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LETTER TO THE EDITOR

Possible localization of sound propagation in hard-sphere gases

Kwang-Hua W Chu

Department of Physics, Northwest Normal University, Gansu, Lanzhou 730070, People's Republic of China

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Abstract

The effects of disorder (or free-orientation) using the discrete velocity model for the possible (dynamical) localization of (plane) sound waves propagating in dilute monatomic hard-sphere gases are presented. Comparison with previous fixed-orientation ($\theta = 0$) results show that there exists a certain gap in the spectra when the disorder or free-orientation exists and when a periodic medium with a gap (in spectra) is (slightly) randomized (like our orientation-free 4-velocity case) possible localization occurs in the vicinity of the edges of the gap.

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1. Introduction

Emerging interest in wave propagation in random, disordered and granular media has recently stimulated intensive research. Work on both theory and measurement is in rapid progress, acoustical analogues considering continuum mechanical and quantum mechanical approaches included [1–3]. Note that studies of classical wave mechanical systems have some important advantages over quantum mechanical wave systems even when there are similarities between them. In a mesoscopic system, where the sample size is smaller than the mean free path for elastic scattering, it is satisfactory for a one-electron model to solve the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V'(\vec{r})\psi = E\psi$$

or (after dividing by $-\hbar^2/2m$)

$$\nabla^2\psi + [q^2 - V(\vec{r})]\psi = 0 \qquad (1)$$

where q is an (energy) eigenvalue parameter, which for the quantum mechanical system is $\sqrt{2mE/\hbar^2}$. Meanwhile, the equation for classical (scalar) waves is

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} = 0$$

or after applying a Fourier transform in time and contriving a system where c (the wave speed) varies with position $\vec{r}$

$$\nabla^2\psi + [q^2 - V(\vec{r})]\psi = 0. \tag{2}$$

Here, the eigenvalue parameter q is ω/c_0, where ω is a natural (or an eigen-)frequency and c_0 is a reference wave speed. Comparing the time dependencies one sees the quantum and classical relation $E = \hbar\omega$ [3].

The control and observability of the classical experimental analogues may be matched by analytical works or numerical simulations. However, classical systems could be used to study time-dependent potential fields and nonlinear effects, which are very difficult and time-consuming to treat numerically or analytically. Motivated by the analogy between electrons in periodic or disordered metals and waves in classical acoustical systems an investigation for observing classical (Anderson) localization [4] using the discrete velocity model was performed and will be presented here.

The plane (sound) wave propagation in dilute monatomic (hard-sphere) gases has been successfully investigated by continuous and/or discrete velocity models since the 1960s [5, 6] (please see the detailed references therein). Relevant initial and/or boundary value problems, i.e. the former being central to the analytical or numerical approach because of the propagation of the forced sound from a certain origin, while the latter being almost related to the experimental environment due to the sensors and transducers somewhere downstream, must be well defined and then solved to obtain the complex spectra or dispersion relations (real part: sound dispersion, imaginary part: sound attenuation or absorption) [5, 6]. In comparison with experiments, results of the continuous velocity approach gave a better fit than the discrete velocity one [5, 6]. The integral form of the former, however, may smooth out some peculiar phenomena or only give *bulk* physical behaviour considering the continuous distribution of molecular velocities. The discrete form of the latter, i.e. molecular velocities (and thus the associated number density) being a finite set while keeping the space and time continuous, provides us possibilities to adjust the discrete velocity, for example its free orientation in the 2D plane (or a kind of disorder for co-planar velocity models), and solve relevant problems to gain more physical insights for specific interests. For instance, a molecular beam interacting with surfaces (solids or liquids) will normally depend on some specific incident or reflecting angles. Sound propagation in random or disordered media might be another case [2, 3]. We noticed that similar efforts, but employing the lattice gas model [7], have been reported recently which, because of the symmetry of the lattice, varied the orientation from $\theta = 0$ to $\pi/4$.

