Waves in Random and Complex Media
Vol. 20, No. 4, November 2010, 634–655

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Effective propagation in a one-dimensional perturbed periodic structure: comparison of several approaches

Agnès Maurel[a]*, P.A. Martin[b] and Vincent Pagneux[c]

[a]*Laboratoire Ondes et Acoustique, Institut Langevin, UMR CNRS 7587, Ecole Supérieure de Physique et de Chimie Industrielles, 10 rue Vauquelin, 75005 Paris, France;* [b]*Department of Mathematical and Computer Sciences, Colorado School of Mines, Golden, CO 80401, USA;* [c]*Laboratoire d'Acoustique de l'Université du Maine, UMR CNRS 6613, Avenue Olivier Messiaen, 72085 Le Mans Cedex 9, France*

(*Received 13 November 2009; final version received 5 May 2010*)

Acoustic scattering by an ensemble of scatterers whose positions are close to the positions of a periodic arrangement (with small and random perturbations in the position of each scatterer) is considered in one dimension. Three methods are compared to obtain the effective wavenumber of the coherent field. The first two methods, the quasi-crystalline approximation (QCA) and the coherent potential approximation (CPA), give the exact Floquet solution in the periodic case. However, in a perturbed almost periodic configuration, they give different dispersion relations. These methods are compared to a perturbation approach and confronted with the results obtained from direct numerical calculations. It is shown that CPA is able to get the first correction to the Floquet dispersion relation due to the introduced perturbation, in agreement with the perturbation approach and with direct numerical results, while QCA is unable to get this correction.

1. Introduction

The description of a multiple scattering medium in terms of an effective medium for the coherent part of the wave is attractive: instead of solving the whole problem, the medium is described in terms of an effective wavenumber K which depends on the parameters of the scatterers (typically, the density and the strength of the scatterers). In many cases, the effective wavenumber is derived perturbatively using a reference medium. When the reference medium is the medium free of scatterers, with k the wavenumber of free space, it is expected that $K \sim k$ or, in other words, the expression for K is expected to be valid for weak scattering effects. To reach strong scattering effects (thus K not close to k), the reference medium has to be changed, and a good candidate is a medium with a periodic set of scatterers.

*Corresponding author. Email: agnes.maurel@espci.fr

ISSN 1745–5030 print/ISSN 1745–5049 online
© 2010 Taylor & Francis
DOI: 10.1080/17455030.2010.494693
http://www.informaworld.com

In one dimension (1D), the dispersion relation gives the wavenumber Q of the Floquet mode ([1], equation (6)), ([2], equation (49.9))

$$\cos Qd = \cos kd + iM \sin kd, \tag{1}$$

for a wave satisfying the Helmholtz equation with point scatterers

$$u''(x) + k^2 u(x) = 2ikM \sum_n \delta(x - x_n) u(x). \tag{2}$$

Here, d is the spacing between scatterers ($x_n = nd$ in the periodic case) and M is the scattering strength. Equation (2) describes the propagation of a wave through scatterers at positions x_n (the wave is described by a continuous field u, the effects of the scatterers being encapsulated in the condition $u'(x_n^+) - u'(x_n^-) = 2ikMu(x_n)$). It represents, for instance, the propagation of waves through an acoustic duct with Helmholtz resonators [3] or the vibrations in beaded strings [4]. It can also be seen as the limit for small scatterers of size a having a contrast in the sound speed $\tilde{c}$ with respect to the sound speed c of the background medium: $M = -(i/2)(1 - \tilde{c}^2/c^2)ka$.

In this paper, we examine the possibility of describing a medium (hereafter referred to as the perturbed periodic medium) close to the periodic medium but where some randomness has been introduced. Unlike previous studies that focus on the phenomenon of localization [5,6], we are interested in the coherent (effective) waves that propagate in such a medium. These waves experience attenuation when they propagate, so they can be measured in practice for sufficiently small slabs (with respect to the localization length). This problem has applications to the design of electromagnetic devices using periodic structures (which are susceptible to some disorder in the periodic material) and has been studied experimentally [7,8].

In the present case, randomness is introduced into the position of the scatterers $x_n = (n + \epsilon_n)d$, where ϵ_n is the random variable (other sources of disorder have been considered in [6] and reference herein). Then, the perturbed periodic medium refers to the (effective) medium averaged over all realizations of randomness. Here, this means the medium averaged over all ϵ_n values, with $|\epsilon_n| \leq \epsilon/2$. A similar configuration has been considered in [9] with perturbations in the scatterer positions except for one scatterer $x_n = x_p + (n + \epsilon_n)d$, x_p at a fixed position (see also [10] in two dimensions). Two methods are studied: the quasi-crystalline approximation (hereafter referred to as QCA) due to Lax [11,12] and the coherent potential approximation (hereafter referred to as CPA) [13]. Both the QCA and the CPA are simple to use, and both have been used widely in the literature on waves in random media (see for instance, a comparison of the two methods in a Green function formalism for 1D uncorrelated point scatterers in [14]). However, both are difficult to justify mathematically. The QCA introduces a certain closure assumption into an infinite hierarchy of equations. The CPA starts from the physical argument that a cell embedded in the effective medium should be transparent (in terms of acoustical properties) if it satisfies statistically the same properties as the effective medium.

Compared to these two empirical methods, some deductive methods are available. The Dyson approach gives a formal exact solution for the effective propagation. However, it is much more involved and, usually, the exact solution is

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

not possible. Another possible approach has been proposed by Parnell and Abrahams [4,15] in the form of an expansion of the solution in the small parameters ϵ_n. We use this expansion as the reference calculation to compare with the QCA and CPA results. Our conclusion is that the CPA dispersion relation agrees with the perturbation expansion result whereas the QCA result does not. Namely, we find the following dispersion relations for the effective wavenumber K

$$\cos Kd = \cos Qd + \frac{M^2}{2(1-M)}\, e^{ikd}\big(1 - \mathrm{sinc}^2 \epsilon kd\big), \quad \text{using QCA}, \tag{3}$$

$$\cos Kd = \cos Qd + \frac{M^2}{2}\, e^{iKd}\big(1 - \mathrm{sinc}^2 \epsilon kd\big), \quad \text{using CPA}, \tag{4}$$

with sinc $x \equiv \sin x/x$. The validity of CPA and of the perturbation calculation is confirmed using direct numerical calculations.

The paper is organized as follows. In Section 2, direct numerical calculations of the effective wave propagating in a perturbed periodic medium are presented and three illustrative examples are given, in terms of the effective wave behaviors and in terms of the dispersion relations when varying the deviation from the periodic situation (i.e. the parameter ϵ). Section 3 presents the derivation of the exact solution for a row of periodic point scatterers; the result is shown to be correctly recovered by using QCA and CPA approaches with $\epsilon_n = 0$ (Section 4). There is a pedagogic interest in explaining the ideas behind the QCA and CPA derivations in the (simpler) periodic case, ideas that are then adapted in Section 5 to the more involved case of the perturbed periodic configuration. Then, we present the perturbation approach, where an expansion in the small deviations ϵ_n with respect to the periodic situation is used. The obtained result in ϵ^2 to leading order agrees with the CPA result, not with the QCA result. Section 6 ends the paper by confronting the dispersion relations given by QCA and CPA with the dispersion relations obtained from direct numerical calculations. This confirms that CPA gives the first correction in the dispersion relation due to the considered deviation (correction in ϵ^2) while QCA is unable to do that. Technical calculations are collected in four appendices. In the paper, the assumed time dependence is $e^{-i\omega t}$.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

2. Numerical results

Direct numerical calculations of the exact wavefield $u(x)$ with N scatterers are performed. Then, $\langle u\rangle(x)$ is deduced by averaging the fields $u(x)$ calculated for N_r realizations of the disordered configurations. A configuration consists of N scatterers $x_n = (n-1+\epsilon_n)d$, $n = 1, \dots, N$, each ϵ_n being randomly chosen with $|\epsilon_n| < \epsilon/2$. All the scatterers have the same scattering strength M. We consider an incident wave coming from the left, $u(x) = e^{ikx}$. At each scatterer, we apply $[u]_{x_n} = 0$ and $[u']_{x_n} = 2ikMu(x_n)$. For $x_{n-1} \le x \le x_n$, the wavefield can be written

$$u(x) = a_n\big[e^{ik(x-x_n)} + Z_n e^{-ik(x-x_n)}\big]. \tag{5}$$

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

To account for the radiation condition after the Nth scatterer, a ghost scatterer is added at $x_{N+1} = x_N$ with $Z_{N+1} = 0$. Then, the conditions $[u]_{x_n} = 0$ and $[u']_{x_n} = 2ikMu(x_n)$ give a recurrence relation for Z_n,

$$Z_n = \frac{Me^{-i\varphi_n} + Z_{n+1}(1+M)e^{i\varphi_n}}{(1-M)e^{-i\varphi_n} - Z_{n+1}Me^{i\varphi_n}}, \tag{6}$$

with $\varphi_n \equiv k(x_{n+1} - x_n)$. Once (Z_n) has been computed, the amplitudes (a_n) are derived starting from $a_1 = e^{ikx_1}$ and using the recurrence

$$a_{n+1} = (MZ_n + 1 + M)e^{i\varphi_n} a_n. \tag{7}$$

The N_r wavefields are averaged to produce the effective wavefield $\langle u \rangle(x)$. Because the scatterers are embedded in a slab, we use the ansatz

$$\langle u \rangle(x) = Tf_\epsilon(x)e^{iKx} + Rg_\epsilon(x)e^{-iKx}, \tag{8}$$

where f_ϵ and g_ϵ are two d-periodic functions and (T, R) are the transmission and reflection coefficients at the entrance and exit of the slab. For the sake of simplicity, we choose configurations in the forbidden bandgap (Q purely imaginary). In that case, the right-going wave is evanescent. For a sufficiently large slab, this wave has decreased in amplitude sufficiently so that its reflection at the end of the slab can be neglected and we can consider $u(x) \simeq T\, f_\epsilon(x)e^{iKx}$. The field $\langle u \rangle(nd) \propto e^{iKnd}$ is used to deduce $K(\epsilon)$.

