Effective propagation in a perturbed periodic structure

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In a recent paper [D. Torrent, A. Hakansson, F. Cervera, and J. Sánchez-Dehesa, Phys. Rev. Lett. **96**, 204302 (2006)] inspected the effective parameters of a cluster containing an ensemble of scatterers with a periodic or a weakly disordered arrangement. A small amount of disorder is shown to have a small influence on the characteristics of the acoustic wave propagation with respect to the periodic case. In this Brief Report, we inspect further the effect of a deviation in the scatterer distribution from the periodic distribution. The quasicrystalline approximation is shown to be an efficient tool to quantify this effect. An analytical formula for the effective wave number is obtained in one-dimensional acoustic medium and is compared with the Berryman result in the low-frequency limit. Direct numerical calculations show a good agreement with the analytical predictions.

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In recent papers, Torrent *et al.*[1,2] used homogenization theory to characterize a cluster made of cylinders with periodical or weakly disordered arrangement. The authors showed that a small amount of disorder does not affect significantly the effective parameters of the perfect ordered system. It is the interest of this Brief Report to quantify the effect of a deviation from a periodic system on the effective wave propagation.

The one-dimensional (1D) configuration is under consideration in the present Brief Report. The simplicity inherent to one-dimensional media on the one hand permits us to gain insights of wave propagation in random media and allows us to perform complete numerical computations. On the other hand, the results obtained from the 1D problem can be applied directly to the physical problems of propagation in disordered media: layered systems,[3,4] transmission lines,[5] nearly periodic beaded strings,[6,7] electromagnetic waveguides,[8] acoustic ducts,[9] and elastic rods.[10]

Starting from a periodic set of scatterers, each scatterer is allowed to move randomly in each cell. This 1D configuration has been studied in Ref. 11 in the low-frequency approximation and for scatterers moving with maximum amplitude ($\epsilon=1$ in the following). In this Brief Report, analytical calculations are performed using multiple-scattering theory in the quasicrystalline approximation,[12,13] hereafter referred to as QCA. The dispersion relation for the effective wave number $K(k,\epsilon)$ is derived, where k is the wave number in free space and ϵ is a measure of the disorder. This 1D configuration with isotropic point scatterers is chosen because it allows us (i) to derive a simple analytical expression for QCA and (ii) to perform complete numerical computations to compare with the QCA results. Our main result is to show that the obtained dispersion relation agrees with direct numerical calculations. In the low-frequency limit, the Berryman prediction[14] is recovered at leading order and the deviation from this static law is derived.

In the literature, perturbative methods have been extensively used to study the effective propagation through scatterers. These methods are based on the knowledge of the wave propagation in a reference or unperturbed medium, say the unperturbed wave number k. The wave number K characterizing the wave propagation in the perturbed medium is then determined perturbatively close to the k value. In general, the reference medium is the medium free of scatterers, which implicitly assumes that the scatterers have a weak effect on the wave. Among the pertubative theories, the QCA by Lax[12,13] has been extensively used to study random distributions of scatterers in the approximation of dilute media. In general, QCA is unreliable since it used a closure assumption that is not clearly justified. However, this assumption being exact for a periodic distribution of scatterers, QCA is a candidate to be an efficient method to study configurations of scatterers weakly disordered with respect to a periodic configuration.

In the following, we consider an ensemble of N discrete isotropic scatterers. The scattering strength of each scatterer can be measured by the quantity M. For the ensemble of scatterers located at x_n, the total field u is the solution of the wave equation,

$$(\Delta + k^2)u(x) = Mk\sum_n \delta(x-x_n)u(x), \qquad (1)$$

where the right-hand side term describes the effect of the scatterers on the wave $u(x)$.

Equation (1) describes for instance the propagation of waves through an acoustic duct with Helmholtz resonators, which has been experimentally studied in Ref. 9, or also the vibrations in beaded strings.[7,10] In order to take into account the effect of finite-size scatterers, we will also consider Eq. (1) as the limit for small scatterer of size a having a contrast in the sound speed $\tilde{c}$ with respect to the sound speed c of the background medium. In that case, Eq. (1) describes the solution $u(x)$ for $a \to 0$ of the problem for finite-size scatterers,

$$(\Delta + k^2)u(x) = k^2(1-c^2/\tilde{c}^2)\sum_n \Pi_a(x-x_n)u(x), \qquad (2)$$

where $\Pi_a(x)=1$ for $|x|<a/2$ and $\Pi_a(x)=0$ for $|x|\geq a/2$. The relation between M and the contrast in sound speed is then

$$M=(1-c^2/\tilde{c}^2)ka. \tag{3}$$

Equation (1) [with Eq. (3)] and Eq. (2) (that accounts for finite-size effects) will be used for numerical calculations.

