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Vibration of two bonded composites: effects of the interface and distinct periodic structures

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Abstract

Small elastic vibrations of two particulate composites that are caused by a non-plane time-harmonic wave are investigated. Effects of the adhesive interface and distinct periodic structures on the transmission and reflection of acoustic waves are rigorously analyzed. A two-scale asymptotic expansion with interfacial correctors is introduced to account for the macro- and micromechanical effects on wave propagation. An efficient algorithm is developed for computing first and second order corrections for the coefficients that depend on the composites microstructure and the interfacial constraint.

Keywords: Vibration of bonded composite materials; Homogenization; Interface effects

1. Introduction

The growing use of advanced materials requires further improvements in the material characterization methods in order to monitor the tailoring of material properties and in-service performance of complex composite systems. Mathematical modeling is instrumental in the ongoing optimization of multi-layer designs and characterization techniques for multifunctional hybrid systems and composite structures (Harik et al., 2000; Almroth et al., 1981). Now, multiple layers of single-purpose materials are being replaced in various structures by their multipurpose counterparts. The full advantage of hybrid composites can be realized only when the microstructural damage is controlled during processing (Harik and Cairncross, 1999), service and repairs.

Acoustic sensing techniques such as acoustic emission (AE), ultrasonic testing and through-transmission ultrasonics (TTU) have been widely used for the non-destructive evaluation (NDE) and material characterization of advanced materials and repaired structures (Harik et al., 2000; Arrington, 1990; Kline, 1992).

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During the NDE, an acoustic wave is introduced into one side of a composite and received by the sensors on the opposite side. The amplitude of the acoustic wave received is analyzed in the evaluation of material (Almroth et al., 1981) and imperfectly contacting interfaces (Harik and Cairncross, 1999) will reduce the amplitude of the received signal and the corresponding transmission coefficients (Kline, 1992). In ultrasonic testing, the frequency bandwidth includes the slow kilohertz and fast megahertz waves (Cracknell, 1980). The TTU characterization of damage is usually performed in the frequency range of about 100 kHz to about 10 MHz (Cracknell, 1980). In composites, a typical attenuation of a wave amplitude is high, so the test frequency is often reduced to compensate. For most high performance thermoplastic composites, the sound wavelength, λ, is on the order of millimeters (Tackett, 1999), while the typical diameter of glass fibers is about 20 μm. The wavelength, λ, is usually much larger than the fiber diameter, $2r_{\mathrm{f}}$ (i.e., $\lambda \gg r_{\mathrm{f}}$). As a result, the propagation of waves may not always be sensitive to individual fibers, but rather to the variations in fiber distribution or significant changes in the fiber or matrix properties as in some bonded hybrid structures.

The basic mathematical tool used in this paper is the theory of homogenization and two-scale asymptotic expansions (Sanchez-Palencia, 1980; Bakhvalov and Panasenko, 1989). Homogenization of equations of linearized elastostatics for a single periodic composite is by now classical. Recent extensions concern non-linear elastostatics (Wu and Ohno, 1999; Jansson, 1992) and non-standard transmission conditions on the boundary separating constituents (Lene and Leguillon, 1982). A method for homogenization of equations of elastodynamics has been proposed in Murakami et al. (1992). In all of the above papers, only the case of a single composite is considered.

In bonded composites, the NDE of the material state is more complex due to the existence of plane interfacial regions along the adhesion line. Interpretation of the AE results and material characterization are inhibited by the unknown interfacial structure and properties and their effect on the transmission of acoustic waves. The TTU is sensitive to a lack of intimate contact caused by the air gaps that result from imperfectly contacting surfaces at the interface (Tackett, 1999). These interfacial defects will reduce the amplitude of transmitted waves by reflecting a portion of the incident acoustic wave train. Similar effects are caused by the sudden changes in the material properties as at the adhesive interfaces between the two bonded composites with distinct material properties. In composites, adhesive zones may form so-called interphase regions with unique mechanical properties that may affect the macroscopic behavior of these materials.

The commonly used formulae for the transmission and reflection coefficients neglect the effect of composite microstructure by employing the average properties of bonded materials (Krautkramer and Krautkramer, 1983). The constraining effect of one bonded composite on another is also neglected. A lack of accessible algorithms for computing the first and second order corrections to the effective reflection and transmission coefficients at the plane interfaces separating different composites is evident. This paper presents a rigorous method for developing the computational algorithms needed.

In this paper, a two-scale asymptotic expansion with interfacial correctors is introduced to account for the effects of the adhesive interface and distinct periodic structures on the transmission and reflection coefficients. To evaluate these coefficients for two vibrating composites, an efficient algorithm is developed for the derivation of first and second order corrections at the interface. In the proposed method, the amount of computation needed to compute the next correction is basically independent of the number of the correction. A different method proposed by Avellaneda et al. (1999) requires solving ever larger linear systems of equations. In contrast to Avellaneda et al., our method involves only solving some periodic or partially periodic cell problems on each step.

2. Mathematical formulation of the problem

The problem of acoustic wave propagation is formulated for a system of two elastic composites separated by an adhesive interface. The volumes of two particulate composites are large. In three dimensions,

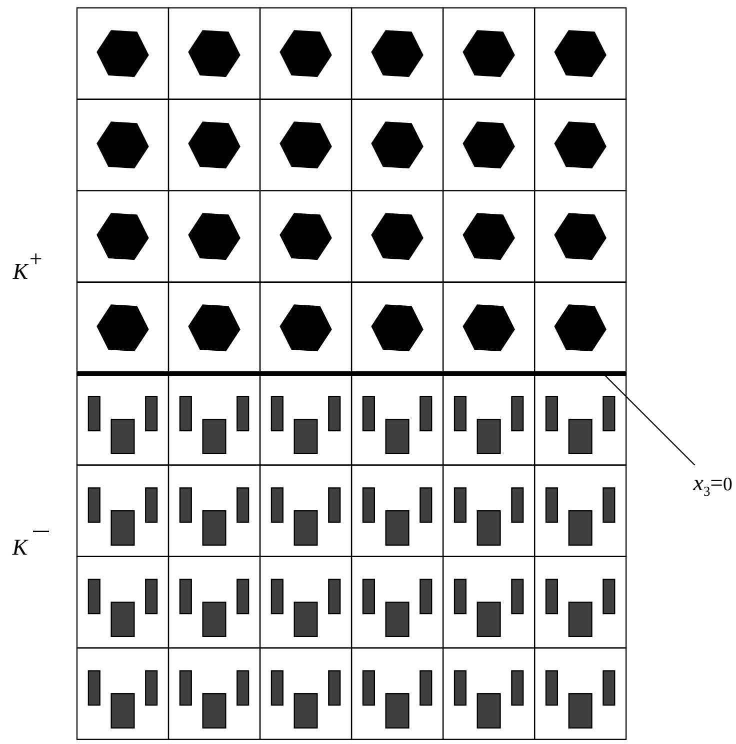

Fig. 1. Two composites separated by a plane interface.

the bonded composites occupy half-spaces $K_+ = \{x_3 > 0\}$ and $K_- = \{x_3 < 0\}$, respectively. The signs + or − will be used below to indicate the half-space in which a quantity is defined. A plane interface between the two materials is located at $x_3 = 0$ (see Fig. 1).