Figure 1 shows the results for different values of M and kd. For non-zero ϵ, between 10^4 and 10^5 realizations have been performed and averaged to obtain the effective, or coherent, field. In each realization, random values of ϵ_n were used.

In the three cases shown, the periodic medium ($\epsilon = 0$) corresponds to a Floquet wavenumber Q that is purely imaginary. Let us comment on the first curve at the top of (a): with a purely imaginary Floquet wavenumber Q, the field $u(nd) \propto e^{iQnd}$ (in black) is exponentially decreasing. In addition in this case, the wavelength being smaller than the space between the scatterers ($kd = 14.2\pi$), we observe the wave $u(x)$ made of left- and right-going waves propagating between two scatterers (in gray), with $e^{\pm ikx}$ dependencies (two scatterers are separated by free space). When the wavelength is decreased (from (a) to (c), where $kd \sim 1$) these waves are no longer visible.

Introducing disorder produces a change in $u(nd)$, with $Q \to K$. K experiences a decrease in the attenuation (imaginary part) and may acquire a real part. Finally, in the first case, the attenuation is not too strong so that the attenuation of the wave occurs over a significant length (50–100 scatterers). Increasing the M-value (as from case (a) to (b)) produces an increase in the attenuation.

The figures at the bottom of Figure 1 show the K-value deduced from the curves at the top (owing to $u(nd) \propto e^{iKnd}$). As will be seen in Section 6, the prediction of the effective wavenumber K applies for small deviation ϵ with respect to the periodic case. This implies that K remains close to Q; when the change becomes significant, this no longer holds (in (a) for $\epsilon \sim 10^{-2}$, in (b) for $\epsilon \sim 10^{-0.5}$).

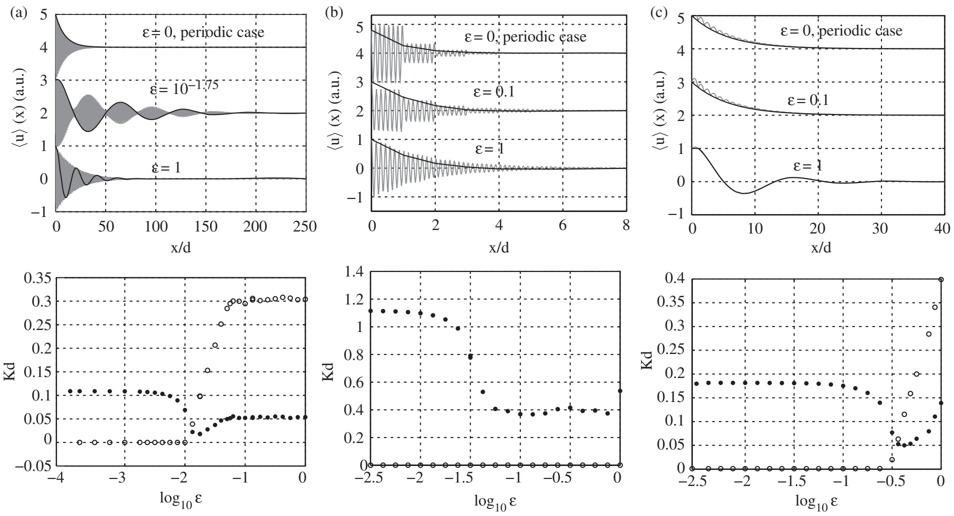

Figure 1. Top panels: mean field $\langle u\rangle(x)$ in gray line for different ϵ-value. In black line, $\langle u\rangle(nd)\propto e^{iKnd}$, used to determined the K-value. Bottom panels: effective wavenumber Kd as a function of ϵ (open circles show the real part of K and solid circles show the imaginary part of K). (a) $kd=14.2\pi$ and $M=0.67/(2i)$, (b) $kd=14.2\pi$ and $M=3/(2i)$, (c) $kd=2\pi/5.1$ and $M=1.45/(2i)$.

3. Periodic row of identical scatterers: exact results

In this section, we briefly recall some known exact results for waves through a periodic row of identical, finite-width scatterers. Suppose that at each point $x=nd$, $n\in\mathbb{Z}$, there is a scatterer of width $2b<d$. Between the scatterers, $u''+k^2u=0$. Concentrating on the scatterer at $x=0$, we can write

$$u(x)=\begin{cases} a_1e^{ikx}+b_1e^{-ikx}, & -d+b<x<-b,\\ a_2\,e^{ikx}+b_2e^{-ikx}, & b<x<d-b,\end{cases}$$

where the coefficients a_1 and a_2 give the amplitudes of the waves going to the right and the coefficients b_1 and b_2 give the amplitudes of the waves going to the left.

To characterize the scattering, introduce the reflection coefficient r_0 and the transmission coefficient t_0 for the scatterer at $x=0$. We assume that r_0 and t_0 are independent of the direction of the incident wave: the scatterer is symmetric. Thus, for an incident wave e^{ikx} and a single scatterer at the origin, the total field is $e^{ikx}+r_0e^{-ikx}$ to the left of the scatterer and it is t_0e^{ikx} to the right. Hence,

$$b_1=r_0a_1+t_0b_2 \quad\text{and}\quad a_2=r_0b_2+t_0a_1. \tag{9}$$

We seek solutions satisfying the Bloch condition,

$$u(x+d)=u(x)e^{iQd}. \tag{10}$$

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

This condition implies that

$$b_2 = b_1 e^{i(Q+k)d} \quad \text{and} \quad a_2 = a_1 e^{i(Q-k)d}. \tag{11}$$

Equations (9) and (11) will have a non-trivial solution provided

$$\cos Qd = \mathcal{A} \cos kd + \mathcal{B} \sin kd, \tag{12}$$

where

$$\mathcal{A} = \frac{1}{2t_0}(t_0^2 - r_0^2 + 1) \quad \text{and} \quad \mathcal{B} = \frac{i}{2t_0}(t_0^2 - r_0^2 - 1). \tag{13}$$

This result is general: to use it, we merely insert the appropriate reflection and transmission coefficients. Notice that $\mathcal{A}$ and $\mathcal{B}$ depend on the scattering properties of a single scatterer.

In the rest of the paper, we consider point scatterers. For this problem, we have two possible, exact, formulations. One is in terms of a scattering coefficient g,

$$u(x) = u^0(x) + g \sum_n e^{ik|x-x_n|} u^e(x_n), \tag{14}$$

$$u^e(x_n) = u^0(x_n) + g \sum_{m \neq n} e^{ik|x_n - x_m|} u^e(x_m), \tag{15}$$

where x_n are the locations of the scatterers and $u^0(x)$ denotes the incident wave.

The second formulation is in terms of potentials (see Equation (2)),

$$u(x) = u^0(x) + 2ikM \sum_n G^0(x - x_n) u(x_n), \tag{16}$$

where $G^0(x) = e^{ik|x|}/(2ik)$. The two formulations are equivalent in 1D owing to $Mu(x_n) = gu^e(x_n)$ and the relation between M and g can be found easily by considering a single scatterer: $g = M/(1-M)$, $M = g/(1+g)$. The reflection and transmission coefficients for a point scatterer at the origin are given by

$$r_0 = g = M/(1-M) \quad \text{and} \quad t_0 = 1 + g = 1/(1-M). \tag{17}$$

Substituting from Equation (17) in Equations (12) and (13) gives the (known) dispersion relation, Equation (1).

If energy is conserved, $\operatorname{Re} g + |g|^2 = 0$ whence $g = ie^{i\varphi} \sin \varphi$ for some real φ, $M = i \tan \varphi$ implying that M is purely imaginary, and Equation (1) reduces to

$$\cos Qd \cos \varphi = \cos (kd + \varphi). \tag{18}$$

Thus, if we assume that Q is real, then k will be real. Alternatively, if we assume that k is real, then Q could be real (pass band) or imaginary (stop band).

