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

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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 \( K \approx k \) 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.
In one dimension (1D), the dispersion relation gives the wavenumber $Q$ of the Floquet mode ([1], equation (6)), ([2], equation (49.9))

$$\cos Qd = \cos kd + iM \sin kd,$$

for a wave satisfying the Helmholtz equation with point scatterers

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

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 $\epsilon_n$ 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 $\epsilon_n$ 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
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 $\epsilon_n$. 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 $K$

\begin{equation} \cos Kd = \cos Qd + \frac{M^2}{2(1 - M)} e^{ikd} (1 - \sin^2 \epsilon k d), \text{ using QCA}, \tag{3} \end{equation}

\begin{equation} \cos Kd = \cos Qd + \frac{M^2}{2} e^{ikd} (1 - \sin^2 \epsilon k d), \text{ using CPA}, \tag{4} \end{equation}

with $\text{sinc } x \equiv \sin x/x$. 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 $\epsilon$). 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 $\epsilon_n$ with respect to the periodic situation is used. The obtained result in $\epsilon^2$ 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 $\epsilon^2$) while QCA is unable to do that. Technical calculations are collected in four appendices. In the paper, the assumed time dependence is $e^{-\text{i}kt}$.

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 $x_n = (n - 1 + \epsilon_n)d$, $n = 1, \ldots, N$, each $\epsilon_n$ 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, $u(x) = e^{\text{i}kx}$. At each scatterer, we apply $[u]_{x_n} = 0$ and $[u']_{x_n} = 2\text{i}kMu(x_n)$. For $x_{n-1} \leq x \leq x_n$, the wavefield can be written

\begin{equation} u(x) = a_n \left[ e^{\text{i}k(x-x_n)} + Z_n e^{-\text{i}k(x-x_n)} \right]. \tag{5} \end{equation}
To account for the radiation condition after the $N$th 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 $Z_n$,

$$Z_n = Me^{-ik_{n+1}x} + Z_{n+1}(1 + M)e^{-ik_nx} \over (1 - M)e^{-ik_nx} - Z_{n+1}Me^{-ik_nx},$$

(6)

with $k_n = k(x_{n+1} - x_n)$. Once $(Z_n)$ has been computed, the amplitudes $(a_n)$ are derived starting from $a_1 = e^{ik_0x}$ and using the recurrence

$$a_{n+1} = (MZ_n + 1 + M)e^{ik_nx}a_n.$$

(7)

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

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

(8)

where $f_\epsilon$ and $g_\epsilon$ are two $\epsilon$-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 $u(x) \sim T f_\epsilon(x)e^{ik_nx}$. The field $\langle u \rangle(nd) \propto e^{ik_\epsilon nd}$ is used to deduce $K(\epsilon)$.

Figure 1 shows the results for different values of $M$ and $kd$. For non-zero $\epsilon$, 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 $\epsilon_n$ 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 $e^{ik_nx}$ 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 $Q \rightarrow K$. $K$ 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 $u(nd) \propto e^{ik_\epsilon nd}$). As will be seen in Section 6, the prediction of the effective wavenumber $K$ applies for small deviation $\epsilon$ with respect to the periodic case. This implies that $K$ remains close to $Q$; when the change becomes significant, no longer holds (in (a) for $\epsilon \sim 10^{-2}$, in (b) for $\epsilon \sim 10^{-0.5}$).
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

\[
  u(x) = \begin{cases} 
    a_1e^{ikx} + b_1e^{-ikx}, & \text{if } -d + b < x < -b, \\
    a_2e^{ikx} + b_2e^{-ikx}, & \text{if } b < x < d - b,
  \end{cases}
\]

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 \( e^{ikx} + r_0 e^{-ikx} \) to the left of the scatterer and it is \( t_0 e^{ikx} \) to the right. Hence,

\[
  b_1 = r_0 a_1 + t_0 b_2 \quad \text{and} \quad a_2 = r_0 b_2 + t_0 a_1.
\]

We seek solutions satisfying the Bloch condition,

\[
  u(x + d) = u(x)e^{iQd}.
\]

Figure 1. Top panels: mean field \( \langle u \rangle(x) \) in gray line for different \( \varepsilon \)-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 \( \varepsilon \) (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

\[
  u(x) = \begin{cases} 
    a_1e^{ikx} + b_1e^{-ikx}, & \text{if } -d + b < x < -b, \\
    a_2e^{ikx} + b_2e^{-ikx}, & \text{if } b < x < d - b,
  \end{cases}
\]