Both composites are periodic with the cubic cells of the edge length l.

The volume of a cell is divided into parts filled by the constituents of a composite. The cells on each side have the same basic shape and size, but otherwise they may be different, both in terms of the geometry of reinforcing phases, and the material properties of particulates and matrices (see Fig. 2).

The structure of two bonded composites has two well separated length scales. The cell size l introduces the microscopic length scale. The second, macroscopic length scale is associated with a size of the whole specimen, or with any other measurement that is large compared to l. These aspects of the problem allow us to use homogenization (or averaging) techniques (Bakhvalov and Panasenko, 1989), and the two-scale asymptotic expansions. In the context of wave propagation, the macroscopic scale is introduced by a typical wave length λ. Although the two-scale description works especially well when λ is much larger than l, i.e.

$$\epsilon = \frac{l}{\lambda}$$

is a small parameter, the method presented can be also useful in the so-called resonance regime when the wave length is comparable with the cell size.

Another straightforward extension of the theory presented in the paper concerns the case of different (non-cubic) cells on opposite sides of the interface. All the mathematical results will apply without change if the cells of periodicity C^+ and C^- adjacent to the interface have a common side of length l_c, and the other sides are different (see Fig. 3).

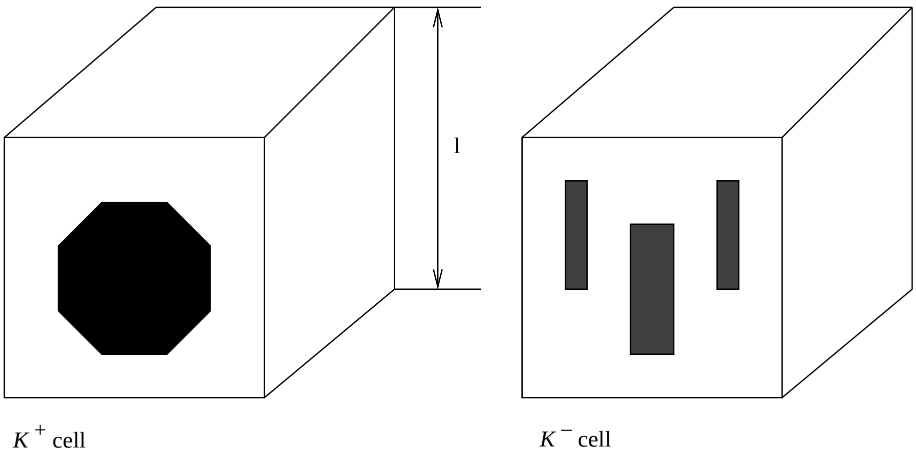

Fig. 2. Periodicity cells.

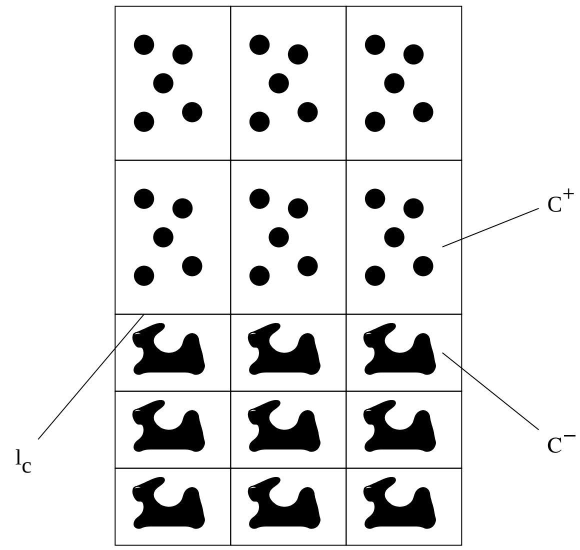

Fig. 3. Different cell structures with the same l_c.

In that case, one simply changes the definition of the small parameter by writing

$$\epsilon = \frac{\lambda}{l_{\max}}$$

where $l_{\max}$ is the largest side length of the cells C^+ and C^-.

Furthermore, our method allows one to treat the case of *different* side lengths at the interface. This situation is schematically represented on Fig. 4. The lengths of the sides adjacent to the interface are denoted by l^+ and l^-, respectively.

Our method of interface homogenization requires existence of an infinite strip which contains periodicity cells on both sides of the interface. The crucial condition which determines applicability of the method is

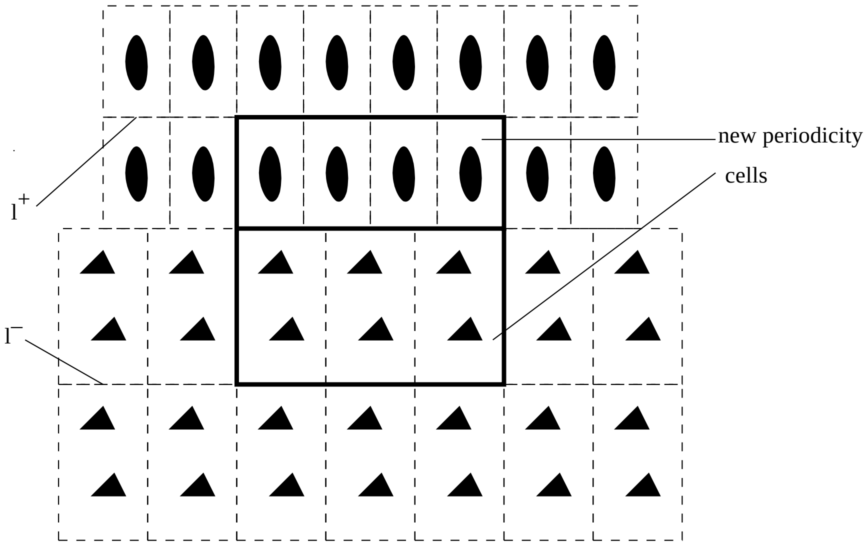

Fig. 4. Different cell structures with ratio $l^+/l^- = 3/4$: boundaries of the new cells shown in bold.

that the ratio of l^+ and l^- is a rational number. In this case there exist two integers m, n such that m cells on one side of the interface exactly match n cells on the other side. The situation on Fig. 4 corresponds to $m = 3$, $n = 4$. To apply the method, one needs to redefine periodicity cells. New periodicity cells must include m "old" cells on one side of the interface, and n cells on the other side. The only drawback of this is the need to enlarge ϵ.