4. Rederiving perfectly periodic results using QCA and CPA

In this section, we show that both QCA and CPA do lead to the known exact dispersion relation when specialized to a periodic row of identical point scatterers.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

4.1. *QCA approach*

The QCA approach consists of a closure assumption on the hierarchy of averaged equations coming from Equation (15). Thus, for N scatterers,

$$\langle u\rangle(x) = u^0(x) + Ng\int \mathrm{d}x_1\; p(x_1)e^{ik|x-x_1|}\langle u^e\rangle_1(x_1), \tag{19}$$

$$\langle u^e\rangle_1(x_1) = u^0(x_1) + (N-1)\,g\int \mathrm{d}x_2\; p(x_2|x_1)e^{ik|x_1-x_2|}\langle u^e\rangle_2(x_2), \tag{20}$$

where

$$\langle u^e\rangle_1(x_1) \equiv \int \mathrm{d}x_2\ldots\mathrm{d}x_N\; p(x_2,\,\ldots,x_N|x_1)u^e(x_1),$$
$$\langle u^e\rangle_2(x_2) \equiv \int \mathrm{d}x_3\ldots\mathrm{d}x_N\; p(x_3,\,\ldots,x_N|x_1,x_2)u^e(x_2).$$

The QCA closure assumption is simply $\langle u^e\rangle_1 = \langle u^e\rangle_2$ leading to

$$\langle u\rangle(x) = u^0(x) + Ng\int \mathrm{d}x_1\; p(x_1)e^{ik|x-x_1|}\langle u^e\rangle(x_1), \tag{21}$$

$$\langle u^e\rangle(x_1) = u^0(x_1) + (N-1)\,g\int \mathrm{d}x_2\; p(x_2|x_1)e^{ik|x_1-x_2|}\langle u^e\rangle(x_2). \tag{22}$$

In the periodic case, we can take $p(x) = N^{-1}\sum_n \delta(x-nd)$ and

$$p(x_2|x_1) = \frac{1}{N-1}\sum_{m\neq n}\delta(x_2-md), \quad x_1 = nd. \tag{23}$$

Then, in the limit $N\to\infty$, Equations (21) and (22) give

$$\langle u\rangle(nd) = u^0(nd) + g\sum_m e^{ik|n-m|d}\langle u^e\rangle(md), \tag{24}$$

$$\langle u^e\rangle(nd) = u^0(nd) + g\sum_{m\neq n} e^{ik|n-m|d}\langle u^e\rangle(md). \tag{25}$$

These equations agree with (the deterministic) Equations (14) and (15) with $\langle u\rangle = u$, $\langle u^e\rangle = u^e$ and $x_n = nd$, from which we deduce that QCA is exact when considering the periodic case. This is because, for periodic scatterers, the positions of all scatterers are known as soon as the position of one scatterer is known. We give in Appendix 1 the derivation of the dispersion relation for the Floquet mode and the derivations of the functions f_0 and g_0 when solutions are sought in the form

$$u(x) = g_0(y)e^{iQx} + f_0(y)e^{-iQx}, \quad x = nd + y, \quad 0 \le y < d, \tag{26}$$

where f_0 and g_0 are d-periodic. We indicate here the main results (for details, see Appendix 1). The wavenumber Q is given by the dispersion relation,

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Equation (1),

$$g_0(y) = Ae^{i(k-Q)y} + Be^{-i(k+Q)y} \quad \text{and} \quad f_0(y) = g_0(d-y), \tag{27}$$

with $A=(1-e^{i(k-Q)d})^{-1}$ and $B=(e^{-i(k+Q)d}-1)^{-1}$. This solution is exact, since it corresponds to the solution of Equation (15): in the periodic case, the QCA closure is not an assumption.

4.2. *CPA approach*

In this case, we consider the cell $[(n-1)d+z, nd+z]$ embedded in the effective periodic medium (Figure 2). Usually, the cell is assumed to contain a scatterer located at its periodic position ($\epsilon_n=0$ in Figure 2), in which case the cell is equivalent to the effective medium and it is transparent for the incident wave coming from the left, say, in the effective medium. No reflection or transmission can occur. Here, we present a more involved calculation with $\epsilon_n \neq 0$. Although it is overly complicated for the resolution of the periodic case, we present it because it is similar to the one used later in the perturbed periodic case.

In our calculation, the cell embedded in the periodic medium contains one scatterer at $x_n=(n+\epsilon_n)d$ (Figure 2). The host periodic medium has right-going waves propagating as $g_0(y)e^{iQx}$ and left-going waves propagating with $f_0(y)e^{-iQx}$, where $x=y+md$ with integer m and $0 \leq y < d$. The position of the interfaces between the host medium and the cell can be set at $(n-1)d+z$ and $nd+z$. The parameter z can vary in the interval $\epsilon_n d < z < d-\epsilon_n d$: the interfaces can move leaving the problem under consideration unchanged. This is because the host medium has a part made of free space (all space apart from the scatterers). When ϵ_n is non-zero, reflection and

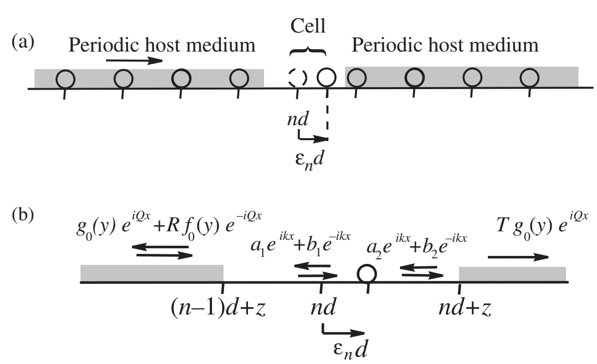

Figure 2. Configuration considered in the CPA approach. (a) A cell is considered, embedded in the periodic medium. (b) Enlargement of the cell and its boundaries. If the scatterer, at $x=nd$ when located at its periodic position, is shifted to $x=(n+\epsilon_n)d$, reflection and transmission by the cell are expected. When the cell satisfies the same properties as the host medium (here, periodic, so $\epsilon_n=0$), it is transparent for the incident wave, $R(0)=0$, $T(0)=1$.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

transmission at the interfaces are expected. Thus, we write

$$v(x)=\begin{cases} g_0(y)e^{iQx}+R(\epsilon_n)f_0(y)e^{-iQx}, & x<(n-1)d+z,\\ a_1e^{ikx}+b_1e^{-ikx}, & (n-1)d+z\le x<(n+\epsilon_n)d,\\ a_2e^{ikx}+b_2e^{-ikx}, & (n+\epsilon_n)d\le x<nd+z,\\ T(\epsilon_n)\,g_0(y)e^{iQx}, & x\ge nd+z. \end{cases} \tag{28}$$

The functions f_0 and g_0 are d-periodic and they do not depend on ϵ_n. The field v and its first derivative are continuous at the boundaries of the cell, $x=(n-1)d+z$ and $x=nd+z$. These conditions give

$$a_1=Ae^{i(Q-k)(n-1)d}+DRe^{-i(Q+k)(n-1)d},\quad b_1=Be^{i(Q+k)(n-1)d}+CRe^{i(k-Q)(n-1)d}, \tag{29}$$

$$a_2=ATe^{i(Q-k)nd},\quad b_2=BTe^{i(Q+k)nd}, \tag{30}$$

where A, B, C and D depend on the functions f_0 and g_0 and their first derivatives:

$$\begin{aligned} A&=[g_0'(z)+i(Q+k)\,g_0(z)]e^{i(Q-k)z}/(2ik),\\ B&=-[g_0'(z)+i(Q-k)\,g_0(z)]e^{i(Q+k)z}/(2ik),\\ C&=-[f_0'(z)-i(Q+k)f_0(z)]e^{i(k-Q)z}/(2ik),\\ D&=[f_0'(z)+i(k-Q)f_0(z)]e^{-i(k+Q)z}/(2ik). \end{aligned}$$

As previously noted, the position of the interfaces, given by z, can be changed without changing the problem. Thus, a_1, a_2, b_1 and b_2 do not depend on z, which implies that A, B, C and D do not depend on z. It follows that g_0 and f_0 have the forms given in Equation (27). These forms also ensure that $g_0(z)e^{iQz}$ and $f_0(z)e^{-iQz}$ satisfy the Helmholtz equation.

At the scatterer position $x_n=(n+\epsilon_n)d$, v satisfies $v(x_n^-)=v(x_n^+)$ and $v'(x_n^+)-v'(x_n^-)=2ikMv(x_n)$. These conditions give

$$a_1=Te^{i(Q-k)nd}\big[(1-M)A-MBe^{-2i\epsilon_nkd}\big], \tag{31}$$

$$b_1=Te^{i(Q+k)nd}\big[MAe^{2i\epsilon_nkd}+(1+M)B\big], \tag{32}$$

using the formulas for a_2 and b_2, Equation (30). Equating the two expressions for a_1 and those for b_1 in Equations (29) and (31), (32) gives

$$\big[1-M-M\mathcal{B}e^{-2i\epsilon_nkd}\big]T(\epsilon_n)-\mathcal{B}e^{-2iQnd}R(\epsilon_n)=e^{i(k-Q)d}, \tag{33}$$

$$\big[Me^{2i\epsilon_nkd}+(1+M)\mathcal{B}\big]T(\epsilon_n)-e^{-2iQnd}R(\epsilon_n)=\mathcal{B}e^{-i(k+Q)d}, \tag{34}$$

where $\mathcal{B}\equiv B/A$. This system of equations has four unknowns, R, T, $\mathcal{B}$ and Q. Note that only R and T depend on ϵ_n since Q and $\mathcal{B}$ characterize the wave propagation in the periodic (host) medium. We solve Equations (33) and (34) by applying the CPA idea: when $\epsilon_n=0$, the cell satisfies the same properties as the host (periodic) medium

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

and therefore it has to be transparent,

$$T(\epsilon_n = 0) = 1, \quad R(\epsilon_n = 0) = 0. \tag{35}$$

Hence, we obtain

$$M\mathcal{B} = 1 - M - e^{i(k-Q)d}, \quad M + [1 + M - e^{-i(k+Q)d}]\mathcal{B} = 0; \tag{36}$$

eliminating $\mathcal{B}$ then gives the dispersion relation for the Floquet mode, Equation (1), as the condition of solvability. We also find that $\mathcal{B} = B/A$ satisfies

$$1 - e^{i(k-Q)d} + \mathcal{B}\left[1 - e^{-i(k+Q)d}\right] = 0. \tag{37}$$

Then, having found Q and $\mathcal{B}$, we can determine R and T from Equations (33) and (34); for example, we obtain

$$T(\epsilon_n) = \left[1 + iM^2 \frac{e^{iQd}}{\sin Qd}(1 - \cos(2\epsilon_n kd))\right]^{-1} \simeq 1 - 2i\epsilon_n^2 \frac{M^2(kd)^2 e^{iQd}}{\sin Qd} \tag{38}$$

for small ϵ_n. This will be used later.