Our previous attempts used fixed-orientation discrete velocity models and, after comparing with experiments, gave rather physical fits, especially for the 4-velocity model [5, 6]. In this paper, we set the 4-velocity model to be orientation-free which could be thought of as a kind of disorder and then re-examine the dispersion relations (complex spectra) for the ultrasound propagation in hard-sphere (monatomic) gases. Sound waves are presumed to be plane waves. We note that, in a certain sense (on some length scale) a vortex could be treated as a combination of concentrated vorticity (core) with its surrounding irrotational fluid (flow) [8]. Thus, they could be, in a certain sense, similar to the hard-sphere particles when the elastic scattering or collisions for a system of them is being considered. Thus, our study here may give clues to sound propagation in a system of discrete vortices or vortex gases. Our preliminary results show that for $\theta = 0$ and $\pi/4$, θ being a disorder parameter, there exist gaps of spectra and possible (dynamical) localization which are similar to those reported in [1–4]. Our (discrete kinetic) approach, as it includes the non-uniform variation of those transport coefficients such as viscosity and thermal conductivity which are related to the mean free path of the gas [6,7] and cannot be handled by using the continuum mechanic or simple quantum mechanic approaches (e.g., that by Kirkpatrick [1]), will thus give researchers greater insight into similar problems.

2. Formulations

We assume that the gas is composed of identical particles of the same mass. The velocities of these particles are restricted to, for example, $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_p$, where p is a finite positive integer. The discrete number density of particles are denoted by $N_i(\boldsymbol{r}, t)$ associated with the velocity $\boldsymbol{u}_i$ at point $\boldsymbol{r}$ and time t. If only nonlinear binary collisions are considered, using the microreversibility property which will be defined later and considering the evolution of N_i, we have

$$\frac{\partial N_i}{\partial t} + \boldsymbol{u}_i \cdot \nabla N_i = \sum_{j=1}^{p} \sum_{(k,l)} (A_{kl}^{ij} N_k N_l - A_{ij}^{kl} N_i N_j) \qquad i = 1, \ldots, p$$

where (k, l) are admissible sets of collisions. We may then define the right-hand side of the above equation as

$$Q_i(N) = \tfrac{1}{2} \sum_{j,k,l} (A_{kl}^{ij} N_k N_l - A_{ij}^{kl} N_i N_j)$$

with $i \in \Lambda = \{1, \ldots, p\}$, and the summation is taken over all $j, k, l \in \Lambda$, where A_{kl}^{ij} are non-negative constants satisfying

$A_{kl}^{ji} = A_{kl}^{ij} = A_{lk}^{ij}$	indistinguishability of the particles in collision
$A_{kl}^{ij}(u_i + u_j - u_k - u_l) = 0$	conservation of momentum in the collision
$A_{kl}^{ij} = A_{ij}^{kl}$	microreversibility condition.

The conditions defined for the discrete velocity above requires that elastic binary collisions, such that momentum and energy are preserved $\boldsymbol{u}_i + \boldsymbol{u}_j = \boldsymbol{u}_k + \boldsymbol{u}_l$, $|\boldsymbol{u}_i|^2 + |\boldsymbol{u}_j|^2 = |\boldsymbol{u}_k|^2 + |\boldsymbol{u}_l|^2$, are possible for $1 \leqslant i, j, k, l \leqslant p$.

The collision operator is now simply obtained by joining A_{ij}^{kl} to the corresponding transition probability densities a_{ij}^{kl} through $A_{ij}^{kl} = S|\boldsymbol{u}_i - \boldsymbol{u}_j|\, a_{ij}^{kl}$, where,

$$a_{ij}^{kl} \geqslant 0 \qquad \sum_{k,l=1}^{p} a_{ij}^{kl} = 1 \qquad \forall i, j = 1, \ldots, p$$

with S being the effective collisional cross-section and the same order of magnitude as that (a, radius of hard-sphere scatters) used by Kirkpatrick [1]. If all q ($p = 2q$) outputs are assumed to be equally probable, then $a_{ij}^{kl} = 1/q$ for all k and l, otherwise $a_{ij}^{kl} = 0$.

The term $S|\boldsymbol{u}_i - \boldsymbol{u}_j|\mathrm{d}t$ is the volume spanned by the molecule with $\boldsymbol{u}_i$ in the relative motion w.r.t. the molecule with $\boldsymbol{u}_j$ in the time interval $\mathrm{d}t$. Therefore, $S|\boldsymbol{u}_i - \boldsymbol{u}_j|N_j$ is the number of j-molecules involved in the collision in unit time.

Collisions which satisfy the conservation and reversibility conditions which have been stated above are defined as an *admissible collision*.

