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Scattering by a slab: an exact calculation

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Abstract
We investigate scattering on an infinite number of point interactions distributed periodically on a finite number of parallel planes. Exact formulae for the transmission coefficients are given and their numerical behaviour is presented. For some values of the interaction parameter the reflection coefficient is close to one for a relatively large set of incident wavelengths.

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1. Introduction

In recent years many papers have been devoted to the study of photonic crystals i.e. periodic structures in which electromagnetic fields cannot propagate for some range of wavelengths and directions [18, 8, 5, 4]. Band gaps have been exhibited numerically for some peculiar periodic structures [12, 13, 14, 11, 19].

Real experiments use, of course, samples which are not infinite periodic structures but slabs or films. So theoretically it is interesting to study not only the spectrum corresponding to these samples but also their scattering properties. Common belief is that the waves whose frequencies are inside the gap for the full infinite structure, will be totally reflected by the slab regardless of their direction, if the width of the slab is sufficiently large. We can also ask if for other frequencies waves can be almost totally reflected for some partial set of directions. The aim of this paper is to solve a model giving us a response to these questions.

In a first attempt we will not look at the electromagnetic situation with Maxwell equations but at the Schrödinger equation. So we will study Hamiltonians corresponding to an infinite number of scatterers distributed over several planes, each of them forming a bidimensional lattice.

Each individual scatterer is described by a point interaction potential, which models an interaction of slow particles with a short range potential supported by a region much smaller than the wavelength. Such a kind of model has been introduced by Bethe and Peierls [3] and Thomas [17] and studied in a mathematically rigorous way by Berezin and Faddeev [2], Grossman, Høegh-Krohn, and Mebkhout [6] and Karpeshina [9]. A detailed review has been given in the book by Albeverio *et al* [1]. This simplification brings the advantage that the scattering by a unique interaction centre is explicitly known and simple. The scattered wavefunction at a point $\vec{x}$ corresponding to the incident plane wave $e^{i\vec{k}\vec{x}}$ is a spherical wave $\frac{e^{i\vec{k}\vec{y}}}{4\pi\alpha - ik}\frac{e^{ik|\vec{x}-\vec{y}|}}{4\pi|\vec{x}-\vec{y}|}$, where $\vec{y}$ is the position of the point scatterer and α is a parameter, positive or negative.

An infinite number of scatterers whose potentials are zero-range potentials have been studied earlier in [10, 15], in particular the study of the spectrum corresponding to a layer can be found in [1].

In section 2, we give the expression for a set of generalized eigenfunctions. They are the sum of the incident plane wave, several scattered plane waves with different wave vectors linked with the two-dimensional reciprocical lattice vectors and surface waves which decrease exponentially as the distance to the layers increases. The amplitudes of the plane waves i.e. the transmission and reflection coefficients can be expressed by series which are well convergent numerically.

In section 3, we give the numerical values for the transmission coefficients for some range of energies in the case of one layer. Playing with the strength of the individual scatterer α, we will see that the most intriguing effect is that, even for a small number of layers, an interval exists for the α near value -0.25, such that for wavelengths larger than twice the distance between the scatterers, the reflection is close to 1. We also give the numerical results for the amplitudes of the resulting scattered plane waves corresponding to ten planes for several strengths of the individual scatterer.

2. The formalism

The point scatterers are located on N two-dimensional parallel planes. Each layer is defined by a vector y_ν, $(\nu = 1, \ldots, N)$, which fixes the seed, and by two independent vectors a_2 and a_3 whose coordinates are $\left(0, a_\ell^2, a_\ell^3\right) \in \mathbb{R}^3$, $\ell = 2, 3$. So the point scatterers in the ν^{th} plane are located on the two-dimensional lattice $\Lambda_{2,\nu} = \{y | y = y_\nu + m_2 a_2 + m_3 a_3 \in \mathbb{R}^3, m = (m_2, m_3) \in \mathbb{Z}^2\}$. As in [1], we denote by Λ_2 the set of vectors $\lambda_m = m_2 a_2 + m_3 a_3 \in \mathbb{R}^3$, $(m_2, m_3) \in \mathbb{Z}^2$ and by $Y = \bigcup_\nu \Lambda_{2,\nu}$ the set of scatterers.

