h^+(x_1, x_2)y_1 + \beta_h^+(x_1, x_2) & , 0 < y_1 \leq \frac{1}{2} \end{cases}$$

Testing at the limit $y_1 = 0$ and per equation (C1,1), functions β_h^- and β_h^+ must be equal. Using this fact and periodicity on y_1 we have

$$\begin{aligned} u_1^{(h)}\left(x_1, x_2, -\frac{1}{2}\right) &= u_1^{(h)}\left(x_1, x_2, \frac{1}{2}\right) \\ \Rightarrow -\frac{1}{2}\alpha_h^-(x_1, x_2) + \beta_h^-(x_1, x_2) &= \frac{1}{2}\alpha_h^+(x_1, x_2) + \beta_h^+(x_1, x_2) \\ \Rightarrow -\alpha_h^-(x_1, x_2) &= \alpha_h^+(x_1, x_2) \end{aligned}$$

and evaluating the partial derivative with respect to y_1 at the same points we have, from equation (D1,1),

$$\begin{aligned} \frac{\partial u_1^{(h)}}{\partial y_1}\left(x_1, x_2, -\frac{1}{2}\right) &= \frac{\partial u_1^{(h)}}{\partial y_1}\left(x_1, x_2, \frac{1}{2}\right) \\ \Rightarrow \alpha_h^-(x_1, x_2) &= \alpha_h^+(x_1, x_2) \end{aligned}$$

Thus u_1 is independent of y_1 since $\alpha_h^- = \alpha_h^+ = 0$. Using the same argument for the “vertical” form on the interval $y_2 \in \left(-\frac{1}{2}, \frac{1}{2}\right)$ for $y_1 = 0$,

$$u_1^{(v)}(x_1, x_2, y_2) = \begin{cases} \alpha_v^-(x_1, x_2)y_2 + \beta_v^-(x_1, x_2) & , -\frac{1}{2} \leq y_2 < 0 \\ \alpha_v^+(x_1, x_2)y_2 + \beta_v^+(x_1, x_2) & , 0 < y_2 \leq \frac{1}{2} \end{cases}$$

testing at the limit $y_2 = 0$ and per equation (C2,1), functions β_v^- and β_v^+ must be equal, and from periodicity on y_2 and equation (D1,1), $\alpha_v^- = \alpha_v^+ = 0$. Combining both results we get that u_1 must be a function of only x_1 and x_2 .

Homogenisation

From our previous result, equation (E1,0) becomes

$$-\nabla_y \cdot \nabla_y u_2(x_1, x_2, y_1, y_2) = \nabla_x \cdot \nabla_x u_0(x_1, x_2) - \lambda u_0(x_1, x_2) - f(x_1, x_2)$$

and averaging over (y_1, y_2) on the unit cell we end up with the homogenised equation:

$$\nabla^2 u_0(x_1, x_2) - \lambda u_0(x_1, x_2) = f(x_1, x_2)$$

4.2 Homogenisation of a “Contrasting Mesh” Periodic Quantum Graph

We define two families of unknown functions, $u_m(y_1)$ acting on all “horizontal” paths of the graph, and $v_n(y_2)$ acting on all “vertical” paths of the graph, both in $H^1(\mathbb{R})$ for $m, n \in \mathbb{Z}$. Similarly to the “contrasting ladder” case we add a contrast of order $O(\epsilon^{-2})$ between the coefficients of the “vertical” and “horizontal” path equations. Taking $f_0(\epsilon y_1, \epsilon y_2)$ and $f_1(\epsilon y_1, \epsilon y_2)$ as known functions in $L^2(\mathbb{R})$, our periodic operator takes the form:

$$v_n''(y_2) - \lambda v_n(y_2) = f_1(\epsilon y_1, \epsilon y_2) \quad , n \in \mathbb{Z}, y_2 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E1})$$

$$\epsilon^{-2} u_m''(y_1) - \lambda u_m(y_1) = f_0(\epsilon y_1, \epsilon y_2) \quad , m \in \mathbb{Z}, y_1 \in \mathbb{R} \setminus \mathbb{Z} \quad (\text{E2})$$

Existence and uniqueness of u_m and v_n can be proved for $\lambda > 0$ by the Lax Milgram Theorem in an analogous way to the “ladder” quantum graphs in Section 3.