When the ratio of the side lengths in question is irrational, the method may not work. It seems, however that the condition mentioned above is sufficiently practical, at least when m and n are small. The larger these numbers, the longer wave lengths will be required for the applicability of the theory presented below.

2.1. Governing equations

In elastic materials, the propagation of acoustic waves can be modeled by the scalar wave equation

$$\rho\Big(\frac{x}{\lambda}\Big)\partial_t^2 U + \operatorname{div}\Big(A\Big(\frac{x}{\lambda}\Big)\nabla U\Big) = 0, \tag{2.1}$$

where ρ is density of the material and A is a symmetric positive definite matrix of material stiffness coefficients. Both ρ and A are assumed to be periodic function with period l with respect to each of the variables x_1, x_2, x_3. We will often refer to such functions as l-periodic.

The model above is chosen mainly to simplify presentation. It already contains all essential difficulties associated with the problem of interface matching. We note, however that most of results of this paper can be carried over to the system of linearized elasticity (see Gilbert and Panchenko, 1999).

The acoustic waves are usually time-harmonic, so we look for periodic in time solutions

$$U(x,t) = e^{i\omega t}\tilde{u}(x,\omega)$$

and then introduce a new unknown $u(x,\omega) = \tilde{u}(x\omega,\omega)$. Then u must satisfy the Helmholtz equation

$$\operatorname{div}\Big(A\Big(\frac{x}{\epsilon}\Big)\nabla u\Big) + \omega^2\rho\Big(\frac{x}{\epsilon}\Big)u = 0. \tag{2.2}$$

On the interface, we prescribe the standard transmission conditions

$$[u] = 0, \tag{2.3}$$

$$[A_{3k}\partial_k u] = 0, \tag{2.4}$$

where brackets denote the jump of the corresponding quantity across the interface. In (2.4) and everywhere below the summation convention is employed.

The problem defined by Eqs. (2.2) can be reduced to an "averaged" model via the classical method of two-scale asymptotic expansions (Sanchez-Palencia, 1980; Bakhvalov and Panasenko, 1989). In this method, the asymptotic solutions have the form of an expansion

$$u(x,\epsilon) = u_0(x) + \epsilon u_1\left(\frac{x}{\epsilon}, x\right) + \epsilon^2 u_2\left(\frac{x}{\epsilon}, x\right) + \cdots \tag{2.5}$$

In the absence of an interface, the theory allows one to calculate effective functions $\langle\rho\rangle$ and $\hat{A}$ such that u_0 from (2.5) is a solution of the averaged equation

$$\hat{A}_{ij}\partial^2_{ij}u_0 + \omega^2\langle\rho\rangle u_0 = 0. \tag{2.6}$$

But this alone does not mean that a solution of the problem (2.2)–(2.4) will be close to v that solves (2.6) and satisfies the transmission conditions

$$[v] = 0, \tag{2.7}$$

$$[\hat{A}_{3k}\partial_k v] = 0. \tag{2.8}$$

In this paper we construct a modified two-scale expansion for a solution of the transmission problem (2.2)–(2.4) that involves interfacial correctors. The leading term v_0 of this new expansion satisfies (2.6)–(2.8). We also find an efficient way to compute corrections of all orders to the transmission and reflection coefficients.

Analysis of cell problems allows us to further reduce the amount of computation. In Section 4, simplified formulae for computing the second term of the asymptotics are derived. It is shown that

$$u(x,\epsilon) = v_0(x) + \epsilon(V(v_0)(x,\epsilon) + v_1(x)) + \mathrm{O}(\epsilon^2),$$

where $V(v_0)$ depends only on v_0 and solutions of certain cell problems. The function v_1 which has a meaning of a genuine macroscopic correction of order ϵ, satisfies the inhomogeneous equation

$$\hat{A}_{ij}\partial^2_{ij}v_1 + \omega^2\langle\rho\rangle v_1 = F(v_0) \tag{2.9}$$

and transmission conditions

$$[v_1] = -[k^{0,i}\partial_i v_0], \tag{2.10}$$

$$[\hat{A}_{3k}\partial_k v_1] = -[t^{2,0}v_0 + \hat{A}_{3k}\partial_k + t^{0,i_1i_2}\partial^2_{i_1i_2}v_0], \tag{2.11}$$

where $k^{0,i}$, $t^{2,0}$, t^{0,i_1i_2} are constants, and $\langle\rho\rangle$ denotes the average density. One of the main results of the paper is the formulae for calculating $F(v_0)$ and the constants in terms of A and solutions of certain cell problems.

3. Two-scale asymptotic solutions

In order to use the method of matched asymptotic expansions, one starts by investigating the asymptotics of solutions on each side of the interface, ignoring interfacial effects for the time being. Then two separate inner expansions are adjusted to achieve interface matching.

We begin by postulating two-scale inner asymptotic expansions (Bakhvalov and Panasenko, 1989)

$$u(x,\epsilon) \sim \sum_{p,l=0}^{\infty} \epsilon^{p+l} \sum_{|i|=l} N^{p,i}\left(\frac{x}{\epsilon}\right) D^i v(x), \tag{3.1}$$

where the functions $N^{p,i}(y)$ are 1-periodic and D^i stands for the operator of partial differentiation corresponding to the multiindex $i_1 i_2 \ldots i_l$ of length l.

The main advantage of (3.1) lies in the fact that one can compute the fast-variable terms $N^{p,i}$ independently of $v(x)$ by solving the so-called unit cell problems.