An approach to write the wave field resulting from the multiple scattering comes from the pioneering works of Foldy.[12,13,15,16] It consists in writing a set of consistent equations,

$$u(x)=u^0(x)+f\sum_{i=1}^{N}G(x-x_i)u^e(x_i),$$

$$u^e(x_i)=u^0(x_i)+f\sum_{j=1,j\neq i}^{N}G(x_i-x_j)u^e(x_j), \tag{4}$$

where $u^0(x)$ is the incident wave and $G(x)\equiv e^{ik|x|}/(2ik)$ is the Green's function of the free space. The first equation gives the total field $u(x)$, with u^e being the field incident on the scatterer centered at x_i, often referred as the *external* field at x_i. The second equation takes into account the multiple scattering in a consistent way. In the limit of isotropic point scatterers, the scattering function f stands for the T matrix. In that limit, the scattering function f is defined as the solution for a unique scatterer located at the origin $u(x)=u^0(x)+fG(x)u^0(0)$. The relation between the scattering function f and the potential M in Eq. (1) is obtained by identifying the solutions for a unique scatterer,

$$f=\frac{Mk}{1+iM/2}. \tag{5}$$

We now consider Eq. (4) for different configurations of the scatterer locations $(x_i)_{i=1\ldots N}$. Averaging Eq. (4) over all configurations leads to a set of N equations that involve more and more information on the statistics of the scatterer distribution. The first two equations of this hierarchy are

$$\langle u\rangle(x)=u^0(x)+Nf\int dx_1p(x_1)G(x-x_1)\langle u^e\rangle_1(x_1),$$

$$\langle u^e\rangle_1(x_1)=u^0(x_1)+(N-1)f\int dx_2p(x_2|x_1)G(x_1-x_2)\langle u^e\rangle_2(x_2). \tag{6}$$

These equations define successive functions of the form

$$\langle u^e\rangle_n(x_i)\equiv\int dx_{n+1}\ldots dx_Np(x_{n+1},\ldots x_N|x_1\ldots x_n)u^e(x_i), \tag{7}$$

where $i=1,\ldots,n$ and $p(x_{n+1},\ldots,x_N|x_1,\ldots,x_n)$ defines the normalized conditional probability of the set of scatterers centered at the $(x_{n+1},\ldots,x_N)$ positions when the set of scatterers centered at the $(x_1,\ldots,x_n)$ positions are fixed. In QCA, a closure assumption is used in which $\langle u^e\rangle_1=\langle u^e\rangle_2$, denoted as $\langle u^e\rangle$ in the following. Within this assumption, $\langle u^e\rangle$ satisfies

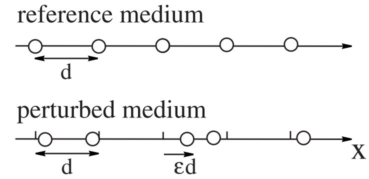

FIG. 1. The periodic lattice of scatterers is the reference medium with the effective Bloch Floquet wave number Q. In the perturbed medium, the embedded lattice is maintained and the scatterer inside each cell is put randomly with amplitude ϵd, with d being the lattice spacing.

$$\langle u^e\rangle(x_1)=u^0(x_1)+(N-1)f\int dx_2p(x_2|x_1)G(x_2-x_1)\langle u^e\rangle(x_2), \tag{8}$$

which constitutes the basic equation in QCA (for details, see, e.g., Ref. 17). Basically, QCA assumes that the joint probability $p(x_2|x_1)$ is sufficient to describe the scatterer distribution. This appears to be exact for periodic distribution; in that case, $p(x_2|x_1)=\sum_{n\neq 0}\delta(x_2-x_1-nd)/(N-1)$, with d being the lattice spacing, and no additional information can be gained on the periodic lattice when the position of one scatterer x_1 and d are known. The periodic lattice is used now as the reference medium. The perturbed medium departs from this reference medium as illustrated in Fig. 1. The embedded lattice is maintained and the scatterer inside each unit cell is put randomly with amplitude ϵd around its reference position. For this distribution, the joint probability is

$$p(x_2|x_1)=\frac{1}{(N-1)\epsilon d}\sum_{n\neq 0}\Pi_{\epsilon d}(x_2-x_1-nd). \tag{9}$$