In conclusion, both the CPA and QCA approaches are able to find the solution for the periodic case, namely the expression of the Floquet wavenumber Q in Equation (1) and the form of the functions $g_0(y)$ and $f_0(y)$ in Equation (27) that characterize the wavefield in the periodic structure.

5. Small deviation in the positions of the scatterers with respect to the periodic case

We apply now the same approaches, QCA and CPA, when the scatterers have small deviations with respect to the periodic configuration, $x_n = (n + \epsilon_n)d$. The effective medium to be characterized corresponds to the average over all realizations of the ϵ_n-values.

5.1. *QCA approach*

The same procedures as in the periodic case may be applied. Define $\Pi_{\epsilon d}(x)$ by

$$\Pi_{\epsilon d}(x) = \begin{cases} 1, & |x| \le \epsilon d/2, \\ 0, & |x| > \epsilon d/2. \end{cases} \tag{39}$$

We take

$$p(x) = \frac{1}{N\epsilon d} \sum_m \Pi_{\epsilon d}(x - md) \tag{40}$$

and

$$p(x_2|x_1) = \frac{1}{(N-1)\epsilon d} \sum_{m \neq n} \Pi_{\epsilon d}(x_2 - md), \quad |x_1 - nd| < \epsilon d/2. \tag{41}$$

As in Section 4.1, start with a doubly-infinite row of scatterers and no incident wave. Then, letting $N \to \infty$ in Equations (21) and (22) gives

$$\langle u \rangle(x) = \frac{g}{\epsilon d} \sum_m \int_{I_m} e^{ik|x-x_1|} \langle u^e \rangle(x_1)\,\mathrm{d}x_1, \tag{42}$$

$$\langle u^e \rangle(x_1) = \frac{g}{\epsilon d} \sum_{m \neq n} \int_{I_m} e^{ik|x_1-x_2|} \langle u^e \rangle(x_2)\,\mathrm{d}x_2, \quad x_1 \in I_n, \tag{43}$$

where I_n is the interval $nd - \epsilon d/2 < x < nd + \epsilon d/2$.

Equation (42) shows that $\langle u \rangle''(x) + k^2 \langle u \rangle(x) = 0$ for $x \notin I_n$, $n \in \mathbb{Z}$, suggesting that the average field $\langle u \rangle$ solves a certain periodic problem, as might be expected. Equation (43) shows that $\langle u^e \rangle''(x) + k^2 \langle u^e \rangle(x) = 0$ for $x \in I_n$, $n \in \mathbb{Z}$. So, write

$$\langle u^e \rangle(x) = a_n e^{ikx} + b_n e^{-ikx}, \quad x \in I_n. \tag{44}$$

Substituting in Equation (43) and equating coefficients of $e^{\pm ikx_1}$ gives

$$a_n = g \sum_{m=-\infty}^{n-1} \left(a_m + b_m \mathcal{S} e^{-2imkd}\right), \quad b_n = g \sum_{m=n+1}^{\infty} \left(b_m + a_m \mathcal{S} e^{2imkd}\right),$$

where $\mathcal{S} = \operatorname{sinc}(k\epsilon d)$. Looking for a solution of these equations in the form

$$a_n = \mathcal{C} e^{i(K-k)nd}, \quad b_n = \mathcal{D} e^{i(K+k)nd}, \tag{45}$$

we find that the constants $\mathcal{C}$ and $\mathcal{D}$ satisfy

$$\mathcal{C} = g(\mathcal{C} + \mathcal{D}\mathcal{S}) \sum_{m=1}^{\infty} e^{i(k-K)md}, \quad \mathcal{D} = g(\mathcal{D} + \mathcal{C}\mathcal{S}) \sum_{m=1}^{\infty} e^{i(k+K)md}.$$

These bear comparison with Equation (64); under the same conditions, we sum the infinite series and then put the resulting 2×2 determinant equal to zero, giving

$$\cos Kd = \mathcal{A}_\epsilon \cos kd + \mathcal{B}_\epsilon \sin kd, \tag{46}$$

where

$$\mathcal{A}_\epsilon = 1 + \frac{g^2 \Phi(k\epsilon d)}{2(1+g)} \quad \text{and} \quad \mathcal{B}_\epsilon = \frac{ig}{1+g}\left[1 + \frac{1}{2} g \Phi(k\epsilon d)\right],$$

with $\Phi(x) = 1 - \operatorname{sinc}^2 x$. Making use of the dispersion relation for the Floquet mode, Equation (65), we can write Equation (46) as Equation (3). The same result is obtained by considering an incident wave and a semi-infinite row of scatterers, as in Section 4.1, a configuration that avoids the divergent sum appearing in $\mathcal{C}$ (see Appendix 2 for details). It can also be obtained using a heuristic argument in which it is assumed that the effective medium is periodic with a row of identical average scatterers (see Appendix 3 for details).

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

5.2. *CPA approach*

For the CPA approach, it is sufficient to consider the host medium as the effective perturbed periodic medium instead of the periodic medium considered in Section 4.2. Thus, the form of the solution in Equation (28) still holds with $g_0 \to g_\epsilon$, $f_0 \to f_\epsilon$, $Q \to K$, $R \to R_\epsilon$ and $T \to T_\epsilon$. This means that we still consider a cell containing one scatterer, the cell being embedded in the effective medium. But here, the effective medium corresponds to the average over all realizations of the scatterers with $(p - \frac{1}{2}\epsilon)d \le x_p \le (p + \frac{1}{2}\epsilon)d$, for all integers p, except the nth scatterer inside the isolated cell. Apart from the nature of the host effective medium (which is encapsulated in K and in the functions f_ϵ and g_ϵ), the problem to solve is exactly the same as in the periodic case until the CPA idea is applied. Thus, we recover the same system as Equations (33) and (34), rewritten here for clarity

$$\left[(1 - M)A_\epsilon - MB_\epsilon e^{-2i\epsilon_n kd}\right]T_\epsilon(\epsilon_n) - B_\epsilon e^{-2iKnd}R_\epsilon(\epsilon_n) = A_\epsilon e^{i(k-K)d}, \tag{47}$$

$$\left[MA_\epsilon e^{2i\epsilon_n kd} + (1 + M)B_\epsilon\right]T_\epsilon(\epsilon_n) - A_\epsilon e^{-2iKnd}R_\epsilon(\epsilon_n) = B_\epsilon e^{-i(k+K)d}. \tag{48}$$

The functions g_ϵ and f_ϵ have the forms in Equation (27),

$$g_\epsilon(y) = A_\epsilon e^{i(k-K)y} + B_\epsilon e^{-i(k+K)y}, \quad f_\epsilon(y) = g_\epsilon(d - y), \tag{49}$$

using the same argument that the positions of the boundaries between the effective medium and the cell must leave the problem unchanged.

As in Section 4.2, we need more information to solve our system. We achieve this by adapting the CPA idea from the case of a periodic host medium to the case of an effective medium with (averaged) perturbed periodic positions. We argue that the cell will be transparent with respect to the perturbed periodic effective medium if an average over all possible positions of the scatterer inside the cell is performed. This leads to the conditions

$$\langle T_\epsilon \rangle = 1, \quad \langle R_\epsilon \rangle = 0, \tag{50}$$

where the average means $\epsilon^{-1}\int_{-\epsilon/2}^{\epsilon/2} \mathrm{d}\epsilon_n$. We use Equation (50) directly on Equations (47) and (48), and so we need $\langle e^{\pm 2ikd\epsilon_n} T_\epsilon(\epsilon_n)\rangle$.

Eliminating $R_\epsilon(\epsilon_n)$ from Equations (47) and (48) shows that $T_\epsilon(\epsilon_n)$ is an even function of ϵ_n. So, a Taylor expansion gives

$$T_\epsilon(\epsilon_n) = c_0 + c_1\epsilon + c_{21}\epsilon_n^2 + c_{22}\epsilon^2 + c_{31}\epsilon\epsilon_n^2 + c_{32}\epsilon^3 + O(\epsilon^4, \epsilon_n^2\epsilon^2, \epsilon_n^4).$$

The periodic case is $T_0(\epsilon_n)$, given by Equation (38). This gives $c_0 = 1$ and c_{21}. Then,

$$\langle T_\epsilon \rangle = 1 + c_1\epsilon + \epsilon^2(c_{22} + c_{21}/12) + \epsilon^3(c_{32} + c_{31}/12) + O(\epsilon^4),$$

which gives $c_1 = 0$, $c_{22} + c_{21}/12 = 0$ and $c_{32} + c_{31}/12 = 0$. Hence,

$$T_\epsilon(\epsilon_n) = 1 + c_{21}\left(\epsilon_n^2 - \frac{\epsilon^2}{12}\right) + c_{31}\epsilon\left(\epsilon_n^2 - \frac{\epsilon^2}{12}\right) + O(\epsilon^4, \epsilon_n^2\epsilon^2, \epsilon_n^4),$$

and $\langle e^{\pm 2ikd\epsilon_n} T_\epsilon(\epsilon_n)\rangle = \mathcal{S} + O(\epsilon^4)$, where $\mathcal{S} = \text{sinc}(kd\epsilon)$. Hence, taking the average of the system (47) and (48) gives

$$(1 - M - e^{i(k-K)d})A_\epsilon - M\mathcal{S}B_\epsilon = 0,$$
$$M\mathcal{S}A_\epsilon + (1 + M - e^{-i(k+K)d})B_\epsilon = 0.$$

We get the dispersion relation from the condition of solvability

$$\cos Kd = \cos Qd + \frac{1}{2}M^2 e^{iKd}\big(1 - \text{sinc}^2(\epsilon kd)\big), \tag{51}$$

which is Equation (4). We can also calculate A_ϵ/B_ϵ from Equation (47) or Equation (48).