The continuity conditions at each vertex simply become:

$$u_m(n) = v_n(m) \quad , \forall m, n \in \mathbb{Z} \quad (\text{C1})$$

The conditions of the sum of the outgoing first derivatives, reflecting the contrast between coefficients, become:

$$\lim_{\sigma \rightarrow 0} \epsilon^{-2} u_m'(n + \sigma) - \epsilon^{-2} u_m'(n - \sigma) + v_n'(m + \sigma) - v_n'(m - \sigma) = 0 \quad (\text{D1})$$

Per the method of multiple scales, we use the following two-scale ansatz:

$$v_n(y_2) = \left[v_0(x_1, x_2, y_2) + \epsilon v_1(x_1, x_2, y_2) + \epsilon^2 v_2(x_1, x_2, y_2) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2}$$

$$u_m(y_1) = \left[u_0(x_1, x_2, y_1) + \epsilon u_1(x_1, x_2, y_1) + \epsilon^2 u_2(x_1, x_2, y_1) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon m}$$

with first derivatives

$$\begin{aligned} v_n'(y_2) &= \left[\frac{\partial v_0}{\partial y_2}(x_1, x_2, y_2) + \epsilon \left(\frac{\partial v_0}{\partial x_2}(x_1, x_2, y_2) + \frac{\partial v_1}{\partial y_2}(x_1, x_2, y_2) \right) + \right. \\ &\quad \left. + \epsilon^2 \left(\frac{\partial v_1}{\partial x_2}(x_1, x_2, y_2) + \frac{\partial v_2}{\partial y_2}(x_1, x_2, y_2) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2} \\ u_m'(y_1) &= \left[\frac{\partial u_0}{\partial y_1}(x_1, x_2, y_1) + \epsilon \left(\frac{\partial u_0}{\partial x_1}(x_1, x_2, y_1) + \frac{\partial u_1}{\partial y_1}(x_1, x_2, y_1) \right) + \right. \\ &\quad \left. + \epsilon^2 \left(\frac{\partial u_1}{\partial x_1}(x_1, x_2, y_1) + \frac{\partial u_2}{\partial y_1}(x_1, x_2, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon m} \end{aligned}$$

and second derivatives

$$\begin{aligned} v_n''(y_2) &= \left[\frac{\partial^2 v_0}{\partial y_2^2}(x_1, x_2, y_2) + \epsilon \left(\frac{\partial^2 v_0}{\partial x_2 \partial y_2}(x_1, x_2, y_2) + \frac{\partial^2 v_1}{\partial y_2^2}(x_1, x_2, y_2) \right) + \right. \\ &\quad \left. + \epsilon^2 \left(\frac{\partial^2 v_0}{\partial x_2^2}(x_1, x_2, y_2) + \frac{\partial^2 v_1}{\partial x_2 \partial y_2}(x_1, x_2, y_2) + \frac{\partial^2 v_2}{\partial y_2^2}(x_1, x_2, y_2) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon n, x_2 = \epsilon y_2} \end{aligned}$$

$$u_m''(y_1) = \left[\frac{\partial^2 u_0}{\partial y_1^2}(x_1, x_2, y_1) + \epsilon \left(\frac{\partial^2 u_0}{\partial x_1 \partial y_1}(x_1, x_2, y_1) + \frac{\partial^2 u_1}{\partial y_1^2}(x_1, x_2, y_1) \right) + \epsilon^2 \left(\frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2, y_1) + \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, x_2, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, x_2, y_1) \right) + O(\epsilon^3) \right]_{x_1 = \epsilon y_1, x_2 = \epsilon m}$$

We will assume that functions u_m (for $m = 0, 1, \dots$), as well as their first derivatives, are 1-periodic in y_1 , and that functions v_n (for $n = 0, 1, \dots$), as well as their first derivatives, are 1-periodic in y_2 .