The dispersion relation is obtained by solving Eq. (8) for $\langle u^e\rangle(x_i)=e^{iKx_i}$ and $i=1,2$ in the absence of incident wave. We obtain the dispersion relation on the QCA wave number K,

$$\frac{iM/2}{1+iM/2}e^{ikd}\left\{\frac{\text{sinc}[(K+k)\epsilon d/2]}{e^{-iKd}-e^{ikd}}+\frac{\text{sinc}[(K-k)\epsilon d/2]}{e^{iKd}-e^{ikd}}\right\}+1=0, \tag{10}$$

where the sinc function is $\text{sinc}\,x\equiv\sin x/x$. When $\epsilon=0$, the scatterers are periodically located and the Bloch Floquet mode $K=Q$ is obtained, leading to

$$\cos Qd=\cos kd+M/2\sin kd. \tag{11}$$

In the limit of nearly periodic structure $\epsilon\to 0$, the effective wave number K departs from Q,

$$Kd=Qd+\epsilon^2\frac{M}{48}\left[(Q^2+k^2)d^2\left(1+\frac{iM}{2}\right)\frac{\sin kd}{\sin Qd}-2kQd^2\right]+O(\epsilon^4). \tag{12}$$

To test the validity of the analytical QCA result, direct numerical simulations of the effective propagation through N scatterers are performed. In the first calculation, hereafter referred to as C_1, the propagation through N point scatterers is calculated by solving Eq. (1) with Eq. (3). The wave field is written $u(x_n\leq x<x_{n+1})=a_n(e^{ikx}+Z_ne^{-ikx})$. The continuity

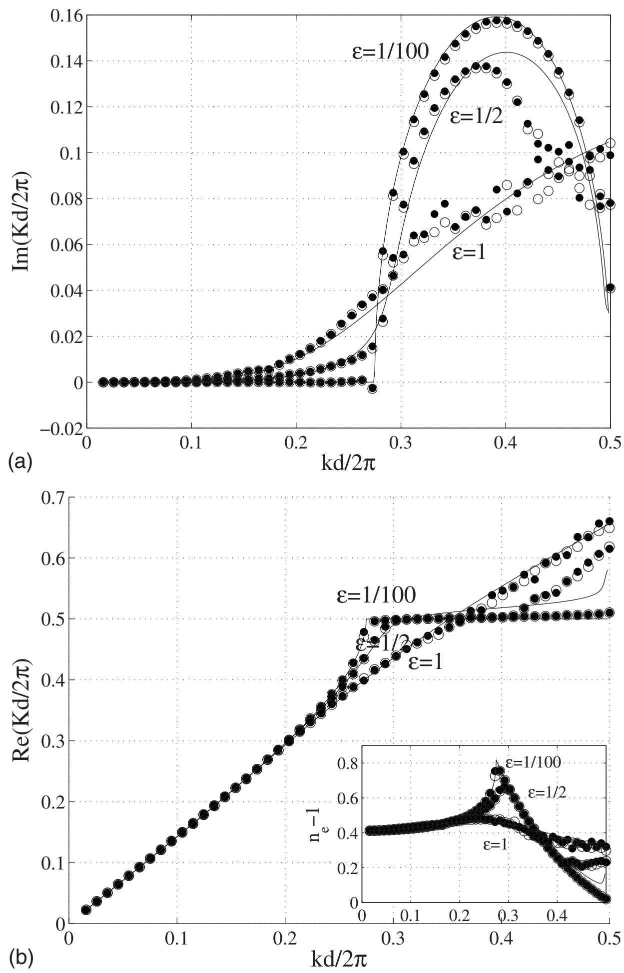

FIG. 2. Dispersion relation $K(k,\epsilon)$ of the perturbed periodic medium. Plain circles correspond to numerical results for the point scatterer model C_1, open circles correspond to numerical results for the finite-size model C_2, and the plain line give the prediction of the analytical model [Eq. (10)]. $c/\tilde{c}=10$ and $\varphi=1\%$.