Thus, the model of the discrete Boltzmann equation [5, 6, 9, 10] is a system of $2n(= p)$ semilinear partial differential equations of the hyperbolic type:

$$\frac{\partial}{\partial t} N_i + \boldsymbol{u}_i \cdot \frac{\partial}{\partial \boldsymbol{x}} N_i = \frac{2cS}{n} \sum_{j=1}^{n} N_j N_{j+n} - N_i N_{i+n} \qquad i = 1, \ldots, 2n \tag{3}$$

where $N_i = N_{i+2n}$ are unknown functions, and $\boldsymbol{u}_i = c(\cos[\theta+(i-1)\pi/n], \sin[\theta+(i-1)\pi/n])$; c is the reference velocity modulus and has the same order of magnitude as that (c, the sound speed in the absence of scatters) used by Kirkpatrick [1], θ is the orientation starting from the positive x-axis to the u_1 direction and could be thought of as a parameter for introducing a *disorder* (cf [5, 6, 9]).

Since passage of the sound wave causes a small departure from equilibrium (Maxwellian type) resulting in energy loss owing to internal friction and heat conduction, we linearize the above equations around a uniform Maxwellian state (N_0) by setting $N_i(t, \boldsymbol{x}) = N_0[1+P_i(t, \boldsymbol{x})]$, where P_i is a small perturbation. After some manipulations [5, 6], we have

$$\left\{\frac{\partial^2}{\partial t^2} + c^2\cos^2\left[\theta + \frac{(m-1)\pi}{n}\right]\frac{\partial^2}{\partial x^2} + 4cSN_0\frac{\partial}{\partial t}\right\}D_m = \frac{4cSN_0}{n}\sum_{k=1}^{n}\frac{\partial}{\partial t}D_k \tag{4}$$

where $D_m = (P_m+P_{m+n})/2, m = 1, \ldots, n$, since $D_1 = D_m$ for $1 = m \pmod{2n}$. We are ready to look for the solutions in the form of the plane wave $D_m = a_m \exp \mathrm{i}(kx-\omega t)$, $(m = 1, \ldots, n)$, with $\omega=\omega(k)$. This is related to the dispersion relations of 1D forced ultrasound propagation of the rarefied gases problem. Consequently we have

$$\left\{1 + \mathrm{i}h - 2\lambda^2\cos^2\left[\theta + \frac{(m-1)\pi}{n}\right]\right\}a_m - \frac{\mathrm{i}h}{n}\sum_{k=1}^{n}a_k = 0 \qquad m = 1, \ldots, n \tag{5}$$

with

$$\begin{aligned}\lambda &= kc/(\sqrt{2}\omega)\\ h &= 4cSN_0/\omega \;\propto\; 1/Kn\end{aligned} \tag{6}$$

where h is the rarefaction parameter of the gas; Kn is the Knudsen number which is defined as the ratio of the mean free path of gases to the wavelength of ultrasound [5, 6].

Let $a_m = \mathcal{C}/(1 + \mathrm{i}h - 2\lambda^2\cos^2[\theta + (m-1)\pi/n])$, where $\mathcal{C}$ is an arbitrary, unknown constant, since here we are only interested in the eigenvalues of the above relation. The eigenvalue problems for different a $2n$-velocity model reduces to $F_n(\lambda) = 0$, or

$$1 - \frac{\mathrm{i}h}{n}\sum_{m=1}^{n}\frac{1}{1 + \mathrm{i}h - 2\lambda^2\cos^2\left[\theta + \frac{(m-1)\pi}{n}\right]} = 0. \tag{7}$$

We only solve $n = 2$ here, i.e. the 4-velocity case. The corresponding eigenvalue equations become of algebraic polynomial form with the complex roots being the results of λ.

For the 2×2-velocity model, we obtain

$$1 - (\mathrm{i}h/2)\sum_{m=1}^{2}1/\{1 + \mathrm{i}h - 2\lambda^2\cos^2[\theta + (m-1)\pi/2]\} = 0. \tag{8}$$

3. Results and discussions

As $\theta \neq 0$, the complex-coefficient polynomial (equation for λ) obtained from equation (8) now has a degree of 4 instead of 2 for the fixed-orientation case ($\theta = 0$) [5, 6]. Note that from equation (8) as $\theta = 0$, $\cos(\pi/2) = 0$ for the $m = 2$ situation, thus we got a second-order polynomial. The complex-root finding procedure thus becomes much more complicated than before. After verifying our new results ($\theta \neq 0$), i.e. once we can recover $\theta = 0$ results from equation (8), we then solve equation (8) step by step to get the complete (complex) spectra from $\theta = 0$ up to $\pi/2$. We only present those of θ up to $\pi/4$ as spectra of orientation effects are symmetric w.r.t. $\theta = \pi/4$ after our checking [9, 10]. They are shown in figures 1–4.