We consider in $\mathbb{R}^3$ the vectors b_2 and b_3 which satisfy $b_i a_j = 2\pi\delta_{ij}$ and denote by $\gamma_n = n_2 b_2 + n_3 b_3$, where $n = (n_2, n_3) \in \mathbb{Z}^2$ a vector of a two-dimensional lattice, called the reciprocical lattice, $\Lambda_2^\perp$.

The Hamiltonian $-\Delta_{\alpha,Y}$ corresponding to this set of scatterers is defined in [1], where it is shown that it can be decomposed in a direct integral of self-adjoint operators $-\Delta_{\alpha,Y}(\theta)$ acting on $H(\theta)$ which is the set of functions $\phi(x_1, x_2, x_3)$ belonging to $L^2(\mathbb{R} \times \mathbb{S}_2)$, ($\mathbb{S}_2$ is the two-dimensional unit cell, $x_2 a_2 + x_3 a_3 \in \mathbb{S}_2$, if $0 < x_2, x_3 < 1$) and such that $\phi(x_1, 1, 1) = e^{i(\theta_2+\theta_3)}\phi(x_1, 0, 0)$, where $\theta = (\theta_2, \theta_3)$ belongs to the two-dimensional Brillouin zone $B_2 = \mathbb{R}^2/\Lambda_2^\perp$.

For $\mathrm{Im}[z] > 0$ the reduced resolvent $(-\Delta_{\alpha,Y}(\theta) - z)^{-1}$ is given in [1], p 213 (1.6.23):

$$(-\Delta_{\alpha,Y}(\theta) - z)^{-1} = g_{\sqrt{z}}(\theta) + \sum_{\nu,\nu'} (\Gamma_{\alpha,Y}(\sqrt{z}, \theta))^{-1}_{\nu\nu'} (g_{\sqrt{z}}(. - y_{\nu'}, \theta), .) g_{\sqrt{z}}(. - y_\nu, \theta), \qquad (2.1)$$

where

$$g_{\sqrt{z}}(x, \theta) = \frac{1}{2}|\mathbb{S}_2|^{-1} \sum_n \frac{e^{-\sqrt{|\gamma_n+\theta|^2 - z}|x_1|}}{\sqrt{|\gamma_n + \theta|^2 - z}} e^{i(\gamma_n+\theta)x_\parallel},$$

see (1.6.12) p 211 in [1], $x \in \mathbb{R} \times \mathbb{S}_2$, ($|\mathbb{S}_2|$ is the area of $\mathbb{S}_2$) and

$$\Gamma_{\alpha,Y}(\sqrt{z},\theta) = (\alpha\delta_{\nu,\nu'} - g_{\sqrt{z}}(y_\nu - y_{\nu'},\theta))_{\nu,\nu'=1}^{N},$$

see (1.6.19) p 212 in [1] and $g_{\sqrt{z}}(\theta)$ is the operator whose kernel is $g_{\sqrt{z}}(x - x',\theta)$.

Then one can show that the Green function of $-\Delta_{\alpha,Y}$ can be expressed as

$$G(x,y,z) = \frac{\mathrm{e}^{\mathrm{i}\sqrt{z}|x-y|}}{4\pi|x-y|} + \int_{B_2} \mathrm{d}\theta \sum_{\nu,\nu'} (\Gamma_{\alpha,Y}(\sqrt{z},\theta))^{-1}_{\nu\nu'} g_{\sqrt{z}}(x-y_\nu,\theta) g_{\sqrt{z}}(y - y_{\nu'},\theta). \quad (2.2)$$

We calculate then $G(x,k,z) = \int G(x,y,z)\,\mathrm{e}^{\mathrm{i}ky}\,\mathrm{d}y$, $k = (k_\perp, k_\parallel) \in \mathbb{R}^3$ and define $\Psi(x,k) = \lim_{\epsilon\to 0} -\mathrm{i}\epsilon G(x,k,k^2+\mathrm{i}\epsilon)$.

