ON RATIONAL BOUNDARY CONDITIONS FOR HIGHER-ORDER LONG-WAVE MODELS

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Abstract: Higher-order corrections to classical long-wave theories enable simple and efficient modelling of the onset of wave dispersion and size effects produced by underlying micro-structure. Since such models feature higher spatial derivatives, one needs to formulate additional boundary conditions when confined to bounded domains. There is a certain controversy associated with these boundary conditions, because it does not seem possible to justify their choice by purely physical considerations. In this paper an asymptotic model for one-dimensional chain of particles is chosen as an exemplary higher-order theory. We demonstrate how the presence of higher-order derivative terms results in the existence of non-physical "extraneous" boundary layer-type solutions and argue that the additional boundary conditions should generally be formulated to eliminate the contribution of these boundary layers into the averaged solution. Several new methods of deriving additional boundary conditions are presented for essential boundary. The results are illustrated by numerical examples featuring comparisons with an exact solution for the finite chain.

Key words: Asymptotics, long waves, strain gradient theories, boundary conditions.

1. INTRODUCTION

The use of long-wave asymptotics in physics and engineering has a long and productive history. Whenever a problem at hand possesses features at two widely different length scales, the natural scale separation may be employed to dramatically simplify the analysis by neglecting the detail at lower observation levels. For example, classical theories of plates and shells de-

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scribe low-frequency dynamics of thin structural elements by disregarding, in particular, variations of stresses and strains across the thickness. Similarly, effective continuum theories for inhomogeneous or discrete media are derived by smoothing out the fine detail of stress and strain field distributions.

It often happens that the influence of micro- and/or meso-scales becomes more pronounced yet still remains a second order. A simple and efficient description of size effects, wave dispersion and other relevant features of the material response may then be achieved by considering higher-order corrections to the leading-order long-wave theory. The resulting higher-order asymptotic models of micro-structure are often termed gradient theories, due to the presence of higher gradients of strain. Similar models for plates and shells are commonly referred to as shear deformation theories.

At the same time, mathematical treatment of the higher-order long-wave models demands a special care and the reason for this is the higher order of the associated differential equations. Additional particular integrals of such governing equations often correspond to short-wave “extraneous” solutions incompatible with the physical assumptions that enabled long-wave expansion. Similar complications are known to arise for higher-order theories of thin elastic plates and shells, see e.g. [1], [2]. Possible solution to the problem involves replacing strain gradient-type terms with the gradients of inertia; however, this method is generally inapplicable in a non-scalar context.

When solving boundary value problems for the aforementioned higher-order models of micro-structure, we have to impose extra boundary conditions in addition to those naturally arising from the original formulations. This paper suggests a rational approach to the derivation of such boundary conditions. It is demonstrated by way of a simple example of a refined asymptotic model for the one-dimensional regular array of particles connected by springs, obtained in [3] and, in a less general form, in [4].

Essentially, general solutions of higher-order models are interpreted as composite asymptotic expansions, combining contributions of long-wave “averaged” solutions and non-physical boundary layers (e.g. extraneous short-wave solutions localised near boundary). Based on this, we propose a principle for deriving additional boundary conditions that is aimed at minimising the effect of the boundary layers on long-wave components of interest. A standard asymptotic procedure (see e.g. [5]) is developed to treat a boundary value problem for the fourth-order ordinary differential equation modelling a finite array with fixed ends. It is worth noting that there always is an ambiguity in the selection of additional boundary conditions. In this paper, we discuss two types of boundary conditions that involve first, second or third spatial derivatives of the displacement. Comparisons with the exact numerical solutions for a finite array demonstrate the efficiency of the proposed methodology.

2. GOVERNING EQUATIONS

Let us consider a regular array of particles of mass m connected by springs with the stiffness K, see Fig. 1. Harmonic oscillations of the nth particle are governed by the finite-difference equation

$$u_{n-1} - (2-\Omega^2)u_n + u_{n+1} = -\frac{q_n}{K}, \tag{1}$$

where $\Omega^2 \equiv m\omega^2 / K$ is the non-dimensional frequency and q_n the mass force. This structure acts as a low-pass filter and does not allow undamped propagation of harmonic waves when $\Omega > 2$, for more details see [6].