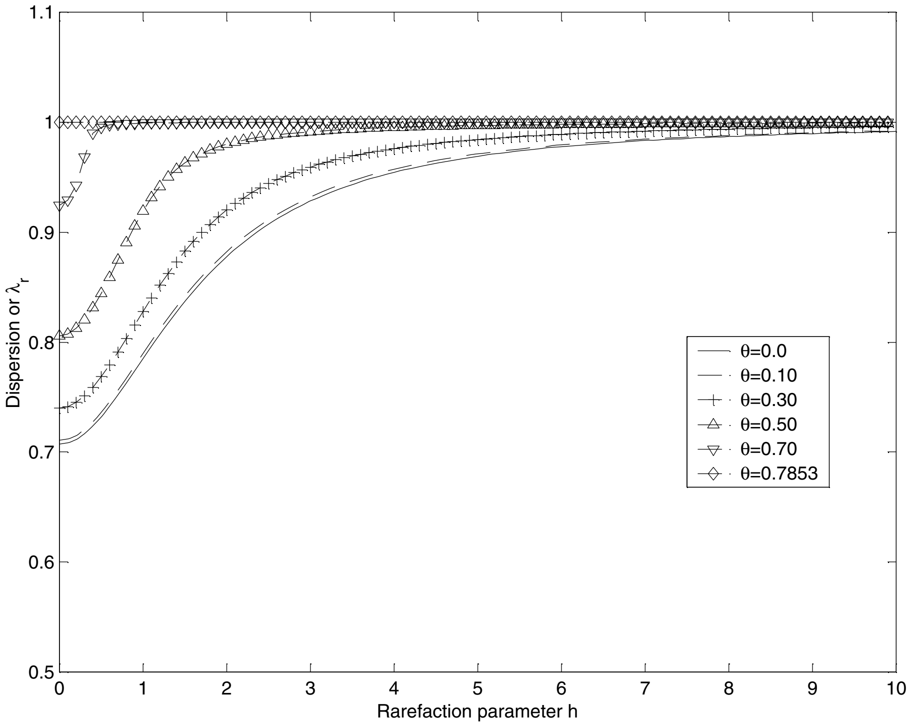

Figure 1. Orientational effects (θ) on the dispersion (λ_r).

We can observe that, the smaller (absolute values of λ) branch (propagation of sound mode) or lower values of both λ_r and λ_i (figures 1 and 2) show a continuous trend as θ increases toward $\pi/4$. The dispersion (λ_r; a relative measure of the sound or phase speed) keeps increasing while the attenuation or absorption (λ_i) keeps decreasing as θ increases from 0. At $\theta = \pi/4$, there is no attenuation and dispersion [9], i.e. $\lambda_r = 1.0$ and $\lambda_i = 0.0$. The latter result, if it is physical, could only be verified by the molecular-beam test, since the molecular distribution for a molecular beam is always in a Maxwellian form [5, 6]. This result also provides a good verification for the experimental side mentioned in [1–3] (acoustical analogue here) as there is no loss for this particular case (θ being a disorder parameter but fixed as $\pi/4$). We also notice that around $h \sim 1$, as shown in figure 2, there exists a trend for the absence of diffusion (λ_i starts decreasing rapidly).

Meanwhile, for the larger (absolute values of λ) branch (the anomalous one which is similar to the propagation of the diffusion mode or entropy wave reported in [5, 6]) or higher values of both real and imaginary roots (figures 3 and 4), there is a discontinuity near $\theta = 0$. Once θ increases from zero, there exists a gap. Spectra (both λ_r and λ_i) will span from the far infinity and then approach the asymptotic case $\theta = 0.7853$ (near $\pi/4$) which accounts for the propagation of the diffusion mode or entropy wave as verified in [5, 6]. Note that from the definition of h or Kn, $h = f_{\text{collision}}/f_{\text{sound}}$, where f_{sound} (cf that used by Kirkpatrick [1]) is related to the classical ω as mentioned in the *introduction* (cf equations (1) and (2)) so that it is relevant to the energy E as defined for the localization, thus we can estimate the localization length from those figures which vary with h. The localization length (ξ depending on the internal frequency) defined by Kirkpatrick [1] is proportional to the (hydrodynamic) mean free path $c \cdot l$ (l also depends on the internal frequency) and, comparing the definition of h here, is

