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Waves around almost periodic arrangements of scatterers: Analysis of positional disorder

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Much is known about the propagation of waves through periodic arrangements of identical scatterers, such as through a photonic crystal. Here, we consider a simple realization: scalar waves through a regular two-dimensional array of identical small circles. We are interested in the effect of random disorder: the circles remain identical, but their centres are given small random displacements. We derive asymptotic approximations that can be used to quantify the effect of positional disorder. Extension to more complicated problems seems feasible and is expected. Copyright © 2010 John Wiley & Sons, Ltd.

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Dedicated to George Hsiao on the occasion of his 75th birthday

1. Introduction

Consider waves in a two-dimensional periodic structure. The structure is defined by a lattice: each cell in the lattice is a parallelogram, each node in the lattice is a scatterer location. For scalar waves governed by the Helmholtz equation, $(\nabla^2+k^2)u=0$, it is known how to calculate the dispersion relation, connecting the wave-number k to the Bloch vector $\mathbf{Q}$: solutions satisfy the Bloch condition $u(\mathbf{r}+\mathbf{r}_j)=u(\mathbf{r})\exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j)$, for every lattice node $\mathbf{r}_j$.

By assumption, all scatterers in the periodic structure are identical. Evidently, the dispersion relation depends on the shape and composition of the scatterers. Asymptotic approximations are also available when the scatterers are small.

The periodic problems outlined above have been studied extensively. One important application concerns photonic crystals [1]. Fabrication of such structures inevitably introduces imperfections, leading to nearly periodic geometries or other forms of disorder. What are the effects of the disorder? There are publications on this question; the main result is that the band-gap phenomena seen with periodic structures are robust to small amounts of random disorder. Representative publications include [2–9]. All these papers include results from numerical simulations. Some [2, 4, 5, 7, 9] use a 'supercell' method, which means that a periodic medium is constructed in which each period contains the same disordered arrangement of circular scatterers; evidently, such a periodic medium is not a random medium, so it is unclear how to interpret the results. The other papers [3, 6, 8] use a finite number of circular scatterers, 169 in [3], 38 in [6] and 1152 in [8]. One paper [5] also includes a simple method for estimating the effect of disorder on k, but it assumes that the scatterers are penetrable and that the fields in the periodic medium are known.

In this paper, we propose an analytical method for estimating the effect of positional disorder on wave propagation. We use the simplest possible model: identical, small, sound-soft circular scatterers, implying isotropic scattering. We calculate the ensemble-averaged field, using the Lax quasi-crystalline approximation (QCA). This leads to an infinite, homogeneous system of linear algebraic equations; setting the determinant to zero yields a method for calculating the allowable wavenumbers in the disordered structure. Known results are recovered when the disorder is absent, and simple explicit approximations are obtained when the disorder is small. Many extensions of the basic approach are anticipated.

2. Periodic case: no scatterers

We start with an infinite two-dimensional lattice Λ. Lattice points $\mathbf{r}_j\in\Lambda$ are defined by

$$\mathbf{r}_j=j_1\mathbf{a}_1+j_2\mathbf{a}_2,\quad j_1,j_2\in\mathbb{Z}, \tag{1}$$

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for given independent constant vectors $\mathbf{a}_1$, $\mathbf{a}_2$. Later, we shall distribute identical scatterers, with scatterer C_j located at (or near) $\mathbf{r}_j$. The origin, O, is at $\mathbf{r}_0$. Let $d = \min\{|\mathbf{a}_1|, |\mathbf{a}_2|\}$; it is the distance from O to the nearest lattice point.

Solutions are sought satisfying the *Bloch condition*,

$$u(\mathbf{r}+\mathbf{r}_j) = u(\mathbf{r}) \exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j), \tag{2}$$

where $\mathbf{Q} = (q_1, q_2)$ is a constant vector and $\mathbf{r} = (x, y)$. Looking for solutions of the Helmholtz equation in the form

$$u_m(\mathbf{r}) = \exp(\mathrm{i}\mathbf{Q}_m\cdot\mathbf{r}) \quad \text{with } k^2 = Q_m^2 \quad \text{and} \quad Q_m = |\mathbf{Q}_m|,$$

we find that the Bloch condition is satisfied if $\mathbf{Q}_m = \mathbf{Q} + \mathbf{L}_m$ for each

$$\mathbf{L}_m = 2\pi(m_1\mathbf{b}_1 + m_2\mathbf{b}_2), \quad m_1, m_2 \in \mathbb{Z},$$

with $\mathbf{a}_i\cdot\mathbf{b}_j = \delta_{ij}$. The vector $\mathbf{L}_m$ is a *reciprocal lattice vector*; it satisfies

$$\mathbf{L}_m\cdot\mathbf{r}_j = 2\pi p \quad \text{for some } p \in \mathbb{Z}. \tag{3}$$

Explicitly, let $\mathscr{A} = |\mathbf{a}_1 \times \mathbf{a}_2|$ be the area of one cell in the lattice. Then, we can take

$$\mathbf{b}_1 = 2\pi\mathscr{A}^{-1}\mathbf{a}_2 \times \mathbf{a}_3 \quad \text{and} \quad \mathbf{b}_2 = 2\pi\mathscr{A}^{-1}\mathbf{a}_3 \times \mathbf{a}_1 \quad \text{with } \mathbf{a}_3 = \mathscr{A}^{-1}\mathbf{a}_1 \times \mathbf{a}_2.$$

We regard the vector $\mathbf{Q}$ as given, and then the calculations above give allowable values for k, namely Q_m. If we write $\mathbf{Q}_m = Q_m(\cos\tau_m, \sin\tau_m)$, we obtain

$$u_m(\mathbf{r}) = \exp\{\mathrm{i}Q_m(x\cos\tau_m + y\sin\tau_m)\}, \tag{4}$$

a plane wave with *lattice wavenumber* Q_m propagating at an angle τ_m to the positive x-axis. In general, there may be M_m distinct reciprocal lattice vectors $\mathbf{L}_m$ giving the same value for $Q_m = |\mathbf{Q} + \mathbf{L}_m|$. In such a case, we shall denote the corresponding propagation angles by τ_m^j, $j = 1, 2, \ldots, M_m$. The number M_m will depend on $\mathbf{Q}$, Q_m and Λ; generically, we expect $M_m = 1$, but larger values may be possible. For example, McIver [10] considers a square lattice with $\mathbf{Q}$ as a multiple of $\mathbf{a}_1$, and he investigates cases with M_m as large as 4.