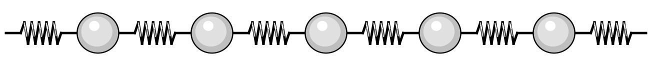

Figure 1. An infinite array of particles connected by springs.

Since we are interested in the behaviour of finite arrays, boundary conditions must be specified. In this paper we will assume the essential (Dirichlet) boundary conditions at the both ends of the array. For arrays of $2N+1$ particles these conditions may be written as

$$u_{-N} = f_{-N}, \; u_N = f_N, \tag{2}$$

with parameters f_{-N} and f_N generally depending on Ω. Equations (1) and conditions (2) form the system of $2N-1$ linear equations in $2N-1$ unknowns u_n, $n = -N+1, \ldots, N-1$. As long as Ω is distinct from one of the natural frequencies, this system has a unique solution that describes configuration of the array subjected to a force excitation at the specified frequency.

It may reasonably be expected that if a long wave is to propagate through such a periodic structure, the resulting motion can be described by a continuum theory. It is easy to see that to the leading order

$$l^2 \frac{\partial^2 u}{\partial x^2} + \Omega^2 u = -\frac{q}{K}, \tag{3}$$

within which $u(x_n) \equiv u_n$ is the continuous displacement field, $q(x_n) \equiv q_n$ the continuous mass force, $x_n = nl$, and l the distance between particles. This leading-order Helmholtz-type approximation does not reproduce any microstructural behaviour and is a form of the effective continuum theory, very similar to the classical rod theory. A more advanced higher-order model that we will use in this paper is derived in [3] and has the following form

$$l^2 \frac{\partial^2 u}{\partial x^2} + \Omega^2 u - \gamma l^4 \frac{\partial^4 u}{\partial x^4} - (\gamma - \alpha) l^2 \Omega^2 \frac{\partial^2 u}{\partial x^2} + \left(\alpha + \frac{1}{12}\right)\Omega^4 u = -\frac{q}{K} + l^2 \frac{(12\gamma+1)}{12K}\frac{\partial^2 q}{\partial x^2} + \frac{(12\alpha+1)}{12K}\Omega^2 q, \tag{4}$$

where α and γ are arbitrary constants and q is assumed to be smooth to the extent that differentiation with respect to x does not change its asymptotic order. Model (4) is strongly elliptic when $\gamma \geq 0$. A particular case of (4) with $\alpha = -1/12$ and $q \equiv 0$ was presented in [4]. It is worth remarking that most long-wave models for longitudinal waves in elastic structures are formally equivalent; thus, after trivial modifications, our results are also valid for higher-order theories of rods and plates.

In the absence of mass forces, the performance of an asymptotic model like (4) may be assessed by comparing its dispersion relation with the exact dispersion relation. For harmonic waves

$$u(x_n) \equiv u_n = U e^{ikx_n} \equiv U e^{i\eta x}, \tag{5}$$

the exact dispersion relation for (1) is given by $\Omega^2 = 2 - 2\cos\eta$, in which $\eta = kl$, $|\eta| \leq \pi$, is the non-dimensional wave number, see [6]. Fig. 2(a) presents typical dispersion curves for the array. Thin straight line that acts as a tangent to the exact solution at $\eta = 0$ corresponds to the leading-order model (3). Dotted line indicates the response of long-wave theory (4) when $\gamma = 0$ and $\alpha = -1/12$. This model produces dispersion and may be expected to accurately simulate behaviour of the array at higher frequencies.

Dispersion relations only characterise the approximation accuracy of asymptotic models on unbounded domains. In order to indicate the performance of theories (3) and (4) when solving boundary value problems, we use a model example of finite array of 25 particles ($N = 12$) with fixed ends $f_{-N} = 1$ and $f_N = -1$. The distance between particles $l = 1/N$ and no mass force is applied $q \equiv 0$. Second-order differential equation (3) may be easily solved subject to (2) with aforementioned parameters. However, fourth-order equation (4) generally requires additional boundary conditions. The choice of these conditions is discussed in Section 3; meanwhile we remark that choice of $\gamma = 0$ reduces the order of (4) and enables solving it subject to (2).