3.1. Micromechanical vibrations

The derivation of the cell problems follows the standard pattern. We first introduce the fast-variable $y = x/\epsilon$ and consider the two-scale expansion

$$u(x,y,\epsilon) \sim \sum_{p,l=0}^{\infty} \epsilon^{p+l} \sum_{|i|=l} N^{p,i}(y) D^i v_{(x)}. \tag{3.2}$$

The two-scale analogue of the differential operator

$$\frac{\partial}{\partial x_j}\left(A_{jk}\left(\frac{x}{\epsilon}\right)\frac{\partial}{\partial x_k}\right)$$

can be written as

$$\epsilon^{-2}\frac{\partial}{\partial y_j}\left(A_{jk}(y)\frac{\partial}{\partial y_k}\right) + \epsilon^{-1}\left(\frac{\partial A_{jk}}{\partial y_j} + A_{jk}\frac{\partial^2}{\partial y_k \partial x_j} + A_{jk}\frac{\partial^2}{\partial y_j \partial x_k}\right) + A_{jk}\frac{\partial^2}{\partial x_j \partial x_k}. \tag{3.3}$$

If we now plug (3.2) into the Helmholtz equation (2.2) and collect the terms, we obtain

$$\sum_{l,p=0} \epsilon^{l+p-2} \sum_{|i|=l} H^{p,i}(y) D^i v \sim 0, \tag{3.4}$$

where $H^{p,i}$ depend on the fast-variable components of the expansion (3.1). The terms of orders ϵ^{-2} and ϵ^{-1} must vanish, hence $H^{0,0} = H^{1,0} = 0$. This yields

$$N^{0,0} = N^{1,0} = 1.$$

For $H^{0,i}$ and $H^{1,i}$ we obtain the expressions

$$\begin{aligned} H^{0,i} &= \operatorname{div}(A\nabla N^{0,i}) + \frac{\partial A_{ik}}{\partial y_k}, \\ H^{1,i} &= \operatorname{div}(A\nabla N^{1,i}) + \frac{\partial A_{ik}}{\partial y_k}. \end{aligned} \tag{3.5}$$

We will also write explicitly and expression for $H^{2,0}$

$$H^{2,0} = -\omega^2 \rho(y) + \operatorname{div}(A\nabla N^{2,0}). \tag{3.6}$$

In a similar fashion, all $H^{p,i}$ can be calculated.

Eq. (3.4) will be useful only if we can guarantee that its left hand side is independent of y. Because of the periodicity assumptions, it is impossible to set all $H^{p,i}$ to zero (we refer to Bakhvalov and Panasenko (1989) for details). Thus we need $H^{p,i}$ to be constant. We also need to be able to choose these constants so that the equations above can be solved for $N^{p,i}$. The requirement of well-posedness for periodic problems then implies that $H^{p,i}$ must be equal to the spatial averages of the expressions on the right of (3.5), (3.6). Since for any 1-periodic function f, the average of $\operatorname{div}(A\nabla f)$ is zero, we obtain the cell problems

$$\begin{aligned} \operatorname{div}(A\nabla N^{0,i}) &= -\frac{\partial A_{ik}}{\partial y_k} + \left\langle \frac{\partial A_{ik}}{\partial y_k} \right\rangle, \\ \operatorname{div}(A\nabla N^{1,i}) &= -\frac{\partial A_{ik}}{\partial y_k} + \left\langle \frac{\partial A_{ik}}{\partial y_k} \right\rangle, \end{aligned} \tag{3.7}$$

and

$$\operatorname{div}(A\nabla N^{2,0}) = \omega^2(\rho(y) - \langle\rho\rangle), \tag{3.8}$$

similar, more complicated problems can be obtained for $N^{p,i}$ of all orders.

3.2. Macromechanical vibrations

Once $N^{p,i}$ nave been determined, one writes the slow variable part as an asymptotic series

$$v(x) = \sum_{q=0}^{\infty} \epsilon^q v_q(x)$$

and uses previously computed functions $N^{p,i}$ to obtain the effective constant coefficient equations for v_q. For the leading term v_0 one obtains the effective Eq. (2.6). The effective quantities are computed by averaging periodic functions. In particular, the effective matrix $\hat{A}$ is calculated by the formula

$$\hat{A}_{ij} = \left\langle A_{ik}\frac{\partial N^{0,j}}{\partial y_k} + A_{ij} \right\rangle, \tag{3.9}$$

$$\langle f \rangle = \frac{1}{|Q|}\int_Q f(x)\,\mathrm{d}x, \tag{3.10}$$

where brackets denote the spatial average.

It is well known (see e.g. Bakhvalov and Panasenko, 1989) that solutions of the periodic problems like (3.7) are unique up to a constant. This means that an expansion (3.1) is "rigid" and does not provide much freedom for interface matching, since we can only change the fast-variable functions $N^{p,i}$ by a constant. This is clearly not enough to match these rapidly oscillating functions across the interface. Therefore we need to mix fast and slow variables while matching. As a consequence, the main advantage of (3.1) evaporates.

A possible way out is the introduction of the so-called boundary layer correctors $S^{p,i}(x/\epsilon)$, 1-periodic in $\hat{x} = (x_1, x_2)$ and exponentially decreasing away from the interface. The modified expansions

$$u(x,\epsilon) \sim \sum_{p,l=0}^{\infty} \epsilon^{p+l} \sum_{|i|=l} \left(N^{p,i}\left(\frac{x}{\epsilon}\right) + S^{p,i}\left(\frac{x}{\epsilon}\right)\right) D^i v(x), \tag{3.11}$$

provides more freedom for matching, but still does not solve the problem. Roughly speaking, the problems for correctors must be well posed and independent of the slow variable x. Since the slow variable parts $D^i v_+$ and $D^i v_-$ are in general different, one ends up with the conditions prescribing the value of both $S^{p,i}$ and $A_{3k}\partial_k S^{p,i}$ at the interface. In elliptic problems these quantities are not independent, so correctors with the desired properties may not exist. To put it differently, our wish to keep the length scales separated can be difficult to fulfill near the interface.

3.3. Asymptotic expansions with interfacial correctors

The main idea of the method proposed in this paper is to look for the asymptotic expansions

$$u(x,\epsilon)^+ \sim \sum_{p,l=0}^{\infty} \epsilon^{p+l} \sum_{|i|=l} (N_+^{p,i} + M_+^{p,i}) D^i v_+ + S_+^{p,i} D^i v_- \tag{3.12}$$

in K^+ and

$$u(x,\epsilon)^- \sim \sum_{p,l=0}^{\infty} \epsilon^{p+l} \sum_{|i|=l} (N_-^{p,i} + M_-^{p,i}) D^i v_- + S_-^{p,i} D^i v_+ \tag{3.13}$$

in K^-. The four functions $M_\pm^{p,i}$ and $S_\pm^{p,i}$ are boundary layer correctors, that is functions periodic in $\hat{x} = (x_1, x_2)$ with period one, and decreasing exponentially away from the interface.