3. Periodic case: circular scatterers

The Bloch solutions described above exist in the absence of scatterers. In order to represent arrays of scatterers, we begin by defining (radiating) wave-functions,

$$\psi_n^H(\mathbf{r}) = H_n(kr)\mathrm{e}^{\mathrm{i}n\theta}, \quad n \in \mathbb{Z},$$

with $H_n \equiv H_n^{(1)}$, $x = r\cos\theta$, $y = r\sin\theta$ and $r = |\mathbf{r}|$. Similarly,

$$\psi_n^J(\mathbf{r}) = J_n(kr)\mathrm{e}^{\mathrm{i}n\theta}, \quad \psi_n^Y(\mathbf{r}) = Y_n(kr)\mathrm{e}^{\mathrm{i}n\theta}, \quad n \in \mathbb{Z}.$$

Then, define

$$G_n(\mathbf{r}) = \sum_{\mathbf{r}_j \in \Lambda} \psi_n^H(\mathbf{r} - \mathbf{r}_j) \exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j). \tag{5}$$

This is a wave-function with a singularity at each lattice point, $\mathbf{r}_j$. Moreover, it is easy to verify that G_n satisfies the Bloch condition (2).

Note that we could replace ψ_n^H by ψ_n^Y in (5). The only reason for using ψ_n^H is to ensure that the Sommerfeld radiation condition (assuming time dependence of $\mathrm{e}^{-\mathrm{i}\omega t}$) is satisfied, but this condition is irrelevant for infinite arrays of scatterers. On the other hand, we could not replace ψ_n^H by ψ_n^J because we know that non-trivial solutions in the presence of scatterers must have singularities inside the scatterers.

We consider a periodic arrangement of circular cylinders, one at each lattice point. Each circle C_j has radius a. We look for solutions in the form

$$u(\mathbf{r}) = \sum_n A_n G_n(\mathbf{r}) \tag{6}$$

where the sum is over all $n \in \mathbb{Z}$ and A_n are unknown coefficients. By construction, u satisfies the Helmholtz equation and the Bloch condition. It remains to impose the boundary conditions on the cylinders. For simplicity, we assume that the cylinders are sound-soft, which means that we impose a Dirichlet condition.

3.1. Sound-soft cylinders

The boundary condition is

$$u(\mathbf{r})=0, \quad \mathbf{r}\in C_j, \quad j\in\mathbb{Z}.$$

It is enough to apply the condition on the circle centred at the origin, $\mathbf{r}_0$. To do this, we begin with Graf's addition theorem,

$$\psi_m^H(\mathbf{r}-\mathbf{r}_j)=\sum_n S_{mn}(-\mathbf{r}_j)\psi_n^J(\mathbf{r}), \quad r<|\mathbf{r}_j|,$$

where $S_{mn}(\mathbf{r})=\psi_{m-n}^H(\mathbf{r})$. Hence, as $\psi_n^H(-\mathbf{r})=(-1)^n\psi_n^H(\mathbf{r})$,

$$G_m(\mathbf{r})=\psi_m^H(\mathbf{r})+\sum_n(-1)^{m+n}\psi_n^J(\mathbf{r})\sigma_{m-n}^H, \quad 0<r<d, \tag{7}$$

where

$$\sigma_n^H=\sigma_n^H(k;\mathbf{Q};\Lambda)=\sum_{\mathbf{r}_j\in\Lambda}{}' \psi_n^H(\mathbf{r}_j)\exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j) \tag{8}$$

and the prime on the summation indicates that the term with $\mathbf{r}_0=\mathbf{0}$ is omitted. Substitution of (7) in (6) gives

$$u(\mathbf{r})=\sum_m\left\{A_m\psi_m^H(\mathbf{r})+\psi_m^J(\mathbf{r})\sum_n A_n(-1)^{m+n}\sigma_{n-m}^H\right\}$$

near C_0. Thus, $u=0$ on $r=a$ combined with orthogonality of $\mathrm{e}^{\mathrm{i}n\theta}$ gives

$$0=A_mH_m(ka)+J_m(ka)\sum_n A_n(-1)^{m+n}\sigma_{n-m}^H, \quad m\in\mathbb{Z}. \tag{9}$$

This is an infinite homogeneous linear system. Setting its determinant to zero then determines k for a specified $\mathbf{Q}$. Later, we shall denote solutions of the periodic problem by k_p.

3.2. Lattice sums

The quantity $\sigma_n^H(k;\mathbf{Q};\Lambda)$, defined by (8), is known as a *lattice sum*. For square arrays, it is denoted by $\mathscr{S}_n(k)$ in [11, Equation (41)] and by $S_n(k,\mathbf{Q})$ in [12, Equation (3.81)]. The special case where the Bloch vector $\mathbf{Q}=\mathbf{0}$ has been studied extensively. For square arrays, see [13, Equation (3.14)], [11, Equation (7)] and [14, Equation (1.5)].