One obtains

$$\Psi(x,k) = \mathrm{e}^{\mathrm{i}kx} + \frac{1}{2}|\mathbb{S}_2|^{-1} \sum_\nu \left(\sum_{\nu'} [\Gamma_{\alpha,Y}(|k|, k_\parallel - \gamma')^{-1}]_{\nu,\nu'}\,\mathrm{e}^{\mathrm{i}ky_{\nu'}} \right)$$
$$\times \left(\sum_{n,|\gamma_n+k_\parallel|<|k|} i \frac{\mathrm{e}^{\mathrm{i}\sqrt{k^2-(\gamma_n+k_\parallel)^2}|x_1-y_{\nu 1}|}}{\sqrt{k^2-(\gamma_n+k_\parallel)^2}}\,\mathrm{e}^{\mathrm{i}(k_\parallel+\gamma_n)(x_\parallel - y_{\nu_\parallel})} \right.$$
$$\left. + \sum_{\gamma_n,|\gamma_n+k_\parallel|>|k|} \frac{\mathrm{e}^{-\sqrt{(\gamma_n+k_\parallel)^2-k^2}|x_1-y_{\nu 1}|}}{\sqrt{(\gamma_n+k_\parallel)^2-k^2}}\,\mathrm{e}^{\mathrm{i}(k_\parallel-\gamma_n)(x_\parallel - y_{\nu_\parallel})} \right), \quad (2.3)$$

where γ' is the reciprocal lattice vector such that $k_\parallel - \gamma'$ belongs to B_2. It is easy to verify that $\Psi(x,k)$ is a solution of the Schrödinger equation:

$$-\Delta_{\alpha,Y}\Psi(x,k) = k^2\Psi(x,k).$$

One can observe that these states consist of a finite number of plane waves (the number depends on energy k^2) plus an infinite number of terms exponentially decreasing in the direction perpendicular to the plane of scatterers. It has been shown in [10] that there exists also another set of generalized eigenfunctions which decrease exponentially in the direction perpendicular to the plane of scatterers. These states are called surface states and they do not participate in the scattering. Using standard arguments [7, 16] one can prove that the two sets form a complete orthogonal system in $L_2(\mathbb{R}^3)$.

Karpeshina proved in [10] that the series

$$\sum_m \mathrm{e}^{\mathrm{i}k_\parallel\lambda_m} \frac{\mathrm{e}^{\mathrm{i}\sqrt{z}|x-\lambda_m|}}{4\pi|x-\lambda_m|}$$

which is evidently convergent for $\mathrm{Im}[z] > 0$ has a limit as $\mathrm{Im}[z] \to 0$. This limit is given by formula (23) in [10].

So the Poisson formula

$$\frac{1}{2}|\mathbb{S}_2|^{-1} \sum_n i \frac{\mathrm{e}^{\mathrm{i}\sqrt{z-(\gamma_n+k_\parallel)^2}|x_1|}}{\sqrt{z-(\gamma_n+k_\parallel)^2}}\,\mathrm{e}^{\mathrm{i}(k_\parallel+\gamma_n)x_\parallel} = \sum_m \mathrm{e}^{\mathrm{i}k_\parallel\lambda_m} \frac{\mathrm{e}^{\mathrm{i}\sqrt{z}|x-\lambda_m|}}{4\pi|x-\lambda_m|}$$

which is true for $\mathrm{Im}[z] > 0$ remains valid for $\mathrm{Im}[z] = 0_+$. This comes from the facts that the elements of the series are continuous with respect to z, the two series are equal for $\mathrm{Im}[z] > 0$ and they converge individually as $\mathrm{Im}[z] \to 0$.

So the scattered wave can also be written as an infinite sum of spherical scattered waves whose centres are the scatterers positions: $y_\nu + \lambda_m$

$$\Psi(x,k) = \mathrm{e}^{\mathrm{i}kx} + \sum_\nu \left(\sum_{\nu'} [\Gamma_{\alpha,Y}(|k|, k_\parallel - \gamma')^{-1}]_{\nu,\nu'}\,\mathrm{e}^{\mathrm{i}ky_{\nu'}} \right) \sum_m \mathrm{e}^{\mathrm{i}k_\parallel\lambda_m} \frac{\mathrm{e}^{\mathrm{i}|k||x-y_\nu-\lambda_m|}}{4\pi|x-y_\nu-\lambda_m|}. \quad (2.4)$$

In [1], p 135 a formula (1.5.1) is given for the scattering wave corresponding to a finite number of centres. One observes that (2.4) is an extension of this formula, to the case the number of scatterers becomes infinite. In our case the index j of formula (1.5.1) in [1] becomes a double index (ν, m). We can interpret $\sum_{\nu'}[\Gamma_{\alpha,Y}(|k|, k_\parallel - \gamma')^{-1}]_{\nu,\nu'}\, \mathrm{e}^{\mathrm{i}k(y_{\nu'}+\lambda_m)}$ in (2.4) as the amplitude $f_{\nu m}$ of the spherical scattered wave at $y_\nu + \lambda_m$.