Fig. 2(b) illustrates the configuration of the array when $\Omega = 0.5$. It is clear that leading-order theory (3) fails to accurately reproduce the array configuration at this frequency, whereas the use of higher-order theory (4) with $\gamma = 0$ and $\alpha = -1/12$ results in a remarkable agreement with the exact solution. Asymptotic model (4) with $\gamma = 0$ is special because it enables solution of boundary value problems without additional boundary conditions.

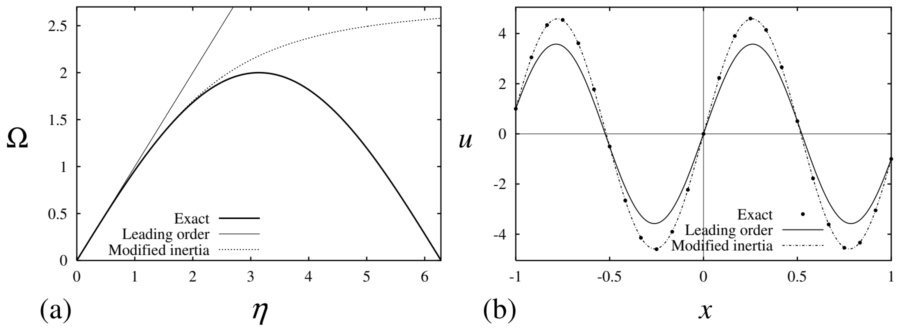

Figure 2. (a) Dispersion curves showing scaled frequency against scaled wave number for exact dispersion relation (thick solid), leading-order theory (thin solid) and theory with modified inertia that uses $\gamma = 0$ and $\alpha = -1/12$ (dotted). (b) Configuration of the array of 25 particles when $\Omega = 0.5$, computed for the same set of theories.

In the context of theories of plates and shells such models are termed "theories with modified inertia", see [1]; we will follow this nomenclature. Unfortunately, it is generally not possible to reduce the order of non-scalar asymptotic theories, see e.g. [3]. At the same time, certain $\gamma > 0$ may result in a better numerical approximation of the exact dispersion relation. Therefore, it would still be useful to develop rational procedure for deriving additional boundary conditions to be used with (4).

It is worth remarking that the considered long-wave theory (4) is somewhat unusual in that it contains two auxiliary parameters α and γ. Any choice of these parameters produces a long-wave model with an equivalent or better truncation error. Such classes of equivalent asymptotic theories may be generated by a simple formal procedure described in [3] for a variety of examples. An alternative approach to homogenisation that also results in parameterised classes of asymptotic theories is described in [4].

3. ESSENTIAL BOUNDARY CONDITIONS

We start by rescaling equation (4) so that differentiation no longer changes asymptotic orders of long-wave quantities. To this end we introduce

$$x = \xi / Nl , \quad c = \Omega / \eta , \quad w = \eta^2 lu , \quad Q = lq / K , \quad F_{\pm 1} = \eta^2 l f_{\pm N} , \tag{6}$$

so that $\Omega \sim \eta$ and, for the sake of determinacy, $c \sim 1$. Please note that this scale results in discrete $\eta = 1/N$. The result of rescaling (4) according to (6) is a non-dimensional representation that reveals the asymptotic structure of the governing equation as well as specifies the implied truncation error:

$$\frac{\partial^2 w}{\partial \xi^2}+c^2 w-\eta^2\left(\gamma\frac{\partial^4 w}{\partial \xi^4}+(\gamma-\alpha)c^2\frac{\partial^2 w}{\partial \xi^2}-\left(\alpha+\frac{1}{12}\right)c^4 w\right)$$
$$=-Q+\eta^2\left(\left(\gamma+\frac{1}{12}\right)\frac{\partial^2 Q}{\partial \xi^2}-\left(\alpha+\frac{1}{12}\right)c^2 Q\right)+O(\eta^4). \tag{7}$$