A way to interpret the "inter-crossed" terms on the right of the above expansions is to view them as the result of "virtual diffusion" of one composite into another. This means that instead of a thin abstract interface we see an interfacial zone of very small thickness where the effects of both composite structures are present. Effective vibrations in each half space influence the outcome of the averaging procedure and the resulting waves on the opposite side of the interface via the interfacial constraint.

The idea behind (3.12), (3.13) is to make use of the fact that the $D^i v_\pm$ are determined by averages of $N^{p,i}$ independent of the correctors. From the mathematical point of view, the new expansion differs from the ones discussed in Section 3, since now the terms $S_+^{p,i}$ and $M_-^{p,i}$ have the same slow variable parts, so for this pair of correctors we can obtain a transmission problem independent of the slow variable. The same reasoning clearly applies to the pair $S_-^{p,i}$, $M_+^{p,i}$.

To deal with the correctors, we first introduce some notations. We denote by $\hat{Q}$ the square $\{0 \leqslant x_j \leqslant 1, j = 1, 2, x_3 = 0\}$ and by Q_∞ the strip of width one which consists of all unit cubes above a given cube adjacent to the interface. Also, we let $Q_{-\infty}$ to be a strip obtained from Q_∞ by reflecting about the interface.

To obtain the cell problems for correctors, we repeat the procedure described in Section 3. The only difference is that now we can choose all $H^{p,i}$ related to correctors to be zero, since for partially periodic functions the equation

$$\operatorname{div}(A\nabla u) = 0$$

can have non-trivial solutions. In particular, we obtain $S^{0,0} = S^{1,0} = M^{0,0} = M^{1,0} = 0$ on both sides of the interface. The cell problems for all other correctors have the same general form

$$\operatorname{div}(A^+\nabla u) = f^+ \tag{3.14}$$

in K^+,

$$\operatorname{div}(A^-\nabla u) = f^-$$

In K^-,

$$[u] = \Phi(\hat{x}), \qquad [A_{3k}\partial_k u] = \Psi(\hat{x}) \tag{3.15}$$

at the interface. We seek solutions $u(\hat{x}, x_3)$, 1-periodic in $\hat{x}$ and rapidly decreasing as $|x_3| \to \infty$ together with their first derivatives.

4. Analysis of the asymptotic solution

4.1. Analysis of the interfacial effects

Available mathematical results (Oleinik and Yosifian, 1982; Oleinik et al., 1992; Gilbert and Panchenko, 1999) show that in order to control behavior of u for large $|x_3|$, one needs to prescribe Ψ in a special way. This crucial fact is known in linear elasticity as a version of the St. Venant principle. For the scalar equation (3.14) we have the following:

If $f^{\pm}$ decay exponentially away from the interface and

$$\int_{\hat{Q}} \Psi(\hat{x})\,\mathrm{d}\hat{x} = \int_{Q_{-\infty}} f^{-}(x)\,\mathrm{d}x - \int_{Q_{\infty}} f^{+}(x)\,\mathrm{d}x, \tag{4.1}$$

then a solution u of the transmission problems (3.14) and (3.15) can be chosen so that it decays exponentially in K^{+}, and approaches a constant k in K^{-} with the exponential rate. Moreover, the first derivatives of u decay exponentially as $|x_3| \to \infty$. The proof for the system of linear elasticity is available in Gilbert and Panchenko (1999). Modulo minor changes, the same method works for the scalar problem at hand.

The solutions constructed in this way are not of the boundary layer type even when the Ψ is chosen as in (4.1). We have a genuine boundary layer only on one side of the interface, while on the other side we can only guarantee that there is a constant k such that $u - k$ is a boundary layer. Contribution of the correctors can not be ignored away from the interface unless the constant k is zero.

Available mathematical theory makes it possible to calculate the constants in terms of solutions of certain auxiliary cell problems (see Oleinik et al. (1992), Chapter 1 Theorem 8.5), but in general the constants will differ from zero. We will always choose $S^{p,i}$ to be the boundary layers, since these terms are responsible for the thickness of the interface transition zone. The correctors $M^{p,i}$ will in general be "exponentially stabilizing."

The above considerations motivate the introduction of the function $\tilde{u}$, equal to u on one side of the interface and to $u - k$ on the other, that solves Eqs. (3.14) and satisfies the transmission conditions

$$[\tilde{u}] = \Phi(\hat{x}) + k, \qquad [A_{3k}\partial_k \tilde{u}] = \Psi(\hat{x}) + t, \tag{4.2}$$

where t is a constant computed by the formula

$$t = -\int_{\hat{Q}} \Psi(\hat{x})\,\mathrm{d}\hat{x} + \int_{Q_{-\infty}} f^{-}(x)\,\mathrm{d}x - \int_{Q_{\infty}} f^{+}(x)\,\mathrm{d}x. \tag{4.3}$$

Below, we will always solve the adjusted cell problems (3.14), (4.2).

The important consequence of the exponential stabilization phenomenon is that constants $k^{p,i}$ will alter the inner expansions, and the constants $t^{p,i}$ will enter the effective transmission conditions.

4.2. An algorithm for computing macroscopic interfacial corrections

Let us now outline the procedure for calculating terms of the modified asymptotic expansions with interfacial correctors.

Step 1. Solve periodic cell problems for $N_{\pm}^{p,i}$. Determine $\hat{A}_{\pm}$.

Step 2. Solve partially periodic problems (3.14), (4.2) to find the correctors $M_{\pm}^{p,i}$ and $S_{\pm}^{p,i}$. Determine the constants $k^{p,i}$, $t^{p,i}$.

Step 3. Use $\hat{A}$, $k^{p,i}$, $t^{p,i}$ to obtain the effective equations and transmission conditions for the slow-variable corrections v_q.

4.3. Approximation of order ϵ

The correctors in (3.12) are not of the boundary layer type in general, as evidenced by the discussion above. We can guarantee that $S_+^{0,i}$ is a boundary layer, and $M_+^{0,i}$ can be written as a sum of a constant $k_+^{0,i}$ and the boundary layer which we still denote by $M_{0,i}^+$. Thus adjusted, the approximation of order ϵ in K^+ is of the form

$$u^+ = v_0^+ + \epsilon\left[v_0^+ + (N_+^{0,i} + k_+^{0,i} + M_+^{0,i})\partial_i v_0^+ + S_+^{0,i}\partial v_0^- + v_1^+\right] + O(\epsilon^2), \tag{4.4}$$

where $M_+^{0,i}$ and $S_+^{0,i}$ are boundary layers. A similar expression is sought in K^-. Eq. (4.4) means in particular that in the far field away from the interface we have the approximation

$$u^+ = v_0^+ + \epsilon\left[v_0^+ + (N_+^{0,i} + k_+^{0,i})\partial_i v_0^+ + v_1^+\right] + O(\epsilon^2). \tag{4.5}$$

The terms corresponding to $k^{0,i}$ represent a non-trivial contribution to the far field due to the interaction between the microstructure and the interface.