As $\psi_n^H=\psi_n^J+\mathrm{i}\psi_n^Y$, we can write $\sigma_n^H=\sigma_n^J+\mathrm{i}\sigma_n^Y$. It turns out that $\sigma_n^J(k;\mathbf{Q};\Lambda)=-\delta_{n0}$, provided k is not a lattice wavenumber, $k^2\neq Q_m^2$. This result was proved by Berry [13, Equation (A.7)] for $\mathbf{Q}=\mathbf{0}$ and by Chin *et al.* [11, Equation (45)] for $\mathbf{Q}\neq\mathbf{0}$. The proofs are for square arrays, but they extend to arbitrary lattices. Consequently, (9) reduces to

$$0=A_mY_m(ka)+J_m(ka)\sum_n A_n(-1)^{m+n}\sigma_{n-m}^Y, \quad m\in\mathbb{Z}, \quad k^2\neq Q_m^2. \tag{10}$$

This is exactly what we would have obtained if we had started with ψ_n^Y in (5) instead of ψ_n^H.

There are many expressions for the lattice sums. We are interested especially in their singularities. We start with a standard integral representation,

$$H_0^{(1)}(kr)=\frac{1}{\mathrm{i}\pi^2}\iint\frac{\mathrm{e}^{\mathrm{i}\mathbf{L}\cdot\mathbf{r}}\,\mathrm{d}\mathbf{L}}{L^2-k^2-\mathrm{i}\varepsilon}. \tag{11}$$

Here, $L=|\mathbf{L}|$ and we let $\varepsilon\to 0+$ at the end of the calculation. Equation (11) is in [13] (put $l=0$ in Equation (B.1)), [11] (middle of p. 4592, without ε) and [15, Equation (2.9.39)]. Then, from (5), we have

$$\begin{aligned}
G_0(\mathbf{r}) &= \sum_{\mathbf{r}_j\in\Lambda}\psi_0^H(\mathbf{r}-\mathbf{r}_j)\exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j)\\
&=\frac{1}{\mathrm{i}\pi^2}\sum_{\mathbf{r}_j\in\Lambda}\iint\frac{\mathrm{e}^{\mathrm{i}\mathbf{L}\cdot(\mathbf{r}-\mathbf{r}_j)}}{L^2-k^2-\mathrm{i}\varepsilon}\mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j}\,\mathrm{d}\mathbf{L}\\
&=\frac{1}{\mathrm{i}\pi^2}\iint\frac{\mathrm{e}^{\mathrm{i}\mathbf{L}\cdot\mathbf{r}}}{L^2-k^2-\mathrm{i}\varepsilon}\sum_{\mathbf{r}_j\in\Lambda}\mathrm{e}^{-\mathrm{i}(\mathbf{L}-\mathbf{Q})\cdot\mathbf{r}_j}\,\mathrm{d}\mathbf{L}\\
&=\frac{4}{\mathrm{i}\mathscr{A}}\iint\frac{\mathrm{e}^{\mathrm{i}\mathbf{L}\cdot\mathbf{r}}}{L^2-k^2-\mathrm{i}\varepsilon}\sum_m\delta(\mathbf{L}-\mathbf{Q}-\mathbf{L}_m)\,\mathrm{d}\mathbf{L}\\
&=\frac{4}{\mathrm{i}\mathscr{A}}\sum_m\frac{\mathrm{e}^{\mathrm{i}\mathbf{Q}_m\cdot\mathbf{r}}}{Q_m^2-k^2}.
\end{aligned} \tag{12}$$

Here, we have used (A1), we have let $\varepsilon\to 0+$, $\mathbf{Q}_m=\mathbf{Q}+\mathbf{L}_m$, $Q_m=|\mathbf{Q}_m|$ and $\mathbf{L}_m$ is a reciprocal lattice vector. For square lattices, the formula (12) is in [11, Equation (39)].

Putting $\mathbf{Q}_m=Q_m(\cos\tau_m,\sin\tau_m)$,

$$e^{i\mathbf{Q}_m\cdot\mathbf{r}}=e^{iQ_m r\cos(\tau_m-\theta)}=\sum_n i^n J_n(Q_m r)e^{in(\tau_m-\theta)}$$

and then (12) gives

$$G_0(\mathbf{r})=\frac{4}{i\mathscr{A}}\sum_n i^n e^{-in\theta}\sum_m \frac{J_n(Q_m r)e^{in\tau_m}}{Q_m^2-k^2}.$$

Also from (5), we have

$$G_0(\mathbf{r})=\psi_0^H(\mathbf{r})+\sum_n(-1)^n\psi_{-n}^J(\mathbf{r})\sigma_n^H=H_0(kr)+\sum_n e^{-in\theta}J_n(kr)\sigma_n^H$$

for $0<r<d$. Comparing these two expressions for $G_0(\mathbf{r})$ gives

$$H_0(kr)+J_0(kr)\sigma_0^H=\frac{4}{i\mathscr{A}}\sum_m \frac{J_0(Q_m r)}{Q_m^2-k^2}$$

and, for $n\neq 0$,

$$J_n(kr)\sigma_n^H=\frac{4}{i\mathscr{A}}i^n\sum_m \frac{J_n(Q_m r)e^{in\tau_m}}{Q_m^2-k^2}.$$

These formulas are in [11, Equation (48)]. They show that

$$\sigma_n^H\simeq\frac{2i^{n+1}}{\mathscr{A}Q_m(k-Q_m)}\sum_{j=1}^{M_m}\exp(in\tau_m^j)\quad\text{when } k\simeq Q_m; \tag{13}$$

recall that there are M_m vectors $\mathbf{Q}_m$ with the same magnitude Q_m (see the discussion following (4)). The approximation is slightly different when $k\simeq -Q_m$, but we shall be interested in positive k and Q_m.