5.3. *Perturbation method*

This method has been developed in [4,15]. Here, we use a modified version.

We consider a semi-infinite row of scatterers, with locations $x_m = md + \epsilon_{md}$, where $m = 1, 2, \ldots$ and $|\epsilon_m| \le \epsilon/2$. A plane wave, e^{ikx}, is incident from the left. The field $v_\epsilon(x; \boldsymbol{\epsilon})$ describes the wave propagating through the scatterers; the vector $\boldsymbol{\epsilon} = (\epsilon_1, \epsilon_2, \ldots)$ (Figure 3(a)). The idea is to write the field $v_\epsilon(x; \boldsymbol{\epsilon})$ as a perturbation around the field $v_0(x) = v_\epsilon(x; \mathbf{0})$, regarding $\boldsymbol{\epsilon}$ as the small parameter. Evidently, $v_0(x)$ corresponds to the periodic situation (which we considered in Section 4.1). Taking the average of the perturbation expansion makes one quantity appear that we are looking for, namely, the effective field $\langle v_\epsilon\rangle(x)$. In addition, we find averages of fields $u(x, \epsilon_n)$: each field $u(x, \epsilon_n)$ corresponds to the situation of Figure 3(b), where all scatterers are located at their periodic positions except the nth scatterer at $x_n = (n + \epsilon_n)d$.

If we had started with an infinite row of scatterers along the whole x-axis (as in Figure 2), the field $u(x, \epsilon_n)$ would correspond to the solution found in Section 5.2.

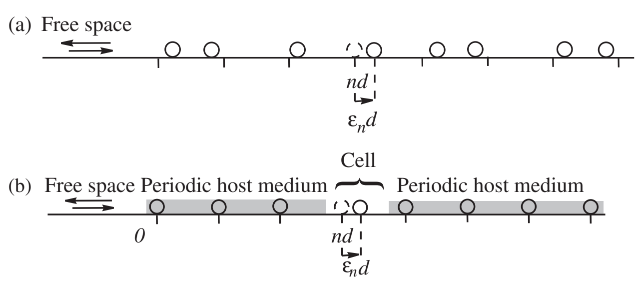

Figure 3. (a) Configuration of interest: the scatterers occupy the half-space $x > 0$ and all have a deviation $\epsilon_n d$ with respect to the periodic positions. The wavefield is $v_\epsilon(x; \boldsymbol{\epsilon})$. Averaging $v_\epsilon(x; \boldsymbol{\epsilon})$ over all realizations of the ϵ_n values leads to the effective medium in $x > 0$. (b) Intermediate configuration needed in the calculation: all scatterers are in their periodic positions (periodic host medium) except the nth scatterer at $x_n = (n + \epsilon_n)d$. The wavefield is $u(x; \epsilon_n)$.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Here, we consider a different configuration, where the host periodic medium and the embedded cell occupy only the half-space $x>0$, and we consider an incident wave, e^{ikx}, coming from the free-space region, $x<0$. We prefer this configuration because it avoids divergent sums that would appear otherwise, a difficulty already encountered in Section 4.1. As the problem of Figure 3(b) is more involved, for simplicity, only those parts of the solution that are useful are given in the following.

We write v_ϵ as a perturbation around v_0, the field of the Floquet mode,

$$v_\epsilon(x,\boldsymbol{\epsilon}) = v_0(x) + \sum_m \epsilon_m \frac{\partial v_\epsilon}{\partial \epsilon_m}(x,\mathbf{0}) + \frac{1}{2}\sum_{m,n}\epsilon_m\epsilon_n \frac{\partial^2 v_\epsilon}{\partial\epsilon_m\partial\epsilon_n}(x,\mathbf{0}) + O(\epsilon^3). \tag{52}$$

This equation holds where $v_\epsilon(x,\boldsymbol{\epsilon})$ has continuous derivatives, that is outside the scatterer positions. The system is now averaged. Starting with N scatterers (the limit $N\to\infty$ will be taken shortly), define

$$\langle v_\epsilon\rangle(x) = \frac{1}{\epsilon^N}\int_{-\epsilon/2}^{\epsilon/2}\cdots\int_{-\epsilon/2}^{\epsilon/2} \mathrm{d}\epsilon_1\cdots \mathrm{d}\epsilon_N v_\epsilon(x,\boldsymbol{\epsilon}). \tag{53}$$

As the nth scatterer occupies the interval I_n (defined below Equation (43)), we choose x outside all such intervals; specifically, we choose x between I_{n_0} and I_{n_0+1} so that $(n_0+\epsilon/2)d<x<(n_0+1-\epsilon/2)d$ and all derivatives are continuous there. As $\langle\epsilon_n\rangle=0$, we get

$$\langle v_\epsilon\rangle(x) = v_0(x) + \frac{1}{2}\langle\epsilon_n^2\rangle\sum_n \frac{\partial^2 v_\epsilon}{\partial\epsilon_n^2}(x,\mathbf{0}) + O(\epsilon^4). \tag{54}$$

In the right-hand side term, the second derivative involves the field $u(x,\epsilon_n) = v_\epsilon(x,\boldsymbol{\epsilon}'_n)$ (where $\boldsymbol{\epsilon}'_n = (0,\ldots,0,\epsilon_n,0,\ldots)$ is a vector of zeros apart from one entry) in the sense that the two fields have the same second derivative,

$$\frac{\partial^2 u_n(x,0)}{\partial\epsilon_n^2} = \frac{\partial^2 v_\epsilon(x,\mathbf{0})}{\partial\epsilon_n^2}. \tag{55}$$

The field u_n describes the wave propagating through a set of scatterers periodically spaced except for the nth scatterer (Figure 3(b)). This field can be found in a separate calculation; see Appendix 4 where this 'u-problem' is solved.

The sum in Equation (54) is approximately $\langle v_\epsilon\rangle(x) - v_0(x)$, and it is $O(\epsilon^2)$ (because $\langle\epsilon_n^2\rangle = \epsilon^2/12$). The field $\langle v_\epsilon\rangle(x)$ describes the wave propagating in the effective medium with perturbed-periodic positions. On average, the configuration of Figure 3(a) corresponds to a single interface between the free space $x<0$ with wavenumber k and the effective medium space with wavenumber K. The effective wave satisfies the radiation condition at $+\infty$ and only a right-going wave propagates in $x=y+n_0d>0$, so

$$\langle v_\epsilon\rangle(x) = t_\epsilon g_\epsilon(y)e^{iKx} \quad \text{for } x>0, \tag{56}$$

with $g_\epsilon(y)$ a d-periodic function. Similarly, through the semi-infinite periodic row, we have

$$v_0(x) = t_0 g_0(y)e^{iQx} \quad \text{for } x>0. \tag{57}$$

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

We expand t_ϵ, g_ϵ and K in powers of ϵ. As $\epsilon=0$ corresponds to the periodic case, we write

$$t_\epsilon = t_0 + \epsilon t_1 + \epsilon^2 t_2 + O(\epsilon^3), \quad g_\epsilon = g_0 + \epsilon g_1 + \epsilon^2 g_2 + O(\epsilon^3),$$
$$K = Q + \epsilon K_1 + \epsilon^2 K_2 + O(\epsilon^3).$$

Hence, with an error that is $O(\epsilon^3)$,

$$\begin{aligned} e^{-iQx}[\langle v_\epsilon\rangle(x) - v_0(x)] = \epsilon[t_0 g_1 + t_1 g_0 + i t_0 g_0 K_1 x] \\ + \epsilon^2\big[t_0 g_2 + t_1 g_1 + t_2 g_0 + iK_1 x(t_0 g_1 + t_1 g_0) \\ + t_0 g_0(iK_2 x - K_1^2 x^2/2)\big]. \end{aligned} \tag{58}$$

In this expansion, the coefficient multiplying ϵ must vanish,

$$t_0 g_1(y) + t_1 g_0(y) + i t_0 g_0(y) K_1 y + i t_0 g_0 K_1 n_0 d = 0,$$

and this should hold for each choice of n_0. Hence, $K_1=0$, $t_0 g_1 + t_1 g_0 = 0$ and Equation (58) reduces to

$$\langle v_\epsilon\rangle(x) - v_0(x) = \epsilon^2[F(y) + i n_0 d K_2 t_0 g_0(y)]e^{iQx}, \tag{59}$$

where $F(y) = t_0 g_2(y) + t_1 g_1(y) + t_2 g_0(y) + iK_2 y t_0 g_0(y)$ does not depend on n_0 and $\epsilon d/2 < y < d - \epsilon d/2$. The key point here is the explicit dependence on n_0 seen in the last term in Equation (59): identifying this term in the solution of the u-problem will enable K_2 to be extracted.