Now consider some particular cases: if there is only one layer ($N = 1$) and we suppose $|\mathbb{S}_2| = 1$, the amplitude of the wave scattered by the centre located at $y_1 + \lambda_m$ is

$$\begin{aligned} f_{1m} &= \mathrm{e}^{\mathrm{i}k(y_1+\lambda_m)}\Gamma_{\alpha,Y}(|k|, k_\parallel - \gamma')^{-1} \\ &= \mathrm{e}^{\mathrm{i}k(y_1+\lambda_m)}(\alpha - g_{|k|}(0, k_\parallel - \gamma'))^{-1} \\ &= \frac{\mathrm{e}^{\mathrm{i}k(y_1+\lambda_m)}}{\alpha + \lim_{\omega\to\infty}\left(\frac{\omega}{4\pi} - \sum_{n,|k_\parallel+\gamma_n|<\omega}\frac{1}{2\sqrt{|k_\parallel+\gamma_n|^2-k^2}}\right)}. \end{aligned} \tag{2.5}$$

If moreover $k_\parallel = 0$ and $y_1 = 0$ then f_{1m} is independent of m, as it is clear from symmetry considerations, and it depends only on $|k|$, we will denote it $f(|k|)$. In this case, the generalized eigenfunction has the expression

$$\begin{aligned} \psi_{\alpha,Y}(x) = \mathrm{e}^{\mathrm{i}kx} + \frac{\mathrm{i}}{2}\frac{f(|k|)}{k}\mathrm{e}^{\mathrm{i}|k_\perp||x_1|} + \frac{\mathrm{i}}{2}f(|k|)\sum_{n,0<|\gamma_n|<k}\frac{\mathrm{e}^{\mathrm{i}\sqrt{k^2-\gamma_n^2}|x_1|}}{\sqrt{k^2-\gamma_n^2}}\mathrm{e}^{\mathrm{i}\gamma_n x_\parallel} \\ + \frac{f(|k|)}{2}\sum_{n,|\gamma_n|>k}\frac{\mathrm{e}^{-\sqrt{\gamma_n^2-k^2}|x_1|}}{\sqrt{\gamma_n^2-k^2}}\mathrm{e}^{\mathrm{i}\gamma_n x_\parallel}. \end{aligned}$$

So in the case $k_\parallel = 0$ the wavefunction is the sum of plane waves with a wave vector whose first component is $\sqrt{k^2-\gamma_n^2}$ (for all the n such that $|\gamma_n| < |k|$) and of surface waves decreasing exponentially with exponent $\sqrt{\gamma_n^2 - k^2}$, $(|\gamma_n| > k)$.

3. Numerical results and conclusion

Let us begin the discussion with the amplitude of the wave scattered at $y_1 + \lambda_m$ in the case of one layer formed by a square lattice of period 1. The behaviour of $|f(|k|)|$ is shown on figure 1. To evaluate $|f(|k|)|$ we used (2.5), where we put $\omega = 10^6$, which is sufficient to get three digit precision. The amplitude vanishes at the values of $|k|$ satisfying $k^2 - (k_\parallel + \gamma_n)^2 = 0$. This implies that they coincide with absolute values of vectors of the reciprocical lattice when k is perpendicular to the plane of scatterers. We show $|f|$ for three different values of α ($\alpha = -1, -0.25, 1$) both in the case of the wave vector perpendicular to the plane of scatterers ($\theta = 0$) and for k tilted *wrt* the plane ($\theta = \pi/3, \phi = \pi/5$). Here, θ is the polar angle measured from the direction perpendicular to the plane towards the plane and ϕ is the azimuthal angle in the plane of scatterers measured from the direction determined by a_2.