We substitute the ansatz into equations (E1) and (E2), and consider independently the terms corresponding to each order of ϵ . At order ϵ^{-2} we get:

$$\frac{\partial^2 u_0}{\partial y_1^2}(x_1, x_2, y_1) = 0 \quad (\text{E2,-2})$$

At order ϵ^{-1} we get:

$$\frac{\partial^2 u_0}{\partial x_1 \partial y_1}(x_1, x_2, y_1) + \frac{\partial^2 u_1}{\partial y_1^2}(x_1, x_2, y_1) = 0 \quad (\text{E2,-1})$$

At order ϵ^0 we get:

$$\frac{\partial^2 v_0}{\partial y_2^2}(x_1, x_2, y_2) - \lambda v_0(x_1, x_2, y_2) = f_1(x_1, x_2) \quad (\text{E1,0})$$

$$\frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2, y_1) + \frac{\partial^2 u_1}{\partial x_1 \partial y_1}(x_1, x_2, y_1) + \frac{\partial^2 u_2}{\partial y_1^2}(x_1, x_2, y_1) - \lambda u_0(x_1, x_2, y_1) = f_0(x_1, x_2) \quad (\text{E2,0})$$

We do the same with the continuity and outgoing derivatives condition equations, with the same considerations for taking $\epsilon n = x_1$, $\epsilon m = x_2$, $m = 0$, and $n = 0$ as in the “simple” case. We thus have at order ϵ^{-2} :

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_0}{\partial y_1}(x_1, x_2, \sigma) - \frac{\partial u_0}{\partial y_1}(x_1, x_2, -\sigma) = 0 \quad (\text{D1,-2})$$

At order ϵ^{-1} we get:

$$\lim_{\sigma \rightarrow 0} \frac{\partial u_0}{\partial x_1}(x_1, x_2, \sigma) + \frac{\partial u_1}{\partial y_1}(x_1, x_2, \sigma) - \frac{\partial u_0}{\partial x_1}(x_1, x_2, -\sigma) - \frac{\partial u_1}{\partial y_1}(x_1, x_2, -\sigma) = 0 \quad (\text{D1,-1})$$

At order ϵ^0 we get:

$$u_0(x_1, x_2, 0) = v_0(x_1, x_2, 0) \quad (\text{C1,0})$$

$$\begin{aligned} & \lim_{\sigma \rightarrow 0} \frac{\partial u_1}{\partial x_1}(x_1, x_2, \sigma) + \frac{\partial u_2}{\partial y_1}(x_1, x_2, \sigma) - \frac{\partial u_1}{\partial x_1}(x_1, x_2, -\sigma) + \\ & - \frac{\partial u_2}{\partial y_1}(x_1, x_2, -\sigma) + \frac{\partial v_0}{\partial y_2}(x_1, x_2, \sigma) - \frac{\partial v_0}{\partial y_2}(x_1, x_2, -\sigma) = 0 \end{aligned} \quad (\text{D1,0})$$

Determination of v_0

From equation (E1,0), taking $\lambda > 0$ we get

$$v_0(x_1, x_2, y_2) = -\frac{1}{\lambda} f_1(x_1, x_2) + \alpha_0(x_1, x_2) e^{\sqrt{\lambda} y_2} + \alpha_1(x_1, x_2) e^{-\sqrt{\lambda} y_2}$$

for unknown functions α_0 and α_1 . From the periodicity condition on the unit cell of v_n with respect to y_2 we have

$$\begin{aligned} v_0\left(x_1, x_2, -\frac{1}{2}\right) &= v_0\left(x_1, x_2, \frac{1}{2}\right) \\ \Rightarrow -\frac{1}{\lambda}f_1(x_1, x_2) + \alpha_0(x_1, x_2)e^{-\frac{1}{2}\sqrt{\lambda}} + \alpha_1(x_1, x_2)e^{\frac{1}{2}\sqrt{\lambda}} &= \\ -\frac{1}{\lambda}f_1(x_1, x_2) + \alpha_0(x_1, x_2)e^{\frac{1}{2}\sqrt{\lambda}} + \alpha_1(x_1, x_2)e^{-\frac{1}{2}\sqrt{\lambda}} & \\ \Rightarrow \alpha_1(x_1, x_2) &= \alpha_0(x_1, x_2) \end{aligned}$$