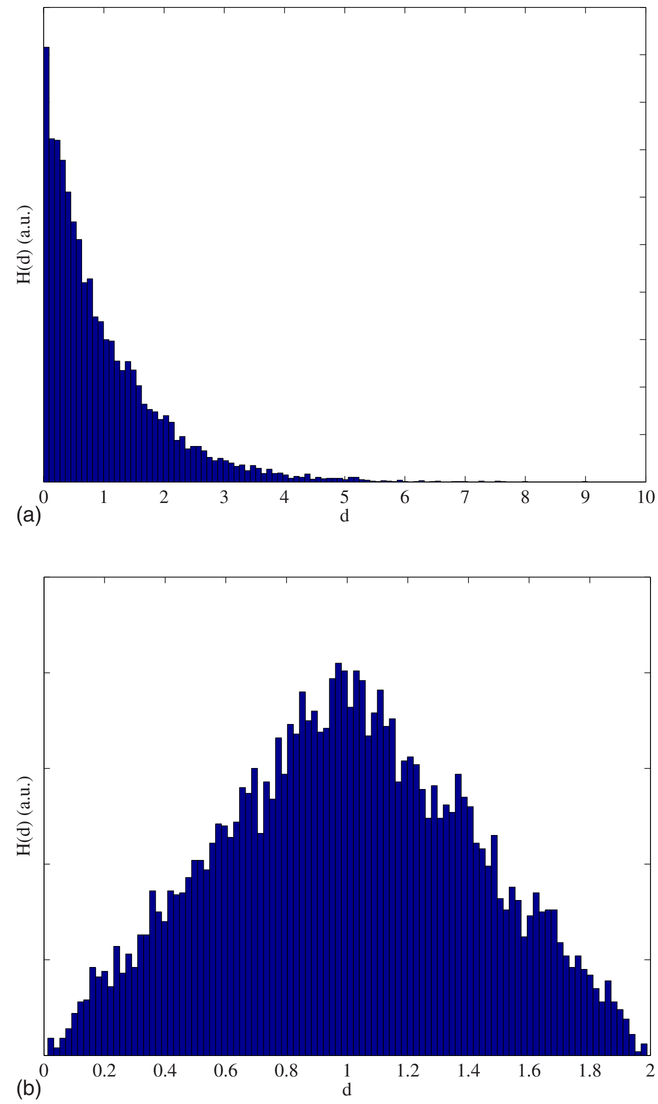

FIG. 3. (Color online) Histograms of the distances between closer scatterers for (a) a random distribution of scatterers (each of the N scatterers have been allowed to take any position in $[0,L]$) and for (b) a distribution of Fig. 1 with $\epsilon=1$.

relations, deduced from Eq. (1), are $[u]_{x_n}=0$ and $[u']_{x_n}=Mku(x_n)$, where $[u]_{x_n}$ stands for $[u]_{x_n}\equiv\lim_{\delta\to 0}[u(x_n+\delta)-u(x_n-\delta)]$. These relations allow us to define two recurrence relations on Z_n and on a_n. The radiation condition $Z_{2N}=0$ and the source condition $a_1=e^{ikx_1}$ at the first scatterer, together with the two recurrence relations, allow us to numerically calculate the field u.

In the second calculation (C_2), the finite size of the scatterers is taken into account owing to the model of Eq. (2). The interfaces between the background medium and the boundaries of the scatterers are denoted as $(y_n)_{n=1\ldots 2N}$, with $y_{2n-1}=x_n-a/2$ and $y_{2n}=x_n+a/2$ for $n=1,\ldots N$ in the wave equation (2). The wave field is written as $u(y_n\leq x<y_{n+1})=a_n(e^{ik_nx}+Z_ne^{-ik_nx})$, with either $k_n=k$ or $k_n=\tilde{k}\equiv kc/\tilde{c}$. The continuity relations for both u and u' (Ref. 18) at the interfaces give the two recurrence relations on Z_n and on a_n, afterward the calculation is the same in C_1.