3.3. Small circular scatterers

The homogeneous system (9) is exact. However, we know that small sound-soft cylinders scatter isotropically [16, §8.2.5], so that approximations can be made. Thus, for $0<ka\ll 1$, we can put $A_n=\delta_{n0}$, whence (6) reduces to

$$u(\mathbf{r})=G_0(\mathbf{r})=\sum_{\mathbf{r}_j\in\Lambda}\psi_0^H(\mathbf{r}-\mathbf{r}_j)e^{i\mathbf{Q}\cdot\mathbf{r}_j} \tag{14}$$

and (9) reduces to

$$0=H_0(ka)+J_0(ka)\sigma_0^H(k;\mathbf{Q};\Lambda) \tag{15}$$

or, equivalently,

$$0=Y_0(ka)+J_0(ka)\sigma_0^Y(k;\mathbf{Q};\Lambda). \tag{16}$$

This is [17, Equation (18.28)] and [12, Equation (3.160)]. From (13), we obtain

$$\sigma_0^H\simeq\frac{2iM_m}{\mathscr{A}Q_m(k-Q_m)}\quad\text{when } k\simeq Q_m, \tag{17}$$

so that (15), $J_0(ka)\simeq 1$ and $H_0(ka)\simeq iY_0(Q_m a)$ give

$$Q_m-k\simeq\frac{2M_m}{\mathscr{A}Q_m Y_0(Q_m a)}, \tag{18}$$

which gives an estimate for the wavenumber ($k=k_p$) in the presence of scatterers, regarded as a correction to the wavenumber for a particular lattice wave (Q_m). Note that the approximation (18) was obtained assuming that $ka\simeq Q_m a\ll 1$, but nothing was assumed about the size of kd.

For small hard cylinders ($ka\ll 1$), the scattering is not isotropic, so that dipole terms are needed. McIver [10] has given results similar to (18), using matched asymptotic expansions, for cylinders of arbitrary cross-section. Similar methods for soft cylinders are developed in [18].

3.4. Foldy's deterministic method

Foldy's method starts by assuming isotropic scattering, so it is appropriate for small soft scatterers [16, Section 8.3]. It begins by supposing that we can write

$$u(\mathbf{r}) = \sum_{\mathbf{r}_j \in \Lambda} \mathscr{B}_j \psi_0^H(\mathbf{r}-\mathbf{r}_j) = \mathscr{B}_i \psi_0^H(\mathbf{r}-\mathbf{r}_i) + u_i^{\mathrm{e}}(\mathbf{r}), \tag{19}$$

where

$$u_i^{\mathrm{e}}(\mathbf{r}) = u(\mathbf{r}) - \mathscr{B}_i \psi_0^H(\mathbf{r}-\mathbf{r}_i) = \sum_{j\neq i} \mathscr{B}_j \psi_0^H(\mathbf{r}-\mathbf{r}_j). \tag{20}$$

The quantity $u_n^{\mathrm{e}}(\mathbf{r})$ is the 'external' or 'exciting' field; it is the field incident on the nth scatterer in the presence of all the other scatterers. Next, suppose that $\mathscr{B}_n = g u_n^{\mathrm{e}}(\mathbf{r}_n)$, where g is the scattering coefficient. Thus, the strength of the field scattered by the nth cylinder is proportional to the external field acting on that cylinder. All our scatterers are identical, so we use the same scattering coefficient for each. Then, evaluating (20) at $\mathbf{r} = \mathbf{r}_i$ gives

$$u_i^{\mathrm{e}}(\mathbf{r}_i) = g \sum_{j\neq i} u_j^{\mathrm{e}}(\mathbf{r}_j) \psi_0^H(\mathbf{r}_i - \mathbf{r}_j), \quad \mathbf{r}_i \in \Lambda, \tag{21}$$

a homogeneous linear system for the numbers $u_j^{\mathrm{e}}(\mathbf{r}_j)$. Looking for a solution in the form

$$u_j^{\mathrm{e}}(\mathbf{r}) = \exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}),$$

the system (21) reduces to

$$1 = g \sum_{j\neq i} \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot(\mathbf{r}_j - \mathbf{r}_i)} \psi_0^H(\mathbf{r}_i - \mathbf{r}_j).$$

As $\mathbf{r}_i - \mathbf{r}_j$ is a lattice point, we can write this as a single equation,

$$1 = g\sigma_0^H(k;\mathbf{Q};\Lambda), \tag{22}$$

where σ_0^H is a lattice sum. Also, $u(\mathbf{r}) = gG_0(\mathbf{r})$.

Comparison of (22) with (15) suggests that we take

$$g = -J_0(ka)/H_0(ka). \tag{23}$$

For a related approach, we could begin with

$$u(r,\theta) = G_0(\mathbf{r}) = H_0(kr) + \sum_n \mathrm{e}^{-\mathrm{i}n\theta} J_n(kr)\sigma_n^H.$$

Then, applying the boundary condition 'on average', $\int_{-\pi}^{\pi} u(a,\theta)\,\mathrm{d}\theta = 0$, gives (15) again.

Returning to (22), if we denote a solution by $k = k_{\mathrm{p}}$, and use the approximation (17), we obtain the estimate

$$k_{\mathrm{p}} - Q_m \simeq \frac{2\mathrm{i}gM_m}{\mathscr{A}Q_m}. \tag{24}$$

If we approximate g, as given by (23), for small ka, we have $g \sim \mathrm{i}/Y_0(ka)$, and then (24) reduces to (18) once we use $ka \simeq Q_m a$.