First question that we ought to ask ourselves is how sensitive our problem is to the choice of additional boundary conditions. Would it actually be possible to guess the correct boundary condition without deriving one? Thus, we begin with a numerical experiment in which we attempt to solve governing equation (7) subject to one of the following sets of boundary conditions

$$w\big|_{\xi=-1}=F_{-1}, \quad w\big|_{\xi=1}=F_1, \quad \left.\frac{\partial w}{\partial \xi}\right|_{\xi=-1}=\left.\frac{\partial w}{\partial \xi}\right|_{\xi=1}=0, \tag{8a}$$

$$w\big|_{\xi=-1}=F_{-1}, \quad w\big|_{\xi=1}=F_1, \quad \left.\frac{\partial^2 w}{\partial \xi^2}\right|_{\xi=-1}=\left.\frac{\partial^2 w}{\partial \xi^2}\right|_{\xi=1}=0. \tag{8b}$$

The resulting solutions are compared with both the exact and leading-order approximate theories in Fig. 3. The left hand plot demonstrates striking 250% error in the magnitude obtained when using theory (7) with boundary conditions (8a). The use of boundary conditions (8b) results in a better agreement with the exact solutions, see the right hand plot, however, the resulting accuracy is still of the same order as obtained with the leading-order "rod" theory (3) subjected to (2). The benefits of using higher-order theory, evident, for example, from the performance of the theory with modified inertia in Fig. 2(b), are no longer apparent. This is especially alarming in view of the fact that the frequency used in Fig. 2(b) is double of that in Fig. 3. Therefore, we must explain the poor performance of the theory (7) in considered boundary value problems as well as attempt to formulate additional boundary conditions that will not distort the solution to such an extent.

First, let us consider the dispersion relation for (7), written as

$$\left(\alpha+\frac{1}{12}\right)\Omega^4+(1+(\gamma-\alpha)\eta^2)\Omega^2=\eta^2(1+\gamma\eta^2). \tag{9}$$

It is a bi-quadratic equation in η, thus, it associates two (right-propagating or decaying as $\xi\to\infty$) wave numbers η to each fixed frequency Ω. Please note that there is only one physical solution branch in the exact problem formulation. Relation (9) is particularly simple to interpret in the low-

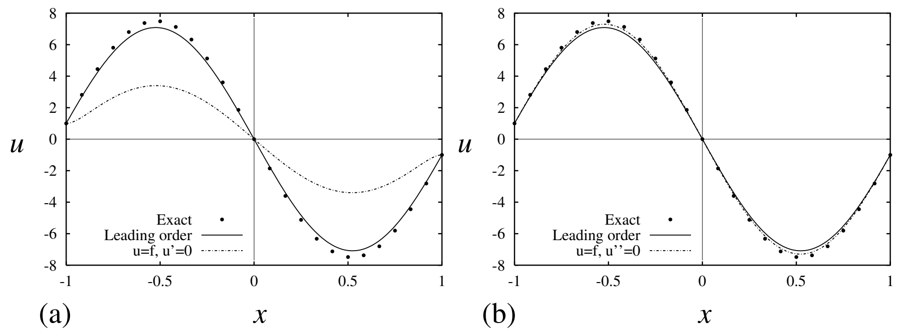

Figure 3. Configurations of the array of 25 particles using exact and asymptotic theories when $\Omega = 0.25$. Dots and thin solid line correspond to the exact solution and leading-order "rod" theory, respectively. Dotted line presents the response of the higher-order theory with $\gamma = 0.5$, $\alpha = -1/12$ and additional boundary condition (8a) and (8b).

frequency limit $\Omega \to 0$. In this case both solutions of (9) are explicit and given by $\eta \sim 0$ and $\eta \sim -i/\sqrt{\gamma}$. The first of the solutions is the expected long-wave component, whereas the second one does not satisfy the long-wave assumption. Particular solution of (7) associated with $\eta \sim -i/\sqrt{\gamma}$ describes an evanescent component that is not relevant for describing wave motion in unbounded array, but produces a boundary layer whenever a boundary condition is imposed. It is worth reiterating that such solutions are short-wave and, therefore, non-physical; they are, essentially, artefacts left after the truncation of an infinite series performed when (7) was formulated. We will refer to these solutions as "extraneous".