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 \( e^{ikx} + r_0 e^{-ikx} \) to the left of the scatterer and it is \( t_0 e^{ikx} \) to the right. Hence,

\[
  b_1 = r_0 a_1 + t_0 b_2 \quad \text{and} \quad a_2 = r_0 b_2 + t_0 a_1.
\]

We seek solutions satisfying the Bloch condition,

\[
  u(x + d) = u(x)e^{iQd}.
\]
This condition implies that
\[ b_2 = b_1 e^{iQ + kd} \quad \text{and} \quad a_2 = a_1 e^{-iQ - kd}. \] (11)

Equations (9) and (11) will have a non-trivial solution provided
\[ \cos Qd = A \cos kd + B \sin kd, \] (12)
where
\[ A = \frac{1}{2f_0} (r_0^2 - r_0^2 + 1) \quad \text{and} \quad B = \frac{i}{2f_0} (r_0^2 - r_0^2 - 1). \] (13)

This result is general: to use it, we merely insert the appropriate reflection and transmission coefficients. Notice that \( A \) and \( B \) 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 \( g \),
\[ u(x) = u^0(x) + g \sum_n e^{ik|x-x_n|} u^r(x_n), \] (14)
\[ u^r(x_n) = u^0(x_n) + g \sum_{m \neq n} e^{ik|x_n-x_m|} u^s(x_m), \] (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)),
\[ u(x) = u^0(x) + 2ikM \sum_n G^0(x-x_n) u^r(x_n), \] (16)
where \( G^0(x) = e^{ik|x|}/(2ik) \). The two formulations are equivalent in 1D owing to \( Mu(x_n) = g u^r(x_n) \) 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
\[ r_0 = g = M/(1-M) \quad \text{and} \quad t_0 = 1 + g = 1/(1-M). \] (17)

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

If energy is conserved, \( \text{Re} \ g + |g|^2 = 0 \) whence \( g = ie^{i \varphi} \sin \varphi \) for some real \( \varphi \), \( M = i \tan \varphi \) implying that \( M \) is purely imaginary, and Equation (1) reduces to
\[ \cos Qd \cos \varphi = \cos (kd + \varphi). \] (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.
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,

$$
\langle u \rangle (x) = u^0(x) + Ng \int dx_1 p(x_1)e^{ik|x-x_1|}\langle u' \rangle_1(x_1),
$$

(19)

$$
\langle u' \rangle_1(x_1) = u^0(x_1) + (N-1) g \int dx_2 p(x_2|x_1)e^{ik|x_2-x_1|}\langle u' \rangle_2(x_2),
$$

(20)

where

$$
\langle u' \rangle_1(x_1) \equiv \int dx_2 \ldots dx_N p(x_2, \ldots, x_N|x_1)u'(x_1),
$$

$$
\langle u' \rangle_2(x_2) \equiv \int dx_3 \ldots dx_N p(x_3, \ldots, x_N|x_1, x_2)u'(x_2).
$$

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

$$
\langle u \rangle (x) = u^0(x) + Ng \int dx_1 p(x_1)e^{ik|x-x_1|}\langle u' \rangle(x_1),
$$

(21)

$$
\langle u' \rangle(x_1) = u^0(x_1) + (N-1) g \int dx_2 p(x_2|x_1)e^{ik|x_2-x_1|}\langle u'^* \rangle(x_2).
$$

(22)

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

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

(23)

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

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

(24)

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

(25)

These equations agree with (the deterministic) Equations (14) and (15) with $\langle u \rangle = u$, $\langle u' \rangle = u'$ 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 I 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

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

(26)

where $f_0$ and $g_0$ are $d$-periodic. We indicate here the main results (for details, see Appendix I). The wavenumber $Q$ is given by the dispersion relation,
Equation (1),
\[ g_0(y) = A e^{i(k-Q)y} + B e^{-i(k+Q)y} \quad \text{and} \quad f_0(y) = g_0(d-y), \]
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 \( (\varepsilon_n=0 \text{ in Figure 2}) \), 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 \( \varepsilon_n \neq 0 \). 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 \( x_n = (n + \varepsilon_n)d \) (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 \( \varepsilon_n d < z < d - \varepsilon_n d \); 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 \( \varepsilon_n \) is non-zero, reflection and

![Figure 2](image-url)