Now, returning to Equation (54), let us evaluate $\langle v_\epsilon\rangle$ at $x = n_0 d + y$, where $\epsilon d/2 < y < z$ so that we are just to the right of the scatterer at $x = n_0 d + \epsilon_{n_0} d$. To do that, we use Equation (55) and our solution for u_n (Appendix 4). We find that

$$\langle v_\epsilon\rangle(x) = v_0(x) + \frac{1}{24}\epsilon^2\big[S_{\text{left}}(x) + S_{\text{cell}}(x) + S_{\text{right}}(x)\big] + O(\epsilon^4)$$

where

$$S_{\text{left}}(x) = \sum_{n=0}^{n_0-1} \frac{\partial^2 u_n(x,\epsilon_n)}{\partial \epsilon_n^2}\bigg|_{\epsilon_n=0} = g_0(y)e^{iQx}\sum_{n=0}^{n_0-1}\frac{\partial^2 T(n,\epsilon_n)}{\partial\epsilon_n^2}\bigg|_{\epsilon_n=0},$$

$$S_{\text{cell}}(x) = \frac{\partial^2 u_{n_0}(x,\epsilon_{n_0})}{\partial\epsilon_{n_0}^2}\bigg|_{\epsilon_{n_0}=0} = e^{ikx}\frac{\partial^2 a_2(n_0,\epsilon_{n_0})}{\partial\epsilon_{n_0}^2}\bigg|_{\epsilon_{n_0}=0} + e^{-ikx}\frac{\partial^2 b_2(n_0,\epsilon_{n_0})}{\partial\epsilon_{n_0}^2}\bigg|_{\epsilon_{n_0}=0},$$

$$\begin{aligned} S_{\text{right}}(x) &= \sum_{n=n_0+1}^{\infty}\frac{\partial^2 u_n(x,\epsilon_n)}{\partial\epsilon_n^2}\bigg|_{\epsilon_n=0} \\ &= g_0(y)e^{iQx}\sum_{n=n_0+1}^{\infty}\frac{\partial^2 t(n,\epsilon_n)}{\partial\epsilon_n^2}\bigg|_{\epsilon_n=0} + f_0(y)e^{-iQx}\sum_{n=n_0+1}^{\infty}\frac{\partial^2 R(n,\epsilon_n)}{\partial\epsilon_n^2}\bigg|_{\epsilon_n=0}. \end{aligned}$$

In these formulas, the quantities T, a_2, b_2, t and R appear in the solution of the u-problem; see Equation (71). Making use of Equation (72), we find that S_{left} and

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

S_{cell} can be combined, giving

$$S_{\text{left}}(x) + S_{\text{cell}}(x) = g_0(y)e^{iQx}\sum_{n=0}^{n_0}\frac{\partial^2 T(n,\epsilon_n)}{\partial\epsilon_n^2}\bigg|_{\epsilon_n=0} = 2g_0(y)e^{iQx}\sum_{n=0}^{n_0}T_2(n),$$

where T_2 is the coefficient of ϵ_n^2 in the expansions of T about $\epsilon_n = 0$ (see Equation (73)). Hence, using similar expansions for R and t, Equations (74) and (75),

$$\langle v_\epsilon\rangle(x) = v_0(x) + \frac{\epsilon^2}{12}f_0(y)e^{-iQx}\sum_{n=n_0+1}^{\infty}R_2(n)$$
$$+\frac{\epsilon^2}{12}g_0(y)e^{iQx}\sum_{n=n_0+1}^{\infty}t_2(n) + \frac{\epsilon^2}{12}g_0(y)e^{iQx}\sum_{n=0}^{n_0}T_2(n) + O(\epsilon^4). \tag{60}$$

Inspecting the dependence on n of T_2, R_2 and t_2 in Equations (73)–(75), we see that only the last sum on the right-hand side of Equation (60) produces a contribution that is linear in n_0, because of the constant term T_{20} in the expression for $T_2(n)$, Equation (73). That contribution is

$$(\epsilon^2/12)\, g_0(y)e^{iQx}(n_0+1)T_{20}.$$

When this is compared with the last term in Equation (59), namely $\epsilon^2 i n_0 d K_2 t_0 g_0(y)e^{iQx}$, we obtain

$$K_2 d = (-i/12)T_{20}/t_0,$$

with T_{20}/t_0 given by Equation (76). This gives the dispersion relation

$$Kd = Qd - \epsilon^2\frac{M^2(kd)^2}{6}\frac{e^{iQd}}{\sin Qd}. \tag{61}$$

5.4. *Conclusion for the perturbed-periodic case*

The QCA approach gives Equation (3) as the dispersion relation. The same formula is obtained by a heuristic argument, in which it is assumed that the effective medium consists of a d-periodic medium in which are embedded scatterers with average scattering properties (see Appendix 3). Expanding Equation (3) in powers of ϵ leads to

$$Kd = Qd - \frac{\epsilon^2}{6}\frac{M^2}{1-M}(kd)^2\frac{e^{ikd}}{\sin Qd}. \tag{62}$$

The CPA approach gives Equation (4). Expanding this formula for small ϵ leads to

$$Kd = Qd - \frac{\epsilon^2}{6}M^2(kd)^2\frac{e^{iQd}}{\sin Qd}. \tag{63}$$

Evidently, Equations (62) and (63) differ. However, the CPA estimate (63) agrees with the perturbation approach, Equation (61), which suggests that QCA has

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

failed for our 1D problem. To confirm this, some numerical experiments were conducted.

6. Numerical experiments

We report the comparison in the effective wavenumber K obtained from the direct numerical calculations. For each set of parameters (kd, M) of Figure 1, the ϵ-value has been changed. The obtained fields (between 10^4 and 10^5) have been averaged and the K-value deduced using $\langle u\rangle(nd) \propto e^{iKnd}$. (We have also checked the periodicity of the function $g_\epsilon(y)$.) The computed wavenumber, denoted K_c here, is compared to the theoretical values of K obtained with the QCA $K = K_{\mathrm{QCA}}$ (plain circles) and CPA $K = K_{\mathrm{CPA}}$ (open circles) approaches. Figure 4 shows the result $|K - K_c|$ as a function of ϵ in the three cases of Figure 1.

In the three cases, a range of ϵ-values clearly appears for which the difference $|K - K_c|$ follows a power law (for instance, in (a), the range is 10^{-3}–10^{-2}): this power law is as ϵ^2 when considering the QCA prediction and it is as ϵ^4 when considering the CPA prediction.

The range of ϵ-values where the CPA prediction compares well with the numerical wavenumber coincides with the range of ϵ-values (strength of the introduced disorder) producing a small change in the Floquet wavenumber Q, as can be seen in Figure 1 (bottom). In case (a), this is roughly until $\epsilon \sim 10^{-2}$, in case (b) until $\epsilon \sim 10^{-1.5}$ and in case (c) until $\epsilon \sim 10^{-0.5}$.

Finally, the comparison between direct numerics and the theoretical prediction confirms that the CPA approach is able to get the first-order correction in ϵ^2 in the wavenumber while QCA is unable to do that.

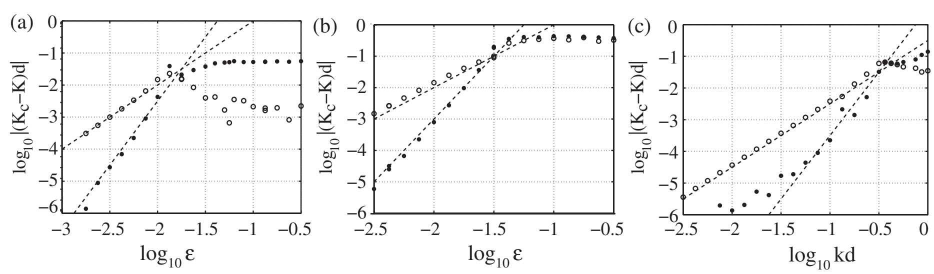

Figure 4. Comparison between the wavenumbers K_c obtained from numerical calculation (see Figure 1) and the wavenumbers given by QCA (open circles) and CPA (plain circles) for the three cases presented in Figure 1: (a) $kd = 14.2\pi$ and $M = 0.67/(2i)$, (b) $kd = 14.2\pi$ and $M = 3/(2i)$, (c) $kd = 2\pi/5.1$ and $M = 1.45/(2i)$. The differences $|K - K_c|$ is plotted as a function of the disorder ϵ in a log-log scale. Dotted lines are guidelines for the power laws in ϵ^2 and ϵ^4.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

7. Conclusion

In this paper, we have considered point scatterers in one dimension, with the *n*th scatterer displaced randomly by a small amount (within $\pm\epsilon/2$) from its periodic position, $x = nd$. The aim was to calculate the first correction (proportional to ϵ^2) to the Floquet wavenumber. We found that QCA and CPA gave different results. The QCA result agrees with a heuristic result, the CPA result agrees with an independent perturbation-based calculation. Moreover, the CPA result agrees with the results obtained by direct numerical simulations.

It is interesting to ask why the QCA approach does not yield the correct result for this problem. It is known that QCA does give good results in some two-dimensional problems, for example. It is also known that the Foldy closure assumption (replace $\langle u^e \rangle_1$ by $\langle u \rangle$ in the right-hand side of Equation (19)) does not lead to the correct dispersion relation for the Floquet mode in a one-dimensional periodic structure.