Because of the linearity of our problem, any of its solutions may be interpreted as a superposition of long-wave $\overline{w}$ and extraneous w_* components:

$$w = \overline{w} + w_* . \tag{10}$$

Essentially, we are treating governing equation (7) as a composite asymptotic expansion. It is clear that in the coordinate system defined by (6) differentiation of the long-wave component $\overline{w}$ does not affect its asymptotic order. Thus, we can say that to the leading order

$$\frac{\partial^2 \overline{w}}{\partial \xi^2} + c^2 \overline{w} + Q = O(\eta^2)\,, \tag{11}$$

as in (3). On the other hand, the extraneous solutions are not long-wave and, therefore, have different asymptotic structure from what is assumed by (7). It is best revealed by rescaling the spatial coordinate as $\zeta = \xi / \eta$ that, to the leading-order, transforms governing equation (7) into

$$\gamma \frac{\partial^2 w_*}{\partial \zeta^2} - w_* = O(\eta^2)\,. \tag{12}$$

Equation (12) is independent of Q because it describes rapidly varying solution. Decaying solution of (12) may be written in the following form

$$w_* = Be^{-\frac{\zeta}{\sqrt{\gamma}}} \equiv Be^{-\frac{\xi}{\sqrt{\gamma}\eta}}\,. \tag{13}$$

We were originally interested in solving (7) subject to essential boundary conditions; let us focus our attention on the left end of the array. Because of assumption (10), whenever we impose

$$w\big|_{\xi=-1} = F_{-1}\,, \quad \text{it results in} \quad \overline{w}\big|_{\xi=-1} = F_{-1} - w_*\big|_{\xi=-1}\,. \tag{14}$$

Therefore, in order to minimise the influence of an extraneous boundary layer we need to minimise its contribution to (14). At the same time, we must formulate an additional boundary condition for governing equation (7). The derivative of boundary layer (13) with respect to ξ is $O(\eta^{-1})$. This presents us with the opportunity to separate contributions of long-wave and extraneous components by using one of boundary conditions given by

$$\left.\frac{\partial^n w}{\partial \xi^n}\right|_{\xi=-1} \equiv \left.\frac{\partial^n \overline{w}}{\partial \xi^n}\right|_{\xi=-1} + \left.\frac{\partial^n w_*}{\partial \xi^n}\right|_{\xi=-1} = \left.\frac{\partial^n \overline{w}}{\partial \xi^n}\right|_{\xi=-1} + \frac{(-1)^n}{\eta^n\sqrt{\gamma^n}} w_*\big|_{\xi=-1} = 0\,, \tag{15}$$

where $n = 1,2,3$. Condition (15) ensures that contribution of the extraneous component is $O(\eta^n)$. It also makes it clear why $O(\eta^2)$ conditions (8b) are so much better at reproducing the exact solution of boundary value problem (1), (2), if compared to $O(\eta)$ conditions (8a). The correction term of higher-order model (7) is $O(\eta^2)$; it would therefore require boundary conditions with an error below $O(\eta^2)$ to achieve accuracy that may compete with the theory with modified inertia (i.e. (4) or (7) with $\gamma = 0$). Condition (15) satisfies this requirement when $n = 3$; thus, we propose our first variant of essential boundary conditions for (4) in the following dimensional form

$$u\big|_{x=\mp Nl} = f_{\mp N}\,, \quad l^3 \left.\frac{\partial^3 u}{\partial x^3}\right|_{x=\mp Nl} = 0\,. \tag{16}$$

Conditions (16) are simple and attractive, however, numerical tests reveal that the theory with modified inertia is still more accurate at higher frequencies. This can be rectified only when we reduce the error in boundary conditions below the model truncation error that is $O(\eta^4)$ for (7).