4. Positional disorder

We introduce perturbations of the periodic arrangement of identical circular cylinders. One option would be to randomly perturb the *radius* of each circular scatterer. Here, we randomly perturb the *location* of each cylinder. Thus, we suppose that the centre of the nth circle is displaced from $\mathbf{r}_n$ to $\mathbf{r}_n'$ with $|\mathbf{r}_n - \mathbf{r}_n'| < \varepsilon d$, where $0 < \varepsilon \ll 1$: each small disc, $\mathscr{D}_n$, of radius εd and centre $\mathbf{r}_n \in \Lambda$, contains exactly one scatterer, centred at $\mathbf{r}_n'$.

For simplicity, we use the Foldy deterministic model, (19) and (21); for a configuration Λ_N' of N cylinders, it gives

$$u(\mathbf{r}) = g \sum_{\mathbf{r}_j' \in \Lambda_N'} u_j^{\mathrm{e}}(\mathbf{r}_j') \psi_0^H(\mathbf{r} - \mathbf{r}_j') \tag{25}$$

where

$$u_i^{\mathrm{e}}(\mathbf{r}_i') = g \sum_{j\neq i} u_j^{\mathrm{e}}(\mathbf{r}_j') \psi_0^H(\mathbf{r}_i' - \mathbf{r}_j'), \quad \mathbf{r}_i' \in \Lambda_N'. \tag{26}$$

The sum in (25) has N terms and the sum in (26) has $N-1$ terms.

Next, we compute the ensemble average $\langle u\rangle$. Suppose that B_N is the region occupied by the N identical circles. We find that (see [16, Section 8.6.2], for example)

$$\langle u(\mathbf{r})\rangle = gN\int_{B_N} p(\mathbf{r}')v_N(\mathbf{r}')\psi_0^H(\mathbf{r}-\mathbf{r}')\,\mathrm{d}\mathbf{r}', \tag{27}$$

$$v_N(\mathbf{r}) = g(N-1)\int_{B_N} p(\mathbf{r}'|\mathbf{r})v_N^{(1)}(\mathbf{r}')\psi_0^H(\mathbf{r}-\mathbf{r}')\,\mathrm{d}\mathbf{r}', \tag{28}$$

and so on, with further equations in a familiar hierarchy, each one involving more information on the statistics of the distribution of the scatterers. (The probability $p(\mathbf{r})$ and the conditional probability $p(\mathbf{r}'|\mathbf{r})$ will be defined below, in (29) and (32), respectively; the function $v_N(\mathbf{r}_1')$ is a conditional average of u_1^{e}). This hierarchy is usually broken with a closure assumption.

At the lowest level, we may try using the Foldy closure assumption, $\langle u\rangle = v_N$, and then (27) becomes an integral equation for $\langle u\rangle$. However, it turns out that this integral equation does not yield a useful result as it cannot recover the known solution for the periodic case.

At the next level, we may use the Lax quasi-crystalline approximation (QCA), $v_N = v_N^{(1)}$, and then (28) becomes an integral equation for v_N. Once v_N has been found, $\langle u\rangle$ can be calculated from the formula (27). This is the approach adopted here. In fact, it is known that: QCA is optimal in a certain variational sense [19, 20]; QCA gives analytical results in agreement with independent calculations for random arrangements of weak scatterers [21]; and QCA gives good agreement with direct numerical simulations [22]. Note that our geometrical configuration is almost periodic: it can truly be described as quasi-crystalline!

To proceed, we must specify the probability $p(\mathbf{r}')$ and the conditional probability $p(\mathbf{r}'|\mathbf{r})$, and then we shall let $N\to\infty$.

Recall that the centre of the nth circle is allowed to move from the lattice point at $\mathbf{r}_n$ to a neighbouring point at $\mathbf{r}_n'$ inside a small disc of radius $R=\varepsilon d$, $\mathscr{D}_n$. Introduce a top-hat function, $\Pi_R(\mathbf{r})$, with $\Pi_R(\mathbf{r})=0$ for $r=|\mathbf{r}|>R$ and $\Pi_R(\mathbf{r})=1$ for $r<R$. Then, we take

$$p(\mathbf{r}') = \frac{1}{N\pi R^2}\sum_{\mathbf{r}_j\in\Lambda_N}\Pi_R(\mathbf{r}'-\mathbf{r}_j). \tag{29}$$

Thus, the probability of finding a scatterer centred at $\mathbf{r}'$ outside all N small discs is zero, whereas it is a certain constant inside any one of the discs; the constant is chosen so that $\int p(\mathbf{r})\,\mathrm{d}\mathbf{r}=1$. Notice that the sum in (25) is over the actual scatterer centres (in the finite, perturbed lattice, Λ_N'), whereas the sum in (29) is over the corresponding finite, periodic lattice Λ_N.

Using (29) in (27) gives

$$\langle u(\mathbf{r})\rangle = \frac{g}{\pi R^2}\int_{B_N} v_N(\mathbf{r}')\sum_{\mathbf{r}_j\in\Lambda_N}\Pi_R(\mathbf{r}'-\mathbf{r}_j)\psi_0^H(\mathbf{r}-\mathbf{r}')\,\mathrm{d}\mathbf{r}'.$$

Let $N\to\infty$ so that B_N becomes the whole plane. Then, writing $v\equiv v_\infty$, we obtain

$$\langle u(\mathbf{r})\rangle = \frac{g}{\pi R^2}\sum_{\mathbf{r}_j\in\Lambda}\int_{\mathscr{D}_j} v(\mathbf{r}')\psi_0^H(\mathbf{r}-\mathbf{r}')\,\mathrm{d}\mathbf{r}'. \tag{30}$$

Equation (30) shows that $\langle u\rangle$ can be written as an acoustic volume potential. This observation has several consequences. First, an application of (∇^2+k^2) to (30) gives

$$(\nabla^2+k^2)\langle u(\mathbf{r})\rangle = \begin{cases} 0, & \mathbf{r}\notin\mathscr{D}_i, \\ [4\mathrm{i}g/(\pi R^2)]v(\mathbf{r}), & \mathbf{r}\in\mathscr{D}_i, \end{cases} \qquad i\in\mathbb{Z}.$$

Thus, $\langle u\rangle$ solves a certain problem for a *periodic* lattice of circular scatterers, each of (small) radius $R=\varepsilon d$. A second consequence is that $\langle u\rangle$ and its normal (radial) derivative are both continuous across the boundary of each $\mathscr{D}_i$. However, as we do not (yet) know v, we do not know the partial differential equation satisfied by $\langle u\rangle$ inside each $\mathscr{D}_i$.