Following the general procedure from Section 4.1 we obtain the effective transmission problem for v_0.

$$\hat{A}_{ik}\partial_{ik}^2 v_0 + \langle\rho\rangle v_0 = 0, \tag{4.6}$$

$$\left[k^{0,0}v_0\right] = 0, \tag{4.7}$$

$$\left[t^{0,i}\partial_i v_0\right] = 0. \tag{4.8}$$

For the next slow variable correction v_1 we find

$$\hat{A}_{ik}\partial_{ik}^2 v_1 + \langle\rho\rangle v_1 = \langle\rho\rangle + \langle A_{ik}\partial_k N^{2,0}\rangle + \hat{A}_{ik}\partial_{ik}^2 v_0, \tag{4.9}$$

$$\left[k^{0,0}v_1\right] = -\left[k^{0,i}\partial_i v_0\right], \tag{4.10}$$

$$\left[t^{0,i}\partial_i v_1\right] = -\left[t^{2,0}v_0 + t^{1,i}\partial_i v_0 + t^{0,i_1 i_2}\partial_{i_1 i_2}^2 v_0\right]. \tag{4.11}$$

Eqs. (4.4)–(4.11) contain functions $N^{0,i}$, $N^{2,0}$ and constants $k^{0,0}$, $k^{0,i}$, $t_\pm^{1,i}$, $t_\pm^{2,0}$ and $t_\pm^{0,i_1 i_2}$.

If one were to follow the general algorithm outlined in the previous subsection, the following cell problems should have been solved.

(1) To obtain $N^{0,i}$ we need to solve the periodic problem (3.7). Similar periodic cell problem (3.8) should be solved to obtain $N^{2,0}$.

(2) The correctors $M_\pm^{0,i}$ and $S_\pm^{0,i}$ are found from the adjusted transmission problem

$$\operatorname{div}\left(A^+\nabla M_+^{0,i}\right) = 0, \tag{4.12}$$

in K^+,

$$\operatorname{div}\left(A^-\nabla S_-^{0,i}\right) = 0$$

in K^-, with the interface conditions

$$\begin{aligned} &N_+^{0,i} + M_+^{0,i} + k_+^{0,i} = S_-^{0,i}, \\ &A_{3k}^+\partial_k(N_+^{0,i} + M_+^{0,i}) = A_{3k}^-\partial_k S_-^{0,i} + t_+^{0,i}. \end{aligned} \tag{4.13}$$

A similar problem can be written for the pair $M_-^{0,i}, S_+^{0,i}$.

(3) The constants $t^{p,i}$ appear in the transmission conditions for the interface correctors $M_\pm^{1,i}$, $S_\pm^{1,i}$, $M_\pm^{2,0}$, $S_\pm^{2,0}$, $M_\pm^{1,i_1 i_2}$, and $S_\pm^{1,i_1 i_2}$, so we would need to solve the corresponding cell problems as well. Thus we have a total of six more problems to solve, two per each pair of the correctors above. The equations and

transmission conditions are similar to those in Eqs. (4.12), (4.13). We emphasize that the correctors are only partially periodic, so we have to deal with problems in unbounded domains. This may be very time-consuming.

4.4. A simplified algorithm for interfacial corrections

Further analysis of the cell problems for correctors can provide useful explicit formulas and substantially reduce the amount of numerics. In this subsection we present some formulas for the constants mentioned above. It is remarkable that to use these formulas, we do not need all the correctors listed at the end of the previous subsection, which leads to an improvement of the method and potentially makes it more effective for computations. The derivation of the formulae can be found in the Appendix A.

First of all, since $N^{0,0} = N^{1,0} = 1$, and $M_{\pm}^{0,0} = S_{\pm}^{0,0} = 0$, we obtain $k_{\pm}^{0,0} = 1$. To determine various t-constants, we make use of the formula (4.3), and the classical formula for the effective matrix $\hat{A}$ (see e.g. Bakhvalov and Panasenko, 1989). Then we find that

$$t_{\pm}^{0,i} = t_{\pm}^{1,i} = \hat{A}_{3i}^{\pm}. \tag{4.14}$$

This means that $t^{0,i}$ and $t^{1,i}$ are found without solving any problems for correctors. All we need is the effective matrix $\hat{A}$ which is determined from the original matrix A and the function $N^{0,i}$.

Next we give the formula for $t_{\pm}^{2,0}$.

$$t_{\pm}^{2,0} = \int_{\hat{Q}} A_{3k}^{\pm} \partial_k N^{2,0}(0, \hat{x})\, \mathrm{d}\hat{x}. \tag{4.15}$$

Again, we need only the periodic function $N^{2,0}$ and the matrix A.

The constants $t_{\pm}^{0,i_1 i_2}$ are found from the formula

$$t_{\pm}^{0,i_1 i_2} = \int_{\hat{Q}} (A_{3i_1}^{\mp} S_{\mp}^{0,i_2} - A_{3i_1}^{\pm} M_{\pm}^{0,i_2})(\hat{x}, 0)\, \mathrm{d}\hat{x} \tag{4.16}$$

that requires the knowledge of A and the correctors $M_{\pm}^{0,i_2}$ and $S_{\pm}^{0,i_2}$.

Now, we have a shortened list of cell problems as follows:

1. Periodic problems for $N^{0,i}$, $N^{2,0}$;
2. Problems for correctors $M^{0,i}$, $S^{0,i}$ that appear explicitly in the asymptotic approximation (4.4). We also need them to determine $k^{0,i}$. Moreover, $M^{0,i}$ and $S^{0,i}$ enter the formula (4.16).

Comparison of this list with the one given in the beginning of the Section 4.1 shows that the item 3 has disappeared. Thus we have six less problems to solve numerically.