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 \( x = (n + \varepsilon_n)d \), reflection and transmission by the cell are expected. When the cell satisfies the same properties as the host medium (here, periodic, so \( \varepsilon_n = 0 \)), it is transparent for the incident wave, \( R(0) = 0, T(0) = 1 \).
transmission at the interfaces are expected. Thus, we write

\[ v(x) = \begin{cases} 
  g_0(y)e^{yQx} + R(\epsilon_n)f_0(y)e^{-yQx}, & x < (n - 1)d + z, \\
  a_1e^{ikx} + b_1e^{-ikx}, & (n - 1)d + z \leq x < (n + \epsilon_n)d, \\
  a_2e^{ikx} + b_2e^{-ikx}, & (n + \epsilon_n)d \leq x < nd + z, \\
  T(\epsilon_n)g_0(y)e^{yQx}, & x \geq nd + z. 
\end{cases} \]

(28)

The functions \(f_0\) and \(g_0\) are \(d\)-periodic and they do not depend on \(\epsilon_n\). 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

\[ a_1 = A e^{i(Q-k)(n-1)d} + D Re^{-i(Q+k)(n-1)d}, \quad b_1 = Be^{i(Q+k)(n-1)d} + C Re^{i(k-Q)(n-1)d}, \]

(29)

\[ a_2 = AT e^{i(Q-k)nd}, \quad b_2 = BT e^{i(Q+k)nd}, \]

(30)

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

\[ A = [g_0'(z) + i(Q + k)g_0(z)]e^{i(Q-k)z}/(2ik), \]

\[ B = -[g_0'(z) + i(Q - k)g_0(z)]e^{i(Q+k)z}/(2ik), \]

\[ C = -[f_0'(z) - i(Q + k)f_0(z)]e^{i(k-Q)z}/(2ik), \]

\[ D = [f_0'(z) + i(k - Q)f_0(z)]e^{-i(k+Q)z}/(2ik). \]

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 \(v'(x_n^-) - v'(x_n^+) = 2ikMr(v(x_n))\). These conditions give

\[ a_1 = T e^{i(Q-k)nd}[(1 - M)A - MBe^{-2i\epsilon_nkd}], \]

(31)

\[ b_1 = T e^{i(Q+k)nd}[MAe^{2i\epsilon_nkd} + (1 + M)B], \]

(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

\[ (1 - M - MB e^{-2i\epsilon_nkd})T(\epsilon_n) - Be^{-2iQmd}R(\epsilon_n) = e^{i(k-Q)d}, \]

(33)

\[ [Me^{-i\epsilon_nkd} + (1 + M)B]T(\epsilon_n) - e^{-2iQmd}R(\epsilon_n) = Be^{-i(k+Q)d}, \]

(34)

where \(B = B/A\). This system of equations has four unknowns, \(R, T, B\) and \(Q\). Note that only \(R\) and \(T\) depend on \(\epsilon_n\) since \(Q\) and \(B\) 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.
and therefore it has to be transparent,
\[ T(\epsilon_n = 0) = 1, \quad R(\epsilon_n = 0) = 0. \] (35)

Hence, we obtain
\[ MB = 1 - M - e^{i(k - Q)d}, \quad M + [1 + M - e^{-i(k + Q)d}]B = 0; \] (36)

eliminating \( B \) then gives the dispersion relation for the Floquet mode, Equation (1), as the condition of solvability. We also find that \( B = B/A \) satisfies
\[ 1 - e^{i(k - Q)d} + B[1 - e^{-i(k + Q)d}] = 0. \] (37)

Then, having found \( Q \) and \( B \), we can determine \( R \) and \( T \) from Equations (33) and (34); for example, we obtain
\[ T(\epsilon_n) = \left[ 1 + iM^2 \frac{e^{iQd}}{\sin Qd}(1 - \cos (2\epsilon_n kd)) \right]^{-1} \simeq 1 - 2i\epsilon_n^2 \frac{M^2(kd)^2 e^{iQd}}{\sin Qd} \] (38)

for small \( \epsilon_n \). 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 \( \epsilon_n \)-values.