Further we denote the amplitude of the plane wave $\mathrm{e}^{\mathrm{i}\sqrt{k^2-|\gamma_{n_1n_2}|^2}x_1}$ by $A_{n_1n_2}$. For k perpendicular to the plane of scatterers we get

$$\begin{aligned} A_{0,0} &= 1 + \frac{\mathrm{i}}{2}\frac{f(|k|)}{|k|} \\ A_{1,0} = A_{0,-1} = A_{0,1} = A_{-1,0} &= \frac{\mathrm{i}}{2}\frac{f(|k|)}{\sqrt{k^2-4\pi^2}} \\ &\vdots \\ A_{n_1n_2} = \cdots = A_{n_2n_1} &= \frac{\mathrm{i}}{2}\frac{f(|k|)}{\sqrt{k^2-4\left(n_1^2+n_2^2\right)\pi^2}}. \end{aligned}$$

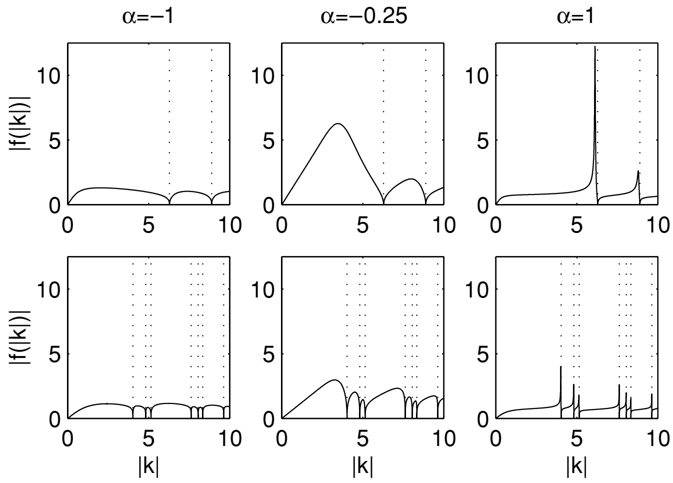

Figure 1. Absolute value of the amplitudes of spherical scattered waves $|f(|k|)|$ are shown for three values of scatterers strength $\alpha = -1, -0.25, 1$. The plane of scattering centres (i.e. $N = 1$) forms a square lattice of period 1 as described in section 2. The upper row corresponds to the situation when the incident plane wave is perpendicular to the plane of scatterers and the lower row to the incident plane wave with the vector k tilted ($\theta = \pi/3$ and $\phi = \pi/5$). In both cases $|f|$ is independent of m, $|f_m| = |f(|k|)|$. The dotted lines mark the positions of $|\gamma_{0,1}| = 2\pi$ and $|\gamma_{1,1}| = 2\sqrt{2}\pi$ in the upper row, while in the lower row they are determined by $k^2 - (k_\parallel + \gamma)^2 = 0$.

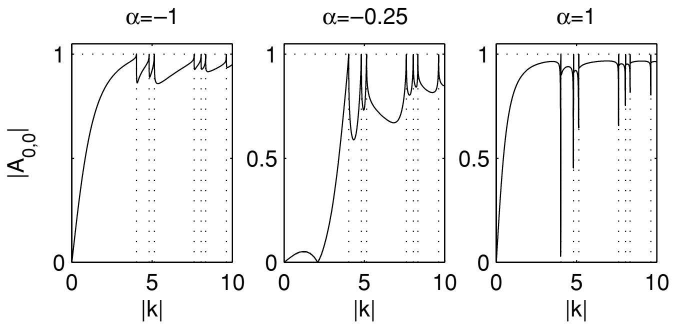

Figure 2. The dependence of the amplitudes of scattered plane waves $|A_{0,0}|$ on $|k|$ for three values of scatterers strengths $\alpha = -1, -0.25, 1$, for an incident plane wave whose direction with respect to the plane of scatterers is given by $\theta = \pi/3$ and $\phi = \pi/5$. The lattice is the same as that in figure 1 ($N = 1$).

There are four plane waves with identical amplitudes $A_{1,0} = A_{0,-1} = A_{0,1} = A_{-1,0}$, etc. If k is tilted, this 'degeneracy' is generally destroyed, i.e. plane waves begin to appear at different values of $|k|$. In figure 2 we present the amplitude of the scattered plane waves $|A_{0,0}|$ for the same three values of α as in figure 1 ($\alpha = -1, -0.25, 1$) in the case when the wave vector is tilted. The values of $|k|$ for which $|A_{0,0}| = 1$ are determined by $k^2 - (k_\parallel + \gamma)^2 = 0$.