4.1. Calculation of v

Equation (30) also shows that we require $v(\mathbf{r})$ for $\mathbf{r}\in\mathscr{D}_i$, $i\in\mathbb{Z}$. If we seek solutions v satisfying the Bloch condition,

$$v(\mathbf{r}+\mathbf{r}_j) = v(\mathbf{r})\exp(\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j), \quad \mathbf{r}\in\mathscr{D}_0, \quad j\in\mathbb{Z}, \tag{31}$$

then it follows that $\langle u\rangle$ also satisfies the Bloch condition.

To find v, we turn to (28). Suppose there is a scatterer at $\mathbf{r}_i'\in\Lambda_N'$. Then, we take

$$p(\mathbf{r}'|\mathbf{r}_i') = \frac{1}{(N-1)\pi R^2}\sum_{j\neq i}\Pi_R(\mathbf{r}'-\mathbf{r}_j), \tag{32}$$

where the sum is over the N lattice points except the one at the centre of the disc in which $\mathbf{r}_i'$ lies, $\mathscr{D}_i$. Then, (28) gives

$$v_N(\mathbf{r}_i') = \frac{g}{\pi R^2}\sum_{j\neq i}\int_{B_N}\Pi_R(\mathbf{r}'-\mathbf{r}_j)v_N(\mathbf{r}')\psi_0^H(\mathbf{r}_i'-\mathbf{r}')\,\mathrm{d}\mathbf{r}', \quad \mathbf{r}_i'\in\mathscr{D}_i.$$

Let $N\to\infty$ and write $v\equiv v_\infty$, whence

$$v(\mathbf{r}_i')=\frac{g}{\pi R^2}\sum_{j\neq i}\int_{\mathscr{D}_j} v(\mathbf{r}')\psi_0^H(\mathbf{r}_i'-\mathbf{r}')\,\mathrm{d}\mathbf{r}',\quad \mathbf{r}_i'\in\mathscr{D}_i.$$

This equation shows that $(\nabla^2+k^2)v=0$ inside each $\mathscr{D}_i$.

Next, put $\mathbf{r}_i'=\mathbf{r}_i+\mathbf{s}$ and $\mathbf{r}'=\mathbf{r}_j+\mathbf{s}'$:

$$v(\mathbf{r}_i+\mathbf{s})=\frac{g}{\pi R^2}\sum_{j\neq i}\int_{\mathscr{D}_0} v(\mathbf{r}_j+\mathbf{s}')\psi_0^H(\mathbf{s}'-\mathbf{s}+\mathbf{r}_j-\mathbf{r}_i)\,\mathrm{d}\mathbf{s}',\quad \mathbf{s}\in\mathscr{D}_0,\quad i\in\mathbb{Z}.$$

Then, using (31) and noting that $\mathbf{r}_j-\mathbf{r}_i$ locates another lattice point, we obtain

$$v(\mathbf{s})=\frac{g}{\pi R^2}\sum_{\mathbf{r}_j\in\Lambda}{}' \mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j}\int_{\mathscr{D}_0} v(\mathbf{s}')\psi_0^H(\mathbf{s}'-\mathbf{s}+\mathbf{r}_j)\,\mathrm{d}\mathbf{s}',\quad \mathbf{s}\in\mathscr{D}_0. \tag{33}$$

As $|\mathbf{r}_j|>2R\geqslant|\mathbf{s}|+|\mathbf{s}'|$, we can use the two-centre expansion of ψ_0^H in the form [16, Theorem 2.14]

$$\psi_0^H(\mathbf{s}'-\mathbf{s}+\mathbf{r}_j)=\sum_n\sum_p(-1)^p\psi_{n-p}^H(\mathbf{r}_j)\psi_{-n}^J(\mathbf{s}')\psi_p^J(\mathbf{s}),$$

and then (33) gives

$$v(\mathbf{s})=g\sum_n\sum_p(-1)^p V_n\sigma_{n-p}^H\psi_p^J(\mathbf{s}),\quad \mathbf{s}\in\mathscr{D}_0, \tag{34}$$

where σ_n^H is a lattice sum (defined by (8)) and

$$V_n=\frac{1}{\pi R^2}\int_{\mathscr{D}_0} v(\mathbf{s})\psi_{-n}^J(\mathbf{s})\,\mathrm{d}\mathbf{s}.$$

Multiplying (34) by $\psi_{-m}^J(\mathbf{s})$ and integrating over $\mathscr{D}_0$ gives

$$V_m=g\sum_n\sum_p V_n\sigma_{n-p}^H\Omega_{mp},\quad m\in\mathbb{Z}, \tag{35}$$

where

$$\Omega_{mp}=\frac{(-1)^p}{\pi R^2}\int_{\mathscr{D}_0}\psi_{-m}^J(\mathbf{s})\psi_p^J(\mathbf{s})\,\mathrm{d}\mathbf{s}=\delta_{mp}\mathscr{J}_m(kR)$$

and

$$\mathscr{J}_m=\mathscr{J}_{-m}=\frac{2}{R^2}\int_0^R J_m^2(ks)s\,\mathrm{d}s=J_m^2(kR)-J_{m-1}(kR)J_{m+1}(kR), \tag{36}$$

using [23, Equation 5.54(2)]. Hence, (35) reduces to

$$V_m=g\mathscr{J}_m(kR)\sum_n V_n\sigma_{n-m}^H(k;\mathbf{Q};\Lambda),\quad m\in\mathbb{Z}. \tag{37}$$

This is an infinite homogeneous system of linear algebraic equations for V_n. Setting its determinant to zero yields the dispersion relation connecting k to $\mathbf{Q}$.