5.1. **QCA approach**

The same procedures as in the periodic case may be applied. Define \( \Pi_{\epsilon d}(x) \) by
\[ \Pi_{\epsilon d}(x) = \begin{cases} 1, & |x| \leq \epsilon d/2, \\ 0, & |x| > \epsilon d/2. \end{cases} \] (39)

We take
\[ p(x) = \frac{1}{N\epsilon d} \sum_m \Pi_{\epsilon d}(x - md) \] (40)

and
\[ p(x_2|x_1) = \frac{1}{(N - 1)\epsilon d} \sum_{m \neq n} \Pi_{\epsilon d}(x_2 - md), \quad |x_1 - nd| < \epsilon d/2. \] (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
\[
\langle u \rangle(x) = \frac{g}{\varepsilon d} \sum_m \int_{I_n} e^{ik|x-x_1|} \langle \tilde{u} \rangle(x_1) \, dx_1,
\]
(42)
\[
\langle u^r \rangle(x_1) = \frac{g}{\varepsilon d} \sum_{m \in I_n} \int_{I_n} e^{ik|x-x_1|} \langle \tilde{u}^r \rangle(x_2) \, dx_2, \quad x_1 \in I_n,
\]
(43)
where $I_n$ is the interval $nd - \varepsilon d/2 < x < nd + \varepsilon d/2$.

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 $\langle u^r \rangle''(x) + k^2 \langle u^r \rangle(x) = 0$ for $x \in I_n$, $n \in \mathbb{Z}$. So, write
\[
\langle u^r \rangle(x) = a_ne^{ikx} + b_ne^{-ikx}, \quad x \in I_n.
\]
(44)
Substituting in Equation (43) and equating coefficients of $e^{\pm ikx}$ gives
\[
a_n = g \sum_{m=-\infty}^{n-1} \left( a_m + b_m S e^{-2imkd} \right), \quad b_n = g \sum_{m=n+1}^{\infty} \left( b_m + a_m S e^{2imkd} \right),
\]
where $S = \text{sinc}(kd)$. Looking for a solution of these equations in the form
\[
a_n = C e^{ikn}, \quad b_n = D e^{ikn},
\]
(45)
we find that the constants $C$ and $D$ satisfy
\[
C = g(C + DS) \sum_{m=1}^{\infty} e^{ikm}, \quad D = g(D + CS) \sum_{m=1}^{\infty} e^{ikm}.
\]
These bear comparison with Equation (64); under the same conditions, we sum the infinite series and then put the resulting $2 \times 2$ determinant equal to zero, giving
\[
\cos Kd = A_e \cos kd + B_e \sin kd,
\]
(46)
where
\[
A_e = 1 + \frac{g^2 \Phi(kd)}{2(1 + g)} \quad \text{and} \quad B_e = \frac{ig}{1 + g} \left[ 1 + \frac{1}{2} g \Phi(kd) \right],
\]
with $\Phi(x) = 1 - \text{sinc}^2 x$. 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 $C$ (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).
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 \( g_0 \rightarrow g_c, f_0 \rightarrow f_c, Q \rightarrow K, R \rightarrow R_c \) and \( T \rightarrow T_c \). 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 \( (p - \frac{1}{2}e)d \leq x_p \leq (p + \frac{1}{2}e)d \) for all integers \( p \), except the \( n \)th scatterer inside the isolated cell. Apart from the nature of the host effective medium (which is encapsulated in \( K \) and in the functions \( f_c \) and \( g_c \)), 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.

\[
(1 - M)A_c - MB_c e^{-2ikd} T_c(\epsilon_n) - B_c e^{-2iknd} R_c(\epsilon_n) = A_c e^{\hat{k}Kd},
\]

\[
M A_c e^{2ikd} + (1 + M) B_c T_c(\epsilon_n) - A_c e^{-2iknd} R_c(\epsilon_n) = B_c e^{-\hat{k}Kd}.
\]  

The functions \( g_c \) and \( f_c \) have the forms in Equation (27),

\[
g_c(y) = A_c e^{\hat{k}Kd} + B_c e^{-\hat{k}Kd}, \quad f_c(y) = g_c(d - y),
\]

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

\[
\langle T_c \rangle = 1, \quad \langle R_c \rangle = 0,
\]

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

Eliminating \( R_c(\epsilon_n) \) from Equations (47) and (48) shows that \( T_c(\epsilon_n) \) is an even function of \( \epsilon_n \). So, a Taylor expansion gives

\[
T_c(\epsilon_n) = c_0 + c_1 \epsilon + c_{21} \epsilon^2 + c_{22} \epsilon^2 + c_{31} \epsilon^3 + c_{32} \epsilon^3 + O(\epsilon^4, \epsilon^2 \epsilon^2, \epsilon^2)
\]