Since the calculations are exactly the same we will drop + and − from now on. To calculate the quantities in the formula (4.4), we need to do the following:

1. *Solve the periodic cell problems for* $N^{0,i}, N^{1,i}$ *and* $N^{2,0}$. At this step, we determine $N^{0,i} = N^{1,i}$ by solving Eqs. (3.3), and $N^{2,0}$ are found from (3.4). Using these functions, we calculate the following constants:
   - the effective matrix $\hat{A}$ by the formula

     $$\hat{A}_{ij} = \langle A_{ik} \partial_k N^{0,i} + A_{ij} \rangle,$$

   - the constants $t^{0,i} = t^{1,i}$ from the formula

     $$t^{0,i} = \hat{A}_{3i},$$

- the constants $t^{2,0}$ from the formula

$$t^{2,0} = \int_{\hat{Q}} (A_{3k}\partial_k N^{2,0})(\hat{x}, 0)\, \mathrm{d}\hat{x}.$$

2. *Solve the partially periodic problem for the adjusted correctors $M_+^{0,i}, S_-^{0,i}$ by solving Eqs. (4.12) with the interface conditions (4.13).* Then one is able to calculate the constants $t^{0,i_1 i_2}$ from the formula (A.16) and also determine the constants $k^{0,i}$.
3. *Write down the effective transmission problems for v_0, v_1*

$$\hat{A}_{ik}\partial^2_{ik} v_0 + \langle\rho\rangle v_0 = 0 \tag{4.17}$$

with the interface conditions

$$[v_0] = 0, \qquad [\hat{A}_{3i}\partial_i v_0] = 0. \tag{4.18}$$

If we use the equations above to simplify the Eqs. (4.9)–(4.11), we obtain

$$\hat{A}_{ik}\partial^2_{ik} v_1 + \langle\rho\rangle v_1 = \langle\rho\rangle(1 - v_0) + \langle A_{ik}\partial_k N^{2,0}\rangle \tag{4.19}$$

with the interface conditions

$$\begin{aligned} &[v_1] = -[k^{0,i}\partial_i v_0], \\ &[\hat{A}_{3i}\partial_i v_1] = -[t^{2,0} v_0 + t^{0,i_1 i_2}\partial^2_{i_1 i_2} v_0]. \end{aligned} \tag{4.20}$$

5. Conclusion

An analysis carried out in Section 4 shows that the leading term of the proposed modified two-scale expansion behaves consistently with respect to homogenization, in the sense that the transmission conditions are generated by the effective matrices. The next correction, however, can potentially exhibit nontrivial interplay between the interface and the microstructure. Amazingly, the localized in space boundary layers may influence the far field through the constants $k^{0,i}$ and the modified transmission conditions (4.20). The main result of Section 4 is a reduction in number of the cell problems needed to be solved. Of course, the bare minimum includes problems for $N^{0,i}$, $M^{0,i}$ and $S^{0,i}$ which appear explicitly in the modified expansion. We were able to show that the only additional problem needed is the periodic cell problem for $N^{2,0}$.

Explicit formulae obtained in Section 4 give expressions for all the constants on the right of (4.20) in terms of the averages of the solutions on the interface. Since these solutions should decay exponentially, one can concentrate on the bounded region near the boundary to obtain a good approximation.

The only parameter for which no convenient formula has been found is $k^{0,i}$. It seems likely that one can express these constants in terms of the boundary traces of the solutions of the original problem and certain auxiliary problems in the spirit of Theorem 8.5 in Chapter 1 of Oleinik et al. (1992). But this approach still requires solving some problems in unbounded domains. From energy decay considerations one should expect $k^{0,i} = 0$ but this does not follow from the theory presented here.

The underlying theoretical considerations are sufficiently general to be applied to the systems of linear elasticity and even certain problems for poroelastic materials (see Gilbert and Panchenko, 1999). It also seems that the method proposed in the paper can lead to an effective numerical algorithm which will be the subject of the future research. We plan to discuss numerics in a separate publication.

Appendix A

A.1. Derivation of the formula (4.14)

Note that from (4.13) one can get

$$t_+^{0,i} = \int_{\hat{Q}} \left(A_{3k}^+ \frac{\partial N_+^{0,i}}{\partial x_k} + A_{3i}^+ \right) \mathrm{d}\hat{x}. \tag{A.1}$$

Let us compare this with the standard formula for the entries of the effective matrix $\hat{A}$:

$$\hat{A}_{3i}^+ = \int_Q \left(A_{3k}^+ \frac{\partial N_+^{0,i}}{\partial x_k} + A_{3i}^+ \right) \mathrm{d}x. \tag{A.2}$$

These equations are almost the same except for the domain of integration. We want to show that $t^{0,i} = \hat{A}_{3i}$. Writing

$$t_+^{0,i} = A_{3i}^+ + \int_{\hat{Q}} B_{3i}^+ \, \mathrm{d}\hat{x}. \tag{A.3}$$

where $B_{3i}^+ = A_{3k}\partial_k N_+^{0,i} + A_{3i} - \hat{A}_{3i}$, we find that the periodic cell equation for $N_+^{0,i}$ can be written as

$$\mathrm{div} B = 0. \tag{A.4}$$

We also note that $\langle B \rangle = 0$. Now integrate (A.4) over $\hat{Q}$ and then integrate in x_3 from zero to some $\alpha < 1$. The integrals containing B_{ji} with $j \neq 3$ will be zero because of periodicity. For the rest of the entries of B we get

$$\int_{\hat{Q}} B_{3i}^+(\alpha, \hat{x}) \, \mathrm{d}\hat{x} = \int_{\hat{Q}} B_{3i}^+(0, \hat{x}) \, \mathrm{d}\hat{x}.$$

This holds for any $\alpha \in [0, 1]$ and therefore the integral of B_{3i}^+ on the right of (A.3) is a constant which we denote by b. Since B_{3i}^+ are periodic, we must have

$$\int_0^1 b \, \mathrm{d}x_3 = \langle B_{3i}^+ \rangle.$$

But the average of B^+ is zero, so $b = 0$ and thus $t_+^{0,i} = \hat{A}_{3i}^+$. Repeating this computation we also get $t_-^{0,i} = A_{3i}^-$.

Next we determine $t_\pm^{1,i}$ since the cell problems for $N_\pm^{1,i}$ are the same as for $N_\pm^{0,i}$, and the problems for correctors with indices $1, i$ are the same as the corresponding problems for $0, i$-correctors, we get $t_\pm^{1,i} = t_\pm^{1,i} = \hat{A}_{3i}^\pm$.

A.2. Derivation of the formula (4.15)

Consider the partially periodic problems for correctors $M_+^{2,0}$, $S_-^{2,0}$:

$$\mathrm{div}(A^+ \nabla M_+^{2,0}) = 0 \tag{A.5}$$

in K^+,

$$\mathrm{div}(A^- \nabla S_-^{2,0}) = 0$$

in K^-, with the interface conditions

$$\begin{aligned} &N_+^{2,0} + M_+^{2,0} = S_-^{2,0}, \\ &A_{3k}^+ \partial_k (N_+^{2,0} + M_+^{2,0}) = A_{3k}^- \partial_k S_-^{2,0} + t_+^{2,0}. \end{aligned} \tag{A.6}$$

Thus $t_+^{2,0}$ is computed from the formula (4.7). Repeating the procedure for the pair $M_-^{2,0}, S_+^{2,0}$ we obtain (4.15).