Further investigations are required. We are looking at the Dyson formalism using the Green function of the periodic medium as reference so as to explore, to any desired order, the effect of randomness with respect to the periodic situation.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

References

[1] R. de L. Kronig and W.G. Penney, *Quantum mechanics of electrons in crystal lattices*, Proc. Roy. Soc. A 130 (1931), pp. 499–513.

[2] H. Levine, *Unidirectional Wave Motions*, North-Holland, Amsterdam, 1978.

[3] O. Richoux and V. Pagneux, *Acoustic characterization of the Hofstadter butterfly with resonant scatterers*, Europhys. Lett. 59 (2002), pp. 34–40.

[4] W.J. Parnell and I.D. Abrahams, *Wave propagation in periodic and random inhomogeneous media: an overview*, in *Proceedings of the GDR 2051 Conference*, M. Deschamps, B. Desoudin, and A. Leger, eds., CNRS ST2I, Giens, France, 2006, pp. 92–99.

[5] P.W. Anderson, *Absence of diffusion in certain random lattices*, Phys. Rev. 109 (1958), pp. 1492–1505.

[6] Y.A. Godin, S. Molchanov, and B. Vainberg, *Wave propagation in a one-dimensional randomly perturbed periodic medium*, Waves Random Complex Media 17 (2007), pp. 381–395.

[7] D. Torrent, A. Hakansson, F. Cervera, and J. Sánchez-Dehesa, *Homogenization of two-dimensional clusters of rigid rods in air*, Phys. Rev. Lett. 96 (2006), 204302.

[8] D. Torrent and J. Sánchez-Dehesa, *Effective parameters of clusters of cylinders embedded in a nonviscous fluid or gas*, Phys. Rev. B 74 (2006), 224305.

[9] A. Maurel and V. Pagneux, *Effective propagation in a perturbed periodic structure*, Phys. Rev. B 78 (2008), 052301.

[10] P.A. Martin and A. Maurel, *Waves around almost periodic arrangements of scatterers: analysis of positional disorder*, preprint (2010), to appear in Math. Methods Appl. Sci. DOI: 10.1002/mma.1333.

[11] M. Lax, *Multiple scattering of waves*, Rev. Modern Phys. 23 (1951), pp. 287–310.

[12] M. Lax, *Multiple scattering of waves. II. The effective field in dense systems*, Phys. Rev. 85 (1952), pp. 621–629.

[13] P. Sheng, *Introduction to Wave Scattering, Localization and Mesoscopic Phenomena*, 2nd ed., Springer, Berlin, 2006.

[14] G.M. Romack and R.L. Weaver, *Monte Carlo studies of multiple scattering of waves in one-dimensional random media*, J. Acoust. Soc. Am. 87 (1990), pp. 487–494.
[15] W.J. Parnell and I.D. Abrahams, *Wave propagation in periodic and random composites; a critique of the use of Lax's Quasi-Crystalline Approximation*, in preparation.
[16] H. Levine, *Reflection and transmission by layered periodic structures*, Quart. J. Mech. Appl. Math. 19 (1966), pp. 107–122.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Appendix 1. QCA in the periodic case

We give a derivation of the Floquet dispersion relation (1) and the form of the solution for the wave $u(x)$ propagating in the periodic set of scatterers. Recall that the QCA approach is not an approximation for the periodic case since the closure is exact. Thus, the solutions for the wavenumber Q and for the field $u(x)$ are exact. To solve this problem, we can try to consider a doubly-infinite periodic row of point scatterers with no incident wave (taking the limit $N \to \infty$ in the correlation functions). Thus, put $u^0 \equiv 0$ and $u^e(nd) = e^{iQnd}$ in Equation (15), with $n \in \mathbb{Z}$. After some calculation, we obtain

$$1 = g\sum_{m=1}^{\infty} e^{i(k+Q)md} + g\sum_{m=1}^{\infty} e^{i(k-Q)md}. \tag{64}$$

When the (geometric) series converge, we can sum them, and then we obtain the expected result,

$$\cos Qd = \cos kd + \frac{ig}{1+g}\sin kd, \tag{65}$$

which is Equation (1) as $M = g/(1+g)$. However, Q can be imaginary for a given real k (see the discussion around Equation (18)), leading to divergent series. This is a well known difficulty. One way to overcome it is to use a continuation argument, where we suppose that $\mathrm{Im}\, k$ is sufficiently positive to ensure convergence of the series, and then allow k to become real in the final result. Another option (not used here) is to use a regularization argument, where G^0 is replaced by another function that decays rapidly; see [2, §51] for details.

Another way is to change the model problem. So, suppose instead that we have a periodic row of point scatterers along the half-line $x > 0$, with an incident wave, $u^0(x) = e^{ikx}$. This problem has been considered by Levine [16], [2, §62]. We look for a solution $u^e(nd) = \mathcal{C}e^{iQnd}$; Equation (15) gives

$$\begin{aligned}\mathcal{C}e^{iQnd} &= e^{iknd} + \mathcal{C}ge^{iknd}\sum_{m=0}^{n-1} e^{i(Q-k)md} + \mathcal{C}ge^{-iknd}\sum_{m=n+1}^{\infty} e^{i(k+Q)md}\\ &= e^{iknd} + \mathcal{C}g\frac{e^{iknd} - e^{iQnd}}{1 - e^{i(Q-k)d}} + \mathcal{C}ge^{iQnd}\sum_{m=1}^{\infty} e^{i(k+Q)md}, \quad n \geq 1.\end{aligned} \tag{66}$$

The last series is convergent for real k and $\mathrm{Im}\, Q > 0$. Summing the series and then balancing the terms proportional to e^{iQnd} gives the dispersion relation of the Floquet mode, Equation (65). Balancing the terms proportional to e^{iknd} gives $\mathcal{C}$:

$$\mathcal{C}g = e^{i(Q-k)d} - 1. \tag{67}$$

Next, consider Equation (21), which reduces to

$$\langle u\rangle(x) = e^{ikx} + \mathcal{C}g\sum_{m=0}^{\infty} e^{ik|x-md|}e^{iQmd}. \tag{68}$$

For $x>0$, write $\langle u\rangle(x)=g_0(y)e^{iQx}$, with $x=y+nd$ and $0\le y<d$ (the function g_0 being d-periodic, consistent with Equation (10)). Then, Equation (68) gives

$$g_0(y)=\mathcal{C}g\left[\frac{e^{i(k-Q)y}}{1-e^{i(k-Q)d}}-\frac{e^{-i(k+Q)y}}{1-e^{-i(k+Q)d}}\right], \tag{69}$$

with $\mathcal{C}g$ defined by Equation (67). In particular, for $0<x<d$, we have

$$\langle u\rangle(x)=\mathcal{C}g\,\frac{e^{ikx}+\mathcal{L}e^{-ikx}}{1-e^{i(k-Q)d}}\quad\text{with}\quad\mathcal{L}=\frac{e^{i(k-Q)d}-1}{1-e^{-i(k+Q)d}}.$$

This should be compared with the exact result obtained in Section 3. Specifically, we should have $\mathcal{L}=b_2/a_2$. Calculating,

$$\frac{a_2\mathcal{L}}{b_2}=\frac{a_2e^{-i(Q-k)d}-a_2}{b_2-b_2e^{-i(Q+k)d}}=\frac{a_1-a_2}{b_2-b_1}=\frac{(1-t_0)a_1-r_0b_2}{(1-t_0)b_2-r_0a_1}=1,$$

as expected, using Equations (9), (11) and (17).

For backward propagation, with $\langle u\rangle(x)=f_0(y)e^{-iQx}$, the solution for f_0 is deduced from that for g_0: $f_0(y)=g_0(d-y)$ for $0\le y<d$.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

Appendix 2. QCA and the perturbed-periodic problem: another derivation

The dispersion relation (3) is also obtained using a more careful derivation, with an incident wave, $u^0=e^{ikx}$, and a semi-infinite row of scatterers, as in Section 4.1. Thus, we start from

$$\begin{aligned}\langle u^e\rangle(x_1)=e^{ikx_1}&+\frac{g}{\epsilon d}\sum_{m=0}^{n-1}\int_{I_m}e^{ik(x_1-x_2)}\langle u^e\rangle(x_2)\,\mathrm{d}x_2\\&+\frac{g}{\epsilon d}\sum_{m=n+1}^{\infty}\int_{I_m}e^{ik(x_2-x_1)}\langle u^e\rangle(x_2)\,\mathrm{d}x_2,\end{aligned}$$

with $x_1\in I_n$, $n=0,1,2,\ldots$. Put $x_1=y_1+nd$ and $x_2=y_2+md$. Then, looking for a solution in the form $\langle u^e\rangle(x)=G(y)e^{iKx}$, where G is d-periodic, we obtain

$$\begin{aligned}G(y_1)e^{iK(nd+y_1)}&=e^{ik(y_1+nd)}+\frac{g}{\epsilon d}\left[e^{ik(y_1+nd)}\sum_{m=0}^{n-1}e^{i(K-k)md}\int_{-\epsilon d/2}^{\epsilon d/2}\mathrm{d}y_2G(y_2)e^{i(K-k)y_2}\right.\\&\qquad\left.+e^{-ik(y_1+nd)}\sum_{m=n+1}^{\infty}e^{i(K+k)md}\int_{-\epsilon d/2}^{\epsilon d/2}\mathrm{d}y_2G(y_2)e^{i(K+k)y_2}\right]\\&=e^{ik(y_1+nd)}+ge^{ik(y_1+nd)}\frac{1-e^{i(K-k)nd}}{1-e^{i(K-k)d}}\,G_-+ge^{-ik(y_1+nd)}\frac{e^{i(K+k)(n+1)d}}{1-e^{i(K+k)d}}\,G_+,\end{aligned} \tag{70}$$

where

$$G_\pm=\frac{1}{\epsilon d}\int_{-\epsilon d/2}^{\epsilon d/2}G(y)e^{i(K\pm k)y}\mathrm{d}y.$$