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

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

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

\[
T_c(\epsilon_n) = 1 + c_{21} \left( \frac{\epsilon^2}{12} \right) + c_{31} \epsilon \left( \frac{\epsilon^2}{12} \right) + O(\epsilon^4, \epsilon^2 \epsilon^2, \epsilon^2),
\]
and \(\langle e^{\pm 2i k d x} T_x(\epsilon_n) \rangle = S + O(\epsilon^4)\), where \(S = \text{sinc}(k d)\). Hence, taking the average of the system (47) and (48) gives
\[
(1 - M - e^{\hat{n} k - k d}) A_e - M S B_e = 0,
MS A_e + (1 - M - e^{-\hat{n} k + k d}) B_e = 0.
\]
We get the dispersion relation from the condition of solvability
\[
\cos K d = \cos Q d + \frac{1}{2} M^2 e^{i K d} (1 - \text{sinc}^2(ek d)),
\]
which is Equation (4). We can also calculate \(A_e/B_e\) 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 \(x_m = md + \epsilon_{m0}\) where \(m = 1, 2, \ldots\) and \(|\epsilon_{m0}| \leq \epsilon/2\). A plane wave, \(e^{i k x}\), is incident from the left. The field \(v(x; \epsilon)\) describes the wave propagating through the scatterers; the vector \(\epsilon = (\epsilon_1, \epsilon_2, \ldots)\) (Figure 3(a)). The idea is to write the field \(v(x; \epsilon)\) as a perturbation around the field \(v_0(x) = v(x; 0)\), regarding \(\epsilon\) 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 \(\langle v_e \rangle(x)\). 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 \(n\)th 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 \(\epsilon_{d0}\) with respect to the periodic positions. The wavefield is \(v_e(x; \epsilon)\). Averaging \(v_e(x; \epsilon)\) over all realizations of the \(\epsilon_n\) 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 \(n\)th scatterer at \(x_n = (n + \epsilon_n)d\). The wavefield is \(u(x; \epsilon_n)\).
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 $v_e$ as a perturbation around $v_0$, the field of the Floquet mode,

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

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

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

As the $n$th scatterer occupies the interval $I_n$ (defined below Equation (43)), we choose $x$ outside all such intervals; specifically, we choose $x$ between $I_n$ and $I_{n+1}$ 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

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

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

$$\frac{\partial^2 u_e(x, 0)}{\partial \epsilon_n^2} = \frac{\partial^2 v_e(x, 0)}{\partial \epsilon_n^2}.$$

The field $u_e$ describes the wave propagating through a set of scatterers periodically spaced except for the $n$th 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 $\langle v_e \rangle(x) - v_0(x)$, and it is $O(\epsilon^3)$ (because $\langle \epsilon_n^2 \rangle = \epsilon^2/12$). The field $\langle v_e \rangle(x)$ 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 $x = y + n_0 d > 0$, so

$$\langle v_e \rangle(x) = t_e g_e(y)e^{ikx} \text{ for } x > 0,$$

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

$$v_0(x) = t_0 g_0(y)e^{iQx} \text{ for } x > 0.$$
We expand $t_\epsilon$, $g_\epsilon$ and $K$ in powers of $\epsilon$. 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 $O(\epsilon^3)$,

$$e^{-iQx}[(v_\epsilon(x) - v_0(x)) = \epsilon[t_0 g_1 + t_1 g_0 + i t_0 g_0 K_1 x]$$

$$+ \epsilon^2[t_0 g_2 + t_1 g_1 + t_2 g_0 + i K_1 x(t_0 g_1 + t_1 g_0)$$

$$+ t_0 g_0(iK_2 x - K^2/(2))]. \quad (58)$$

In this expansion, the coefficient multiplying $\epsilon$ 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

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

where $F(y) = t_0 g_2(y) + t_1 g_1(y) + t_2 g_0(y) + i K_2 y t_0 g_0(y)$ does not depend on $n_0$ and $\epsilon d/2 < y < -\epsilon d/2$. 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 $x = n_0 d + \epsilon_0 d$. To do that, we use Equation (55) and our solution for $u_n$ (Appendix 4). We find that

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

where

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

$$S_{cell}(x) = \frac{\partial^2 u_{n_0}(x, \epsilon_{n_0})}{\partial \epsilon_{n_0}^2} \bigg|_{\epsilon_{n_0} = 0} = \epsilon_0 \frac{\partial^2 a_2(n_0, \epsilon_{n_0})}{\partial \epsilon_{n_0}^2} \bigg|_{\epsilon_{n_0} = 0} + \epsilon_0 \frac{\partial^2 b_2(n_0, \epsilon_{n_0})}{\partial \epsilon_{n_0}^2} \bigg|_{\epsilon_{n_0} = 0},$$