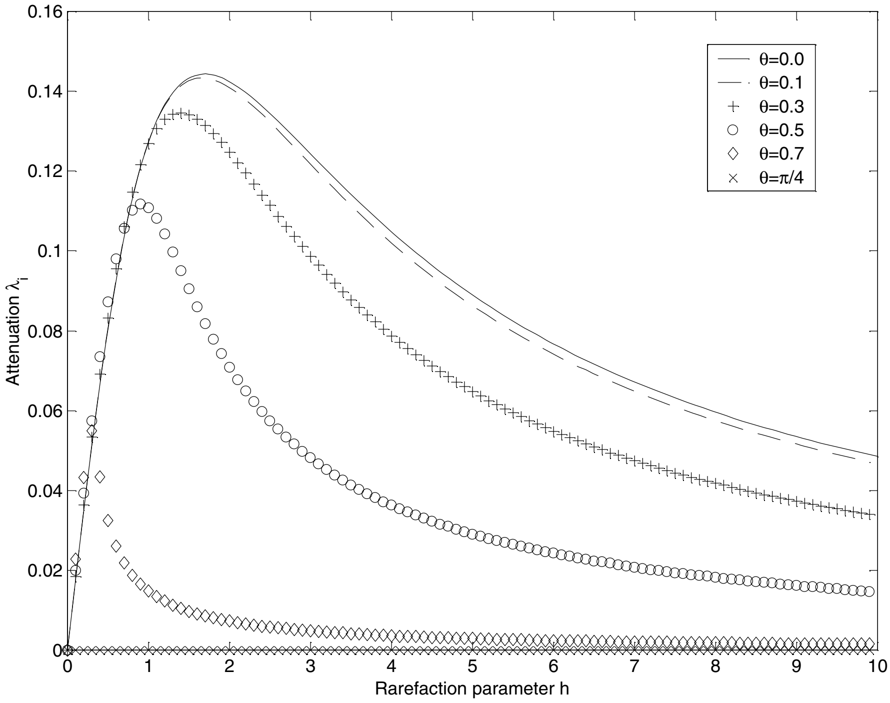

Figure 2. Orientational effects (θ) on the attenuation (λ_i).

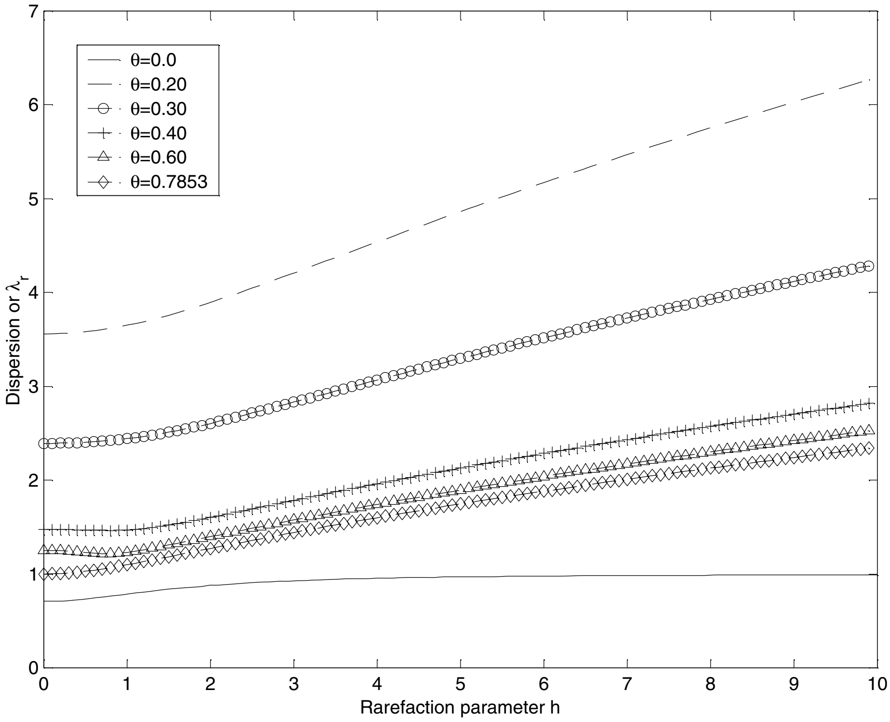

Figure 3. Orientational effects (θ) on the anomalous dispersion (λ_r).