It is perhaps worth noting that, at this stage, we have not used the fact that ε is small, apart from requiring that the discs $\mathscr{D}_n$ do not overlap ($\varepsilon<\frac{1}{2}$). However, when ε *is* small, we can approximate (37); see Section 4.3.

4.2. Calculation of $\langle u\rangle$

Once $v(\mathbf{r})$ has been found for $\mathbf{r}\in\mathscr{D}_0$, we can calculate $\langle u(\mathbf{r})\rangle$ everywhere. Of most interest, perhaps, is $\langle u(\mathbf{r})\rangle$ inside $\mathscr{D}_0$. From (30) and (31), we have

$$\langle u(\mathbf{r})\rangle=\frac{g}{\pi R^2}\sum_{\mathbf{r}_j\in\Lambda}\mathrm{e}^{\mathrm{i}\mathbf{Q}\cdot\mathbf{r}_j}\int_{\mathscr{D}_0} v(\mathbf{s}')\psi_0^H(\mathbf{s}'-\mathbf{r}+\mathbf{r}_j)\,\mathrm{d}\mathbf{s}'.$$

Then, if $\mathbf{r}\in\mathscr{D}_0$, comparison with (33) shows that

$$\langle u(\mathbf{r})\rangle=v(\mathbf{r})+\frac{g}{\pi R^2}\int_{\mathscr{D}_0} v(\mathbf{s}')\psi_0^H(\mathbf{s}'-\mathbf{r})\,\mathrm{d}\mathbf{s}',\quad \mathbf{r}\in\mathscr{D}_0.$$

The remaining integral can be evaluated explicitly, using Graf's addition theorem, but we do not need the result here.

4.3. Approximations for small disorder

For very small disorder, we can approximate the function $\mathscr{J}_m(kR)$ occurring in (37). Immediately, we see from (36) that $\mathscr{J}_m(0)=\delta_{0m}$, so that (37) reduces correctly to (22) in the absence of disorder. Let us now refine this approximation. We have

$$\mathscr{J}_0(kR)\sim 1-(kR)^2/4, \quad \mathscr{J}_1(kR)=\mathscr{J}_{-1}(kR)\sim(kR)^2/8 \quad \text{as } kR=\varepsilon kd\to 0,$$

all other $\mathscr{J}_m$ being asymptotically smaller. Then, (37) shows that we should retain V_0 and $V_{\pm 1}$, and that these quantities satisfy

$$V_0=g\mathscr{J}_0\{V_0\sigma_0^H+V_1\sigma_1^H+V_{-1}\sigma_{-1}^H\}, \tag{38}$$

$$V_1=g\mathscr{J}_1\{V_0\sigma_{-1}^H+V_1\sigma_0^H+V_{-1}\sigma_{-2}^H\}, \tag{39}$$

$$V_{-1}=g\mathscr{J}_1\{V_0\sigma_1^H+V_1\sigma_2^H+V_{-1}\sigma_0^H\}. \tag{40}$$

To leading order, (39) and (40) show that $V_{\pm 1}\simeq g\mathscr{J}_1V_0\sigma_{\mp 1}^H$, and then (38) gives

$$\begin{aligned}1&=g\mathscr{J}_0\{\sigma_0^H+2g\mathscr{J}_1\sigma_1^H\sigma_{-1}^H\}\simeq g\mathscr{J}_0\sigma_0^H+2g^2\mathscr{J}_1\sigma_1^H\sigma_{-1}^H\\ &\simeq g\sigma_0^H(k)+\varepsilon^2(g/4)(kd)^2\{-\sigma_0^H(k)+g\sigma_1^H(k)\sigma_{-1}^H(k)\}.\end{aligned} \tag{41}$$

To leading order in ε, this equation gives $1=g\sigma_0^H(k)$, as expected. Denote the solution of this equation by $k_{\rm p}$, so that $\sigma_0^H(k_{\rm p})=g^{-1}$. Let $\sigma_0'(k)=({\rm d}/{\rm d}k)\sigma_0^H(k)$ and put

$$k=k_{\rm p}+\varepsilon^2\kappa, \tag{42}$$

so that $\sigma_0^H(k)\simeq g^{-1}+\varepsilon^2\kappa\sigma_0'(k_{\rm p})$. Then, the terms in ε^2 from (41) give

$$0=4\kappa\sigma_0'(k_{\rm p})+(k_{\rm p}d)^2\{-g^{-1}+g\sigma_1^H(k_{\rm p})\sigma_{-1}^H(k_{\rm p})\}. \tag{43}$$

This gives an estimate for κ, which then gives an estimate of $k-k_{\rm p}$; see (42).