and from the periodicity condition on the unit cell of v_n' with respect to y_2 we have

$$\begin{aligned} \frac{\partial v_0}{\partial y_2}\left(x_1, x_2, -\frac{1}{2}\right) &= \frac{\partial v_0}{\partial y_2}\left(x_1, x_2, \frac{1}{2}\right) \\ \Rightarrow -\frac{1}{\lambda}f_1(x_1, x_2) + \sqrt{\lambda}\alpha_0(x_1, x_2)e^{-\frac{1}{2}\sqrt{\lambda}} - \sqrt{\lambda}\alpha_1(x_1, x_2)e^{\frac{1}{2}\sqrt{\lambda}} &= \\ -\frac{1}{\lambda}f_1(x_1, x_2) + \sqrt{\lambda}\alpha_0(x_1, x_2)e^{\frac{1}{2}\sqrt{\lambda}} - \sqrt{\lambda}\alpha_1(x_1, x_2)e^{-\frac{1}{2}\sqrt{\lambda}} & \\ \Rightarrow \alpha_1(x_1, x_2) &= -\alpha_0(x_1, x_2) \end{aligned}$$

which together imply $\alpha_0 = \alpha_1 = 0$, and hence

$$v_0(x_1, x_2, y_2) = -\frac{1}{\lambda}f_1(x_1, x_2)$$

Determination of u_0

From equation (E2,-2), and using the same logic as in the ‘‘simple ladder’’ case from section 3.1, we find that u_0 is independent of y_1 . Hence equation (E2,-1) becomes

$$\frac{\partial^2 u_1}{\partial y_1^2}(x_1, x_2, y_1) = 0$$

and using the same logic as for u_0 , we find that u_1 is also independent of y_1 . Hence equation (E2,0) becomes:

$$\frac{\partial^2 u_2}{\partial y_1^2}(x_1, x_2, y_1) = f_0(x_1, x_2) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2) + \lambda u_0(x_1, x_2)$$

Homogenisation

Integrating this last equation on a representative unit cell with respect to y_1 on $(-\frac{1}{2}, 0) \cup (0, \frac{1}{2})$, we have

$$\begin{aligned} &\lim_{\sigma \rightarrow 0} \frac{\partial u_2}{\partial y_1}(x_1, x_2, -\sigma) - \frac{\partial u_2}{\partial y_1}\left(x_1, x_2, -\frac{1}{2}\right) + \frac{\partial u_2}{\partial y_1}\left(x_1, x_2, \frac{1}{2}\right) - \frac{\partial u_2}{\partial y_1}(x_1, x_2, \sigma) \\ &= \int_{-1/2}^{1/2} \left(f_0(x_1, x_2) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2) + \lambda u_0(x_1, x_2) \right) dy_1 = f_0(x_1, x_2) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2) + \lambda u_0(x_1, x_2) \end{aligned}$$

Eliminating the terms that cancel out by periodicity, and using equation (D1,0) and our previous results for v_0 and u_1 , we get

$$\begin{aligned} f_0(x_1, x_2) - \frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2) + \lambda u_0(x_1, x_2) &= 0 \\ \Rightarrow \frac{\partial^2 u_0}{\partial x_1^2}(x_1, x_2) - \lambda u_0(x_1, x_2) &= f_0(x_1, x_2) \end{aligned}$$

Further constraints

Plugging our results into continuity condition equation C(1,0) we get

$$u_0(x_1, x_2) = -\frac{1}{\lambda} f_1(x_1, x_2)$$

which establishes the following condition required for the system to be consistent:

$$\frac{\partial^2 f_1}{\partial x_1^2}(x_1, x_2) - \lambda f_1(x_1, x_2) = -\lambda f_0(x_1, x_2)$$

Acknowledgements

I would like to give special thanks to the following people:

My supervisor Dr. Ilia Kamotski, for his guidance and seemingly infinite patience.

My tutor Dr. Sergei Timoshin, for always being open to any questions and discussions.

Prof. Valéry Smyshlyaev, for his lectures and summary notes on Homogenisation.

And last but not least my parents, for their unwavering support for my decisions regardless of whether they actually agree with them.

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