To find $G_\pm$, we multiply through by $e^{\pm iky_1}$ and integrate over $|y_1|<\epsilon/2$ giving

$$\begin{aligned}G_+&=e^{i(k-K)nd}\mathcal{S}+g\mathcal{S}G_-\frac{e^{i(k-K)nd}-1}{1-e^{i(K-k)d}}+\frac{gG_+e^{i(K+k)d}}{1-e^{i(K+k)d}},\\G_-&=e^{i(k-K)nd}+gG_-\frac{e^{i(k-K)nd}-1}{1-e^{i(K-k)d}}+\frac{g\mathcal{S}G_+e^{i(K+k)d}}{1-e^{i(K+k)d}}.\end{aligned}$$

The dependence on n is eliminated by taking $gG_- = e^{i(K-k)d} - 1$, and then

$$G_+ = \frac{1 - e^{i(K+k)d}}{1 - (1+g)e^{i(K+k)d}}\mathcal{S}$$

with K given by Equation (46). Equation (70) gives $G(y)e^{iKy} = \mathcal{C}e^{iky} + \mathcal{D}e^{-iky}$ with $\mathcal{C} = 1$ and $\mathcal{D} = g\mathcal{S}G_+$. Having found $\langle u^e \rangle$, we can then calculate $\langle u \rangle$ from Equation (42).

Appendix 3. A heuristic argument for the perturbed-periodic problem

We show that the dispersion relation predicted by QCA, Equation (46), is also predicted by using an intuitive argument. Although our computations indicate that the QCA prediction is incorrect, the heuristic argument does have some independent interest.

The dispersion relation predicted by QCA, Equation (46), has the form of the exact dispersion relation for a periodic row of finite-width scatterers, Equation (12), with coefficients $\mathcal{A}$ and $\mathcal{B}$ defined by Equation (13). Those coefficients involve reflection and transmission coefficients for an isolated 'scatterer', r_0 and t_0. Intuitively, we should replace r_0 and t_0 in Equation (13) by averaged reflection and transmission coefficients, $\langle r \rangle$ and $\langle t \rangle$. Recall that r_0 and t_0 are the reflection and transmission coefficients for a scatterer located at $x = 0$. It is easy to see that if the scatterer is moved to $x = c$, then the new reflection coefficient is $r_c = r_0 e^{2ikc}$ but the transmission coefficient is unchanged. Thus, $\langle t \rangle = t_0$ and

$$\langle r \rangle = \frac{1}{\epsilon d}\int_{-\epsilon d/2}^{\epsilon d/2} r_c \, \mathrm{d}c = \frac{r_0}{\epsilon d}\int_{-\epsilon d/2}^{\epsilon d/2} e^{2ikc} \, \mathrm{d}c = r_0 \mathcal{S}.$$

Replacing r_0 by $\langle r \rangle$ in Equation (13), and making use of the point-scatterer expressions, Equation (17), we do indeed recover Equation (46).

Appendix 4. The *u*-problem

In the sum of Equation (54), we need the solution of the following problem (Figures 3(b) and 5). There is a fictitious interface at $x = -d + z_0$, $0 < z_0 < d$. To the left, there is free space with an incident wave and a reflected wave. To the right, there is the periodic (homogenized) medium, apart from a single cell, $(n-1)d + z < x < nd + z$ $(0 < z < d)$, in which there is a single scatterer at $x_n = (n + \epsilon_n)d$ $(-d + z < \epsilon_n d < z)$. Thus, we can write

$$u_n(x, \epsilon_n) = \begin{cases} e^{ikx} + r(n, \epsilon_n)e^{-ikx}, & x < -d + z_0, \\ t(n, \epsilon_n)\, g_0(y)e^{iQx} + Rf_0 e^{-iQx}, & -d + z_0 \le x < (n-1)d + z, \\ a_1(n, \epsilon_n)e^{ikx} + b_1(n, \epsilon_n)e^{-ikx}, & (n-1)d + z \le x < (n + \epsilon_n)d, \\ a_2(n, \epsilon_n)e^{ikx} + b_2(n, \epsilon_n)e^{-ikx}, & (n + \epsilon_n)d \le x < nd + z, \\ T(n, \epsilon_n)\, g_0(y)e^{iQx}, & x \ge nd + z, \end{cases} \tag{71}$$

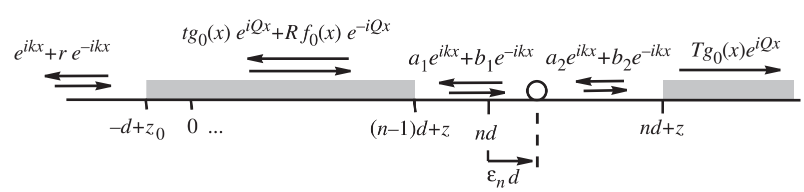

Figure 5. Configuration of the intermediate *u*-problem.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010

with u_n and its first derivative being continuous across the three interfaces, at $x=-d+z_0$, $x=(n-1)d+z$ and $x=nd+z$. Also, at the scatterer position, $x=x_n=(n+\epsilon_n)d$, $u_n(x_n^-)=u_n(x_n^+)$ and $u_n'(x_n^+)-u_n'(x_n^-)=2ikMu_n(x_n)$. In these formulas, f_0 and g_0 are d-periodic, defined for $0<y<d$ by

$$g_0(y)=Ae^{i(k-Q)y}+Be^{-i(k+Q)y}, \quad f_0(y)=Ae^{i(k-Q)(d-y)}+Be^{-i(k+Q)(d-y)}.$$

Applying the eight continuity equations gives the following equations:

$$\begin{aligned}
&1=tAe^{i(k-Q)d}+RB, \quad r=tBe^{-i(k+Q)d}+RA,\\
&a_1=tAe^{i(k-Q)(d-nd)}+RBe^{-i(k+Q)nd}, \quad b_1=tBe^{-i(k+Q)(d-nd)}+RAe^{i(k-Q)nd},\\
&a_2=ATe^{i(Q-k)nd}, \quad b_2=BTe^{i(Q+k)nd},\\
&a_1=Te^{i(Q-k)nd}\big[(1-M)A-MBe^{-2i\epsilon_n kd}\big],\\
&b_1=Te^{i(Q+k)nd}\big[MAe^{2i\epsilon_n kd}+(1+M)B\big].
\end{aligned} \tag{72}$$

These equations are readily solved. In particular, we find

$$\begin{aligned}
&AT(n,\epsilon_n)=\Delta^{-1}e^{-2iQnd}\big\{\mathcal{B}^2e^{-2ikd}-1\big\},\\
&AR(n,\epsilon_n)=\Delta^{-1}\big\{[1-M-M\mathcal{B}e^{-2i\epsilon_n kd}]\mathcal{B}e^{-2ikd}-[Me^{2i\epsilon_n kd}+(1+M)\mathcal{B}]\big\},\\
&At(n,\epsilon_n)=\Delta^{-1}e^{-2iQnd}e^{i(Q-k)d}\big\{(1+M)\mathcal{B}^2+M-1+2M\mathcal{B}\cos(2\epsilon_n kd)\big\}
\end{aligned}$$

with $\mathcal{B}=B/A$ and $\Delta(n,\epsilon_n)$ given by

$$\Delta=[1-M-M\mathcal{B}e^{-2i\epsilon_n kd}][\mathcal{B}^2e^{-2ikd}-e^{-2iQnd}]-\mathcal{B}[1-e^{-2iQnd}][Me^{2i\epsilon_n kd}+(1+M)\mathcal{B}].$$

These formulas are exact. They can be expanded in powers of ϵ_n. We find that these expansions have the form (with an error that is $O(\epsilon_n^3)$)

$$T(n,\epsilon_n)=t_0+\epsilon_n T_1(n)+\epsilon_n^2T_2(n), \quad T_2(n)=T_{20}+T_{22}e^{2inQd}+T_{24}e^{4inQd}, \tag{73}$$

$$R(n,\epsilon_n)=\epsilon_n R_1(n)+\epsilon_n^2R_2(n), \quad R_2(n)=R_{22}e^{2iQnd}+R_{24}e^{4iQnd}, \tag{74}$$

$$t(n,\epsilon_n)=t_0+\epsilon_n t_1(n)+\epsilon_n^2t_2(n), \quad t_2(n)=t_{22}e^{2iQnd}+t_{24}e^{4iQnd}, \tag{75}$$

where $t_0=T(n,0)=t(n,0)=A^{-1}e^{i(Q-k)d}$. All the coefficients in these expansions can be calculated but we shall not need any of them apart from T_{20}:

$$T_{20}=\frac{4M\mathcal{B}(kd)^2e^{2i(Q-k)d}}{A(\mathcal{B}^2e^{-2ikd}-1)}=-2i(Mkd)^2\frac{t_0\,e^{iQd}}{\sin Qd}, \tag{76}$$

after using $At_0=e^{i(Q-k)d}$ and Equation (37) for $\mathcal{B}$.

Downloaded By: [Colorado School of Mines] At: 19:07 15 November 2010