We can approximate further. From (13), we have

$$\sigma_0^H(k)\simeq\frac{2{\rm i}M_m}{\mathscr{A}Q_m(k-Q_m)}, \quad \sigma_{\pm 1}^H(k)\simeq\frac{\mp 2T_m^{\pm}}{\mathscr{A}Q_m(k-Q_m)} \quad \text{with } T_m^{\pm}=\sum_{j=1}^{M_m}\exp(\pm{\rm i}\tau_m^j),$$

when $k\simeq Q_m$. If we also use the estimates (17) and (24), we find that

$$\kappa\simeq\frac{gM_m(k_{\rm p}d)^2}{2{\rm i}\mathscr{A}Q_m}\left(1-\frac{T_m^+T_m^-}{M_m^2}\right). \tag{44}$$

This estimate yields $\kappa=0$ when $M_m=1$ showing that, generically, $k-k_{\rm p}=o(\varepsilon^2)$ as $\varepsilon\to 0$: recall that the present analysis is based on isotropic scattering. When $M_m=2$, (44) gives

$$\kappa\simeq\frac{g(k_{\rm p}d)^2}{2{\rm i}\mathscr{A}Q_m}(1-\cos(\tau_m^1-\tau_m^2)) \quad (M_m=2).$$

5. Discussion and conclusion

We have given a method for estimating the effect of positional disorder on wave propagation when the original periodic structure consists of identical small soft circular scatterers located at the nodes of a regular lattice of parallelograms. This represents a first step as, clearly, much can be done to improve, verify and generalize the basic approach. To begin, the results could be compared with direct (Monte Carlo) numerical simulations; see [22]. In our analysis, we used the Lax QCA as a closure assumption: it should be possible to provide an independent check, at least for weak scatterers (penetrable scatterers with an interior wavenumber that is close to the exterior wavenumber, k); see [21]. Our analysis also assumed isotropic scattering. It is expected that this assumption can be removed, using appropriate multipole expansions, much as was done in [24] and elsewhere for related problems. This extension would permit other boundary conditions on the scatterers; the scatterers would not have to be small, and other shapes could be handled using T-matrix methods [16]. Extensions to three dimensions and to vector problems (such as electromagnetic and elastodynamic problems) are also feasible. We are currently working on some of these aspects of positional disorder in periodic structures.

Appendix A

In Section 3.2, we used the following formula:

$$\sum_j e^{-i\mathbf{r}\cdot\mathbf{r}_j} = \frac{(2\pi)^2}{\mathscr{A}} \sum_m \delta(\mathbf{r}-\mathbf{L}_m). \tag{A1}$$

To test this formula, multiply by $f(x,y)$ and integrate over all x and y, i.e. integrate over $\mathbf{r}$. On the right, we get

$$\sum_m \int f(x,y)\delta(\mathbf{r}-\mathbf{L}_m)\,d\mathbf{r} = \sum_m f(L_x^m, L_y^m)$$

where $\mathbf{L}_m = L_x^m \mathbf{i} + L_y^m \mathbf{j}$. On the left, we get

$$\sum_j \int f(x,y) \exp\{-i[x(\mathbf{i}\cdot\mathbf{r}_j)+y(\mathbf{j}\cdot\mathbf{r}_j)]\}\,dx\,dy. \tag{A2}$$

Expand the exponent, using (1) and $\mathbf{a}_l = a_x^l \mathbf{i} + a_y^l \mathbf{j}$, $l=1,2$:

$$x(\mathbf{i}\cdot\mathbf{r}_j)+y(\mathbf{j}\cdot\mathbf{r}_j) = j_1(xa_x^1+ya_y^1)+j_2(xa_x^2+ya_y^2).$$

This suggests using the Poisson summation formula,

$$\sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} f(u) e^{-imu}\,du = 2\pi \sum_{m=-\infty}^{\infty} f(2m\pi).$$

So, change variables in (A2) from x,y to x',y', with $x' = xa_x^1 + ya_y^1$ and $y' = xa_x^2 + ya_y^2$; inverting gives $x = (x'a_y^2 - y'a_y^1)/\Delta$ and $y = (y'a_x^1 - x'a_x^2)/\Delta$ with $\Delta = a_x^1 a_y^2 - a_x^2 a_y^1$. Note that $|\Delta| = |\mathbf{a}_1 \times \mathbf{a}_2| = \mathscr{A}$. Also, $dx\,dy = |J|\,dx'\,dy'$ where J is the Jacobian,

$$J = \begin{vmatrix} \partial x/\partial x' & \partial y/\partial x' \\ \partial x/\partial y' & \partial y/\partial y' \end{vmatrix} = \begin{vmatrix} a_y^2/\Delta & -a_x^2/\Delta \\ -a_y^1/\Delta & a_x^1/\Delta \end{vmatrix} = \frac{1}{\Delta}.$$

Hence, (A2) becomes

$$\sum_{j_1,j_2} \int f\left(\frac{x'a_y^2 - y'a_y^1}{\Delta}, \frac{y'a_x^1 - x'a_x^2}{\Delta}\right) e^{-i(j_1x'+j_2y')} \frac{dx'\,dy'}{\mathscr{A}} = \frac{(2\pi)^2}{\mathscr{A}} \sum_{n_1,n_2} f\left(\frac{2\pi}{\Delta}(n_1a_y^2 - n_2a_y^1), \frac{2\pi}{\Delta}(n_2a_x^1 - n_1a_x^2)\right).$$

To conclude, we check that the arguments of f on the right-hand side are the components of a reciprocal lattice vector, $\mathbf{L}_m$, by checking (3). Thus, using (1), we compute

$$\frac{2\pi}{\Delta}(n_1a_y^2 - n_2a_y^1)(j_1a_x^1 + j_2a_x^2) + \frac{2\pi}{\Delta}(n_2a_x^1 - n_1a_x^2)(j_1a_y^1 + j_2a_y^2) = 2\pi(j_1n_1 + j_2n_2),$$

which is (3) with $p = j_1n_1 + j_2n_2$.

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