The accuracy may be improved if we choose to reformulate boundary conditions (15) is a slightly different manner. Specifically, let us seek

$$\left.\frac{\partial^n w}{\partial \xi^n}\right|_{\xi=-1} \equiv \left.\frac{\partial^n \overline{w}}{\partial \xi^n}\right|_{\xi=-1} + \frac{(-1)^n}{\eta^n \sqrt{\gamma^n}} w_*\big|_{\xi=-1} = P_n , \quad n = 1,2,3 , \tag{17}$$

with parameter P_n given by $P_n = (\partial^n \overline{w} / \partial \xi^n)_{\xi=-1}$. This suggests a two-step numerical scheme for solving (7). At the first step leading-order equation (11) is solved subject to (2), which gives $\overline{w}$ with $O(\eta^2)$ error. At the second step equation (7) is solved subject to (17) using $\overline{w}$ known from the first step. Corresponding dimensional boundary conditions for (4) have the form

$$u\big|_{x=\mp Nl} = f_{\mp N} , \quad l^n \left.\frac{\partial^n u}{\partial x^n}\right|_{x=\mp Nl} = l^n \left.\frac{\partial^n \overline{u}}{\partial x^n}\right|_{x=\mp Nl} , \tag{18}$$

where $n = 1,2,3$. These boundary conditions would result in $O(\eta^{n+2})$ error. The described technique is rather general and may be extended to higher-order governing equations, where it would require additional iteration steps, and non-scalar problems with, potentially, more complex boundary layers.

For some models it may also be possible to re-formulate boundary conditions (17) analytically. For example, if the additional condition is sought as

$$\left.\frac{\partial^2 w}{\partial \xi^2}\right|_{\xi=-1} \equiv \left.\frac{\partial^2 \overline{w}}{\partial \xi^2}\right|_{\xi=-1} + \frac{w_*\big|_{\xi=-1}}{\gamma \eta^2} = P_2 , \tag{19}$$

then we can use leading-order governing equation (11) together with condition (14) to conclude that the error is $O(\eta^4)$ provided $P_2 = -Q - c^2 F_{-1}$. In terms of the original dimensional variables this yields

$$u\big|_{x=\mp Nl} = f_{\mp N} , \quad l^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_{x=\mp Nl} = -l \frac{q}{K} - l\Omega^2 f_{\mp N} . \tag{20}$$

The efficiency of boundary conditions (20) is demonstrated in Fig. 4, where model (4) exhibits the accuracy comparable with the modified inertia theory used in Fig. 2(b). Similar numerical tests were also performed for boundary

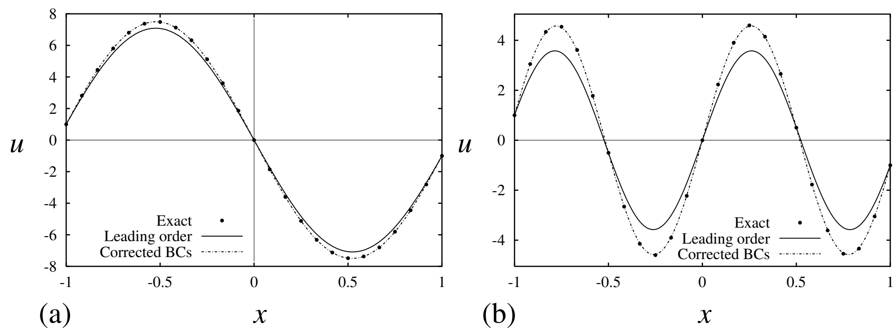

Figure 4. Configurations of the array of 25 particles using exact and asymptotic theories when $\Omega = 0.25$. Dots and thin solid line correspond to the exact solution and leading-order "rod" theory, respectively. Dotted line presents the response of the higher-order theory with $\gamma = 0.5$, $\alpha = -1/12$ and additional boundary conditions (20). (a) $\Omega = 0.25$. (b) $\Omega = 0.5$.

conditions (16) and (18). The asymptotic accuracy estimates presented in this paper seem to correlate well with the results of these computations.

4. CONCLUDING REMARKS

Presence of extraneous solutions, typical to higher-order theories, may significantly distort predictions of long-wave models considered on bounded domains. Thus, the formidable task of deriving additional boundary conditions ought to be perceived as an opportunity to eliminate the influence of these extraneous solutions. Considered model problem for a periodic lattice structure clearly demonstrates the benefits of the proposed approach.

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