We note that this makes it necessary to solve periodic cell problem for $N^{2,0}$

$$\partial_k (A_{kj} \partial_j N^{2,0}) = (\rho - \langle \rho \rangle). \tag{A.7}$$

A.3. Derivation of the formula (4.16)

The procedure is exactly the same for $t_+^{0,i_1 i_2}$ and $t_-^{0,i_1 i_2}$, so we may drop the superscript. To use the formula (4.3) we need to determine the value of

$$\int_{\hat{Q}} \left(A_{3k} \partial_k N^{0,i_1 i_2} + A_{3i_1} N^{0,i_1} \right) \mathrm{d}\hat{x} \tag{A.8}$$

at the interface. The function $N^{0,i_1 i_2}$ is the solution of the cell problem

$$\partial_k (A_{kj} \partial_j N^{0,i_1 i_2} + A_{ki_1} N^{0,i_2}) = -f + \langle f \rangle, \tag{A.9}$$

where

$$f = A_{ki_1} \partial_k N^{0,i_2} + A_{i_1 i_2}.$$

Using the formula for the effective matrix $\hat{A}$ we find that

$$\langle f \rangle = \hat{A}_{i_1 i_2}.$$

Note that in the process of calculating $t^{0,i}$ we showed that the integral of the right hand side over $\hat{Q}$ is zero. Thus, after integrating (A.9) over $\hat{Q}$ in $\hat{x}$ and then from 0 to α in x_3 we obtain

$$\sigma(\alpha) - \sigma(0) = 0, \tag{A.10}$$

where

$$\sigma(\alpha) = \int_{\hat{Q}} \left(A_{3j} \partial_j N^{0,i_1 i_2} + A_{3i_1} N^{0,i_2} \right)(\hat{x}, \alpha) \, \mathrm{d}\hat{x},$$

which means that $\sigma(\alpha)$ is constant. Integrating in α from 0 to 1 we find that

$$\sigma(0) = \langle A_{3j} \partial_j N^{0,i_1 i_2} + A_{3i_1} N^{0,i_2} \rangle. \tag{A.11}$$

Now we note that the solution of the problem (A.9) is unique up to a constant. We always choose a constant to be zero, which makes the solution unique. The divergence of the vector

$$A_{kj} \partial_j N^{0,i_1 i_2} + A_{ki_1} N^{0,i_2}$$

on the left of (A.9) does not depend on the average values of its components. Choosing the average of the third component arbitrarily we do not change the solution. Hence, by uniqueness we conclude that

$$\sigma(\alpha) = 0. \tag{A.12}$$

Furthermore, the pair $M_+^{0,i_1i_2}, S_-^{0,i_1i_2}$ is a solution of the partially periodic cell problem

$$\begin{aligned}\operatorname{div}(A^+\nabla M_+^{0,i_1i_2}) &= -A^+_{i_1k}\partial_k M_+^{0,i_2} - \partial_k(A^+_{i_1k}M_+^{0,i_2}),\\ \operatorname{div}(A^-\nabla S_-^{0,i_1i_2}) &= -A^-_{i_1k}\partial_k S_-^{0,i_2} - \partial_k(A^-_{i_1k}S_-^{0,i_2})\end{aligned} \tag{A.13}$$

with the interface conditions

$$A^+_{3k}\partial_k(N_+^{0,i_1i_2} + M_+^{0,i_1i_2}) + A^+_{3i_1}(N_+^{0,i_2} + M_+^{0,i_2}) = A^-_{3k}\partial_k S_-^{0,i_1i_2} + A^-_{3i_1}S_-^{0,i_2}. \tag{A.14}$$

Now (4.3) yields

$$\begin{aligned} t_+^{0,i_1i_2} = &-\int_{\hat{Q}}(A^+_{3k}\partial_k N_+^{0,i_1i_2} A^+_{3i_1}N_+^{0,i_2})(\hat{x},0)\,\mathrm{d}\hat{x} + \int_{\hat{Q}}(A^-_{3k}\partial_k S_-^{0,i_1i_2} + A^-_{3i_1}S_-^{0,i_2})(\hat{x},0)\,\mathrm{d}\hat{x}\\ &-\int_{\hat{Q}}(A^+_{3k}\partial_k M_+^{0,i_1i_2} + A^+_{3i_1}M_+^{0,i_2})(\hat{x},0)\,\mathrm{d}\hat{x} + \int_0^\infty\int_{\hat{Q}} A^+_{i_1k}\partial_k M_+^{0,i_2} + \partial_k(A^+_{i_1k}M_+^{0,i_2})\,\mathrm{d}\hat{x}\,\mathrm{d}x_3\\ &-\int_0^\infty\int_{\hat{Q}} A^-_{i_1k}\partial_k S_-^{0,i_2} + \partial_k(A^-_{i_1k}S_-^{0,i_2})\,\mathrm{d}\hat{x}\,\mathrm{d}x_3. \end{aligned} \tag{A.15}$$

The first integral in (A.15) is equal to $\int \sigma(x_3)\,\mathrm{d}x_3$ and is zero in view of (A.12). Next we integrate (A.13) over K_+ and K_- and use periodicity in $\hat{x}$ and exponential decay of derivatives in x_3 to deduce

$$\int_0^\infty\int_{\hat{Q}} A^+_{i_1k}\partial_k M_+^{0,i_2} + \partial_k(A^+_{i_1k}M_+^{0,i_2})\,\mathrm{d}\hat{x}\,\mathrm{d}x_3 = \int_{\hat{Q}} A_{3k}\partial_k M_+^{0,i_1i_2}(\hat{x},0)\,\mathrm{d}\hat{x} \tag{A.16}$$

and a similar equation for the terms depending on S_-^{0,i_1i_2}, S_-^{0,i_2} in (A.15). Thus, (A.15) reduces to

$$t_+^{0,i_1i_2} = \int_{\hat{Q}}(A^-_{3i_1}S_-^{0,i_2} - A^+_{3i_1}M_+^{0,i_2})(\hat{x},0)\,\mathrm{d}\hat{x}. \tag{A.17}$$

Clearly, a similar formula holds for t_-^{0,i_1i_2}.

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