In the numerical computations, $N=60$ (for kd/π approaching unity) to 200 scatterers are placed in a segment of length $L=Nd$ and the total field is calculated as described above (either in C_1 or C_2 numerical schemes). Several fields are calculated and averaged until the convergence is obtained for $\langle u\rangle(x)$. For the results presented here, the convergence is obtained after an average on 500–1000 realizations. The real and imaginary parts of K are deduced by estimating, respectively, the periodicity and the exponential decrease in $\langle u\rangle(x)$. Figure 2 shows the relation dispersions $K(k,\epsilon)$. A good agreement is found between the theoretical predictions in Eq. (10) and the numerical results, even for ϵ close to unity. For $\epsilon=1/100$, the configuration is very close to the periodic case. In that case, the agreement between the theoretical value and the numerical value is better than 1.8% (the error is measured by $|K^{\mathrm{num}}-K|/|K|$). The agreement for $\epsilon=1/2$ and 1 remains very good, with an error equal, respectively, to 6% and 7%, even for the k values corresponding to the band gap in the periodic case.

Incidentally, from Eq. (12), the low-frequency limit $kd\to 0$ of the QCA wave number K gives

$$\frac{K^2}{k^2} = 1 - \varphi + \varphi\frac{c^2}{\tilde{c}^2} + \frac{(ka)^2}{24}(1 - c^2/\tilde{c}^2)^2[2 + \epsilon^2(1 + iA)], \tag{13}$$

where $\varphi \equiv a/d$ is the filling fraction and $A \equiv ka[2/\varphi-(1-c^2/\tilde{c}^2)]/2$. In 1D, Berryman[14] predicted that the effective-mass density ρ_e and the inverse of the effective bulk modulus $1/(\rho_e c_e^2)$ are equal to the volume average mass density and the volume average inverse bulk modulus: $D_e=(1-\varphi)D+\varphi\tilde{D}$, with $D=\rho$ or $D=1/(\rho c^2)$. It follows that

$$\frac{1}{c_e^2} = \frac{\varphi}{\tilde{c}^2} + \frac{1-\varphi}{c^2}, \tag{14}$$

that coincides with our Eq. (13) at leading order. Also, it can be seen that the contribution of the disorder at low frequency is indeed small, as experimentally obtained in Refs. 1 and 2. We find a contribution in $(ka)^2\epsilon^2$.

It has been shown in the present Brief Report that QCA is well adapted to study the effective propagation through scatterers having a deviation with respect to reference periodic positions. Namely, this excludes configurations where many scatterers occupy the same unit cell, as it is possible for purely random configurations. This aspect was discussed by Lax[13] in terms of the pertinence of QCA for propagation of light in crystals, liquids, or gas, which is precisely in terms of the pertinence of a periodic medium as a reference medium. Of course, the use of QCA is very attractive since it allows us to account for the strong scattering effect, the small parameter being the deviation from a periodic medium. Experimental tests of our results could be performed in 1D nearly periodic systems such as beaded string systems[7] or acoustic ducts with Helmholtz resonators.[9] More generally, in any disordered system, QCA might be applied by measuring how close the set of scatterers is from a periodic structure. This is illustrated in Fig. 3 in 1D: from a gas type situation, where all scatterers can move randomly in the whole space to a crystal-type situation that has been considered here, the histogram of the distances between nearest scatterers goes from a Poisson distribution to a triangular distribution with a length that is a measure of the ϵ value.

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[18] In C_2, the continuity of the field u and its first derivative at the interfaces corresponds to the usual continuity relations of, say, the pressure (u) and the normal velocity (u'), when the contrast is in the sound speed only (namely, only a contrast in the mass density produces a discontinuity of the normal velocity u'). In C_1, the continuity relations are less straightforward: they correspond to the linearization of the continuity relations in C_2 for small ka. To see that it is sufficient to consider a unique scatterer of size a occupying $0 \leq x \leq a$. The reflection and transmission coefficients are $R=-ika(1-c^2/\tilde{c}^2)/2+O[(ka)^2]$ and $T=1+ika(c^2/\tilde{c}^2-3)+O[(ka)^2]$. Then, the discontinuity relations are $[u]=Te^{ika}-(R+1)=O[(ka)^2]$ and $[u']=ik[Te^{ika}-(1-R+)]=k^2a(1-c^2/\tilde{c}^2)+kO[(ka)^2]$. These conditions are the same than the conditions deduced from Eqs. (1)–(3) [where we have used $[u]=0$, $[u']=Mku(a/2)=k^2a(1-c^2/\tilde{c}^2)$, and we have used $u(a/2)=1+O(ka)$].