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

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...
$S_{\text{cell}}$ can be combined, giving

$$S_{\text{left}}(x) + S_{\text{cell}}(x) = g_0(y)e^{iQx} \sum_{n=0}^{m_0} \frac{\partial^2 T(n, \epsilon_n)}{\partial \epsilon_n^2} \bigg|_{\epsilon_n=0} = 2g_0(y)e^{iQx} \sum_{n=0}^{m_0} T_2(n),$$

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

$$\langle v_e(x) \rangle = v_0(x) + \frac{\epsilon^2}{12} f_0(y)e^{-iQx} \sum_{n=n_0+1}^{\infty} R_2(n) + \frac{\epsilon^2}{12} g_0(y)e^{iQx} \sum_{n=n_0+1}^{\infty} t_2(n) + \frac{\epsilon^2}{12} g_0(y)e^{iQx} \sum_{n=0}^{m_0} T_2(n) + O(\epsilon^4). \quad (60)$$

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

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

When this is compared with the last term in Equation (59), namely $\epsilon^2 i n_0 K_{20} g_0(y)e^{iQx}$, we obtain

$$K_{2d} = (-i/12)T_{20}/t_0,$$

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

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

### 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 $\epsilon$ leads to

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

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

$$Kd = Qd - \frac{\epsilon^2}{6} \frac{M^2}{1 - M^2(kd)^2} \frac{e^{iQd}}{\sin Qd}. \quad (63)$$

Evidently, Equations (62) and (63) differ. However, the CPA estimate (63) agrees with the perturbation approach, Equation (61), which suggests that QCA has
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 $\epsilon$-value has been changed. The obtained fields (between $10^4$ and $10^5$) have been averaged and the $K$-value deduced using $\langle u \rangle_{(nd)} \propto e^{i km}$. (We have also checked the periodicity of the function $g_s(y)$.) The computed wavenumber, denoted $K_c$, here, is compared to the theoretical values of $K$ obtained with the QCA $K = K_{QCA}$ (plain circles) and CPA $K = K_{CPA}$ (open circles) approaches. Figure 4 shows the result $|K - K_c|$ as a function of $\epsilon$ in the three cases of Figure 1.

In the three cases, a range of $\epsilon$-values clearly appears for which the difference $|K - K_c|$ follows a power law (for instance, in (a), the range is $10^{-2} - 10^{-7}$): this power law is as $\epsilon^2$ when considering the QCA prediction and it is as $\epsilon^4$ when considering the CPA prediction.

The range of $\epsilon$-values where the CPA prediction compares well with the numerical wavenumber coincides with the range of $\epsilon$-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 $\epsilon^2$ 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 $M = 0.67/(2\iota)$, (b) $kd = 14.2\pi$ and $M = 3/(2\iota)$, (c) $kd = 2\pi/5.1$ and $M = 1.45/(2\iota)$. The differences $|K - K_c|$ is plotted as a function of the disorder $\epsilon$ in a log-log scale. Dotted lines are guidelines for the power laws in $\epsilon^2$ and $\epsilon^4$. 
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 $\epsilon^2$) 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 $\langle \mu \rangle$ by $\langle \mu \rangle$ 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.

References

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 \( u^0 = 0 \) and \( u'(nd) = e^{Qnd} \) in Equation (15), with \( n \in \mathbb{Z} \). After some calculation, we obtain

\[
1 = g \sum_{m=1}^{\infty} e^{i(k+Qnym)} + g \sum_{m=1}^{\infty} e^{i(k-Qnym)}. \tag{64}
\]

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 \( \text{Im} k \) 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 \( G^d \) 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, \( u'(x) = e^{ikx} \). This problem has been considered by Levine [16], [2, §62]. We look for a solution \( u'(nd) = e^{Qnd} \), Equation (15) gives

\[
Ce^{Qnd} = e^{iknd} + Cg e^{iknd} \sum_{m=0}^{n-1} e^{i(Q-k)ym} + Cge^{-iknd} \sum_{m=n+1}^{\infty} e^{i(k+Q)ym} \\
= e^{iknd} + g \frac{e^{iknd} - e^{Qnd}}{1 - e^{-i(k-Q)d}} + Cge^{Qnd} \sum_{m=1}^{\infty} e^{i(k-Q)ym}, \quad n \geq 1. \tag{66}
\]