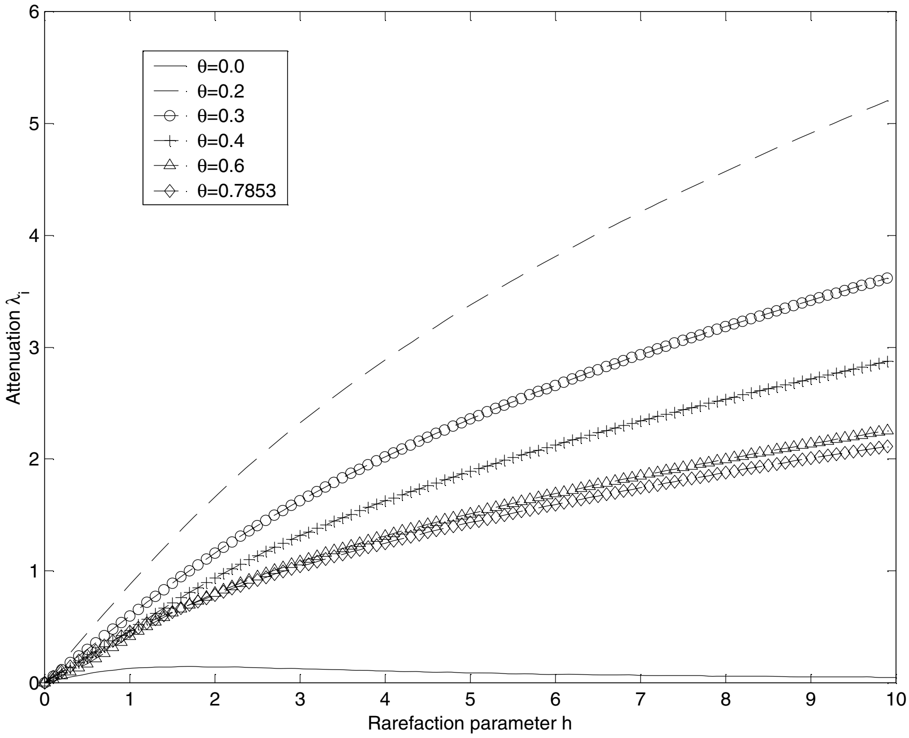

Figure 4. Orientational effects (θ) on the anomalous attenuation (λ_i).

thus related to the inverse of h we used. In fact, Kirkpatrick [1] obtained the expression of ξ by setting $\omega \to 0$ (cf equation (5.1b) therein). Based on these considerations and equations (1) and (2), the relation for the (possible) localization length versus the frequency extracted from our results (especially in figure 2; the attenuation or absorption defined here is related to the *inverse* measure of (say, one wave) length; the maximum absorption then corresponds to the minimum localization length in figure 5(a) of [1] by Kirkpatrick) length is qualitatively similar to that reported by Kirkpatrick [1].

To briefly conclude, since our calculations are orientation dependent, they may also give more clues to the reconstruction of a time-reversed acoustic field (via the angular spectrum), an experimental set-up for ultrasound transducers or the understanding of sound propagation in microscopically random, disordered or granular media [11]. The possible localized behaviour of the spectra (for the larger values) near $\theta = 0$ and $\pi/4$ for different branches of the spectra seems to be the same as the acoustic analogue of the *localization* found elsewhere [1–4] since the physical length-scale parameter used here is the mean free path of the molecular gases subjected to continuous collisions. The results presented here, in fact, as the characteristics of our approach are similar to that mentioned by Figotin and Klein [4], show that when a periodic medium with a gap (in resulting spectra) is (slightly) randomized (like our orientation-free 4-velocity case) [12], possible (Anderson) localization occurs in the vicinity of the edges of the gap (like that of $\pi/4$ here) [13]. As we only consider plane waves propagating in a hard-sphere gas, which is a kind of hard (Neumann) scatterer [13], then it is interesting that our results for the dispersion relation [10] resemble those of the Neumann cases (especially figure 9 in [13]) presented by Condat and Kirkpatrick.

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