As was already stated we verify that for $\alpha = -0.25$ the transmission is very small for a wide range of $|k|$, ($0 < |k| < \pi$). This phenomenon is also noticeable for α in an interval around -0.25: $(-0.3, -0.2)$. Let us recall here that the differential scattering cross section for one point interaction is smaller as $|\alpha| \to \infty$. $\alpha = -0.25$ corresponds to an interaction giving a larger scattering cross section than those corresponding to $\alpha = \pm 1$. It appears in

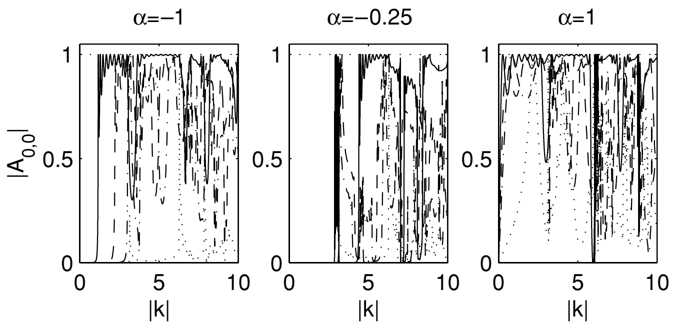

Figure 3. Scattering by $N = 10$ planes regularly spaced with spacing 1. The dependence of the amplitudes of scattered plane waves $|A_{0,0}|$ on $|k|$ is presented for three values of scatterers strengths $\alpha = -1, -0.25, 1$ and for four directions of the incident plane wave, $((\theta = 0, \phi = 0)$ the full line, $(\theta = \pi/3, \phi = 0)$ the dashed line, $(\theta = 2\pi/5, \phi = 0)$ the dash-dotted line and $(\theta = 49\pi/100, \phi = 0)$ the dotted line).

figure 2 that stronger scattering effects (strong reflection at low energies) appear for $\alpha = -0.25$ than for $\alpha = \pm 1$.

In figure 3 we present the values for the transmission coefficients for several directions of the incident wave vector. We only consider the case when the distance between the planes is constant, the individual α are all equal and $y_\nu^2 = y_\nu^3 = 0$ for all ν. We choose the distance equal to 1, $\alpha = -1, -0.25, 1$, and the number of planes $N = 10$.

For a given direction of the incident wave vector, as the number of planes increases, the transmission coefficients decrease in some intervals. When $N = 10$ they are close to zero in some intervals. This fact is reminiscent of the behaviour of the transmission coefficient in one dimension with a finite number of δ-functions (see [1], p 275). There, as the number of scatterers tends to infinity the values of $|k|$ for which the transmission coefficient becomes close to zero correspond to energies in the gaps of the spectrum of the Kronig–Penney operator. These values are multiples of the half of the reciprocal lattice vector length of the one-dimensional crystal. But here the corresponding energies and the gaps in the spectrum are no more related, since in the three-dimensional infinite crystal there is at most one gap (see [1, 9]). This means that, in general, if we change the direction of the incident wave vector, the energies at which the transmission coefficient is small will change. We can observe that each curve for $A_{0,0}$ presents pronounced dips in some wavelength intervals, and there is one dip which is common to all the directions considered.

We have calculated the gap for $\alpha = -0.25$, it corresponds to the interval of energies $(-8.515, 8.19)$ and we can see that the common dip is under the value 2.7 which is near $\sqrt{8.19} = 2.86$. So there is a coincidence between the common dip energies and the gap of the three-dimensional crystal. When for some energy interval and some direction of the incident wave vector the transmission coefficient $|A_{00}|$ is small, changing the incident wave vector direction we observe numerically that the transmission coefficient remains small in some solid angle.

In conclusion, we have given the formulae for the amplitudes of the plane waves and evanescent waves which form the total scattered wave. We have established the link between the transmission coefficients for a layer with a finite number of planes and the spectral properties of the full infinite crystal in three dimensions. For the values of α for which the three-dimensional crystal gap, Δ_2, overlaps the positive energy axis ($\alpha = -0.25$ is close to the value giving the largest second band bottom for the full infinite crystal operator), as the number of planes increases the transmission coefficients, for the energies in Δ_2, decrease. We also note that for α close to -0.25 and these energies transmission coefficient is quite small even for a single plane.

Acknowledgments

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