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

\[
Cg = e^{i(Q-k)d} - 1. \tag{67}
\]

Next, consider Equation (21), which reduces to

\[
\langle u \rangle(x) = e^{ikx} + Cg \sum_{m=0}^{\infty} e^{i(k-Q)x-md} e^{Qnd}. \tag{68}
\]
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For $x > 0$, write $(u)(x) = g_0(y)e^{iQx}$, with $x = y + nd$ and $0 \leq y < d$ (the function $g_0$ being $d$-periodic, consistent with Equation (10)). Then, Equation (68) gives

$$g_0(y) = Cg \left[ \frac{e^{ik-\Omega y}}{1 - e^{ik-\Omega y}} - \frac{e^{-ik+\Omega y}}{1 - e^{-ik+\Omega y}} \right],$$

with $Cg$ defined by Equation (67). In particular, for $0 < x < d$, we have

$$(u)(x) = Cg e^{ikx} + \mathcal{L} e^{-ikx} \quad \text{with} \quad \mathcal{L} = \frac{e^{ik-\Omega d} - 1}{1 - e^{-ik+\Omega d}}.$$  

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

$$\frac{a_2 \mathcal{L}}{b_2} = \frac{a_2 e^{-ik-\Omega d} - a_2}{b_2 - b_2 e^{-ik+\Omega d}} = \frac{a_1 - a_2}{b_2 - b_1} = \frac{(1 - t_0)a_1 - n_0 b_2}{(1 - t_0)b_2 - n_0 a_1} = 1,$$

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

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

### 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, $u' = e^{ikx}$, and a semi-infinite row of scatterers, as in Section 4.1. Thus, we start from

$$(u')(x_1) = e^{ikx_1} + \frac{g}{ed} \sum_{n=0}^{\infty} \int_{I_n} e^{ik(x_1-x_2)} (u')(x_2) \, dx_2$$

$$+ \frac{g}{ed} \sum_{n=1}^{\infty} \int_{I_n} e^{ik(x_2-x_1)} (u')(x_2) \, dx_2,$$

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

$$G(y)e^{iK(\alpha + y_1)} = e^{iK(y_1 + nd)} + \frac{g}{ed} \sum_{n=0}^{\infty} e^{iK(nd)} \int_{-d/2}^{d/2} dy_2 \frac{G(y_2)e^{iK(y_2)}}{1 - e^{iK(y_2)}}$$

$$+ e^{-iK(y_1 + nd)} \sum_{n=1}^{\infty} e^{iK(nd)} \int_{-d/2}^{d/2} dy_2 \frac{G(y_2)e^{iK(y_2)}}{1 - e^{iK(y_2)}}$$

$$= e^{iK(y_1 + nd)} + ge^{iK(nd)} \frac{1 - e^{-iK(y_1 + nd)}}{1 - e^{-iK(y_1 + nd)}} G_+ + ge^{iK(nd)} \frac{1 - e^{iK(y_1 + nd)}}{1 - e^{iK(y_1 + nd)}} G_-,$$

where

$$G_\pm = \frac{1}{ed} \int_{-d/2}^{d/2} G(y)e^{iK(y_1 + y)} \, dy.$$  

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

$$G_+ = e^{iK(y_1 + y) + \frac{g}{ed} G_+ e^{iK(y_1 + y)}}$$

$$G_- = e^{iK(y_1 + y) + \frac{g}{ed} G_- e^{iK(y_1 + y)}}.$$  

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

\[
G_+ = \frac{1 - e^{(K-K)d}}{1 - (1 + g)e^{(K-K)d}} S
\]

with \( K \) given by Equation (46). Equation (70) gives \( G(y)e^{iky} = C e^{iky} + D e^{-iky} \) with \( C = 1 \) and \( D = gSG_+ \). Having found \( \langle u \rangle \), 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 \( A \) and \( B \) 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

\[
\langle r \rangle = \frac{1}{ed} \int_{-d/2}^{d/2} r_c \, dc = \frac{r_0}{ed} \int_{-d/2}^{d/2} e^{2ikc} \, dc = r_0 S.
\]

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 \( x_n = (n + \varepsilon_n)d \) \( (-d + z < \varepsilon_n d < z) \). Thus, we can write

\[
u_n(x, \varepsilon_n) = \begin{cases} 
e \frac{e^{ikx} + r(n, \varepsilon_n)e^{-ikx}}{t(n, \varepsilon_n)g_0(y)e^{ikx} + Rf_0e^{-ikx}}, & x < -d + z_0, \\
e \frac{a_1(n, \varepsilon_n)e^{ikx} + b_1(n, \varepsilon_n)e^{-ikx}}{a_2(n, \varepsilon_n)e^{ikx} + b_2(n, \varepsilon_n)e^{-ikx}}, & -d + z_0 \leq x < (n-1)d + z, \\
e \frac{t(n, \varepsilon_n)g_0(y)e^{ikx}}{a_2(n, \varepsilon_n)e^{ikx}}, & (n-1)d + z \leq x < (n + \varepsilon_n)d, \\
e \frac{T(n, \varepsilon_n)g_0(y)e^{ikx}}{x \geq nd + z}, \end{cases}
\]

(71)

Figure 5. Configuration of the intermediate \( u \)-problem.
with \( u \) 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, \( x = x_n = (n + \epsilon_n)d \), \( u_{x_n}(x_{n}^+ \rangle = u_n(x_{n}^+) \) and \( u_{x_n}(x_{n}^- \rangle - u_n(x_{n}^+) = 2iM u_n(x_{n}) \). In these formulas, \( f_0 \) and \( g_0 \) are \( d \)-periodic, defined for \( 0 < y < d \) by

\[
g_0(y) = A e^{i(k-Q) y} + B e^{-i(k+Q) y}, \quad f_0(y) = A e^{i(k-Q(d-y))} + B e^{-i(k+Q(y-d))}.
\]

Applying the eight continuity equations gives the following equations:

\[
\begin{align*}
1 &= t A e^{i(k-Q) d} + R B, \quad r = t B e^{-i(k+Q) d} + R A, \\
a_1 &= t A e^{i(k-Q(d-nd))} + R B e^{i(k+Q) nd}, \quad b_1 = t B e^{-i(k+Q(d-nd))} + R A e^{i(k-Q) nd}, \\
a_2 &= A T e^{i(Q-k) nd}, \quad b_2 = B T e^{i(Q+k) nd}, \\
a_3 &= T e^{i(Q-k) nd} (1 - M) A - M B e^{-2i\epsilon_n k d}], \\
b_3 &= T e^{i(Q+k) nd} [M A e^{2i\epsilon_n k d} + (1 + M) B],
\end{align*}
\]

These equations are readily solved. In particular, we find

\[
\begin{align*}
AT(n, \epsilon_n) &= \Delta^{-1} e^{-2\epsilon_n k d} [B^2 e^{-2k d} - 1], \\
AR(n, \epsilon_n) &= \Delta^{-1} \left[1 - M - M B e^{-2i\epsilon_n k d} B e^{-2k d} - [M e^{2i\epsilon_n k d} + (1 + M) B] \right], \\
A(n, \epsilon_n) &= \Delta^{-1} e^{-2\epsilon_n k d} e^{i(Q-k) d} \left(1 + M) B^2 + M - 1 + 2M B \cos(2\epsilon_n k d) \right)
\end{align*}
\]

with \( B = B/A \) and \( \Delta \) given by

\[
\Delta = [1 - M - M B e^{-2i\epsilon_n k d}] [B^2 e^{-2k d} - e^{-2\epsilon_n k d}] - B [1 - e^{-2\epsilon_n k d} [M e^{2i\epsilon_n k d} + (1 + M) B]]
\]

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

\[
\begin{align*}
T(n, \epsilon_n) &= t_0 + \epsilon_n T_1(n) + \epsilon_n^2 T_2(n), \quad T_2(n) = T_{20} + T_{22} e^{-2\epsilon_n Q d} + T_{24} e^{4\epsilon_n Q d}, \\
R(n, \epsilon_n) &= \epsilon_n R_1(n) + \epsilon_n^2 R_2(n), \quad R_2(n) = R_{22} e^{-2\epsilon_n Q d} + R_{24} e^{4\epsilon_n Q d}, \\
t(n, \epsilon_n) &= t_0 + \epsilon_n t_1(n) + \epsilon_n^2 t_2(n), \quad t_2(n) = t_{22} e^{-2\epsilon_n Q d} + t_{24} e^{4\epsilon_n Q d},
\end{align*}
\]

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 \( T_{20} ^\prime = \Delta^{-1} e^{i(Q-k) d} \).

\[
T_{20} = \frac{4M B (kd)^2 e^{2i(Q-k) d} A (B^2 e^{-2k d} - 1)}{\sin Q d},
\]

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