Multiple scattering and possible localization of sound propagation in hard-sphere gases

2002 J. Phys. A: Math. Gen. 35 1919

(http://iopscience.iop.org/0305-4470/35/8/309)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 1919–1926 PII: S0305-4470(02)31426-4

Multiple scattering and 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

Received 29 November 2001, in final form 17 December 2001
Published 15 February 2002
Online at stacks.iop.org/JPhysA/35/1919

Abstract

Effects of the disorder (or free-orientation) on the multiple scattering situation by using discrete velocity models for the possible (dynamical) localization and/or delocalization of (plane) sound waves propagating in dilute monatomic hard-sphere gases are presented. After comparing with previous free-orientation ($n = 2$) results, we show that there also exists a certain gap of the spectra for the relevant periodic (wave-propagating) operator when the disorder or free-orientation exists and when a periodic medium with a gap (in spectra) is (slightly) randomized (like our orientation-free 6- and 8-velocity cases) then possible localization and/or delocalization occur in a vicinity of the edges of the gap, even when multiple scattering is being considered.

PACS numbers: 34.10.+x, 02.30.Jr, 02.30.Mv, 34.50.-s, 43.35.Ae, 43.20.El

1. Introduction

The multiple scattering of particles and waves was intensively studied around the early 1950s [1]. The relationship between the multiple scattering and localization, however, to the best knowledge of the author, is still open. Localization of classical waves occurs when the scale of the coherent scattering reduces to the wavelength itself. Recently studies of micro-scale and nano-scale phenomena have arisen in the interdisciplinary research areas of materials physics and chemistry or biology, where it is even more necessary to perform investigations at the atomic and molecular level by using modern technologies or smart sensing techniques for the wave scattering in complex, porous or heterogeneous media [2]. Special attention has been paid to the study of static or dynamical localization [2–8]. The former (Anderson localization) normally links to the phenomenon that at some site the wavefunction has a maximum amplitude and decreases exponentially away from that site. Both theory and experiment are in a state of rapid progress, including acoustical analogues considering continuum mechanic and quantum mechanic approaches [5–7]. Note that studies of classical wave mechanical systems have some important advantages over quantum mechanical wave systems even though 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 to use a one-electron model to solve the time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V'(\vec{r})\psi = E\psi \qquad \text{or} \qquad \nabla^2\psi + [q^2 - V(\vec{r})]\psi = 0 \tag{1}$$

(after dividing by $-\hbar^2/2m$), 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 dependences 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 [8] using discrete velocity models was performed and will be presented here.

The problem for plane (sound) waves propagating in dilute monatomic (hard-sphere) gases 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) [9–11]. In comparison with experiments, results of the continuous velocity approach gave a better fit than the discrete velocity one [9–11]. The integral form of the former, however, may smooth out some peculiar phenomena or only give *bulk* physical behaviour considering the continuous distribution of the particles' velocities. The discrete form of the latter, i.e. the particles' velocities (and thus the associated number density) being a finite set while keeping the space and time continuous, provides possibilities to adjust the discrete velocity, for example, the free orientation of it in the two-dimensional plane (or a kind of disorder for co-planar velocity models), and then solve relevant problems to gain more physical insights for specific interests. For instance, sound propagation in random or disordered media might be such a case [6, 7].

Our previous attempts using free-orientation discrete velocity models ($2n$-velocity models, where n stands for the possible number of incident or scattered velocity directions) gave rather physical results about the newly found localization [3], especially for the $n = 2$ case which might correspond to the single-scattering situation [9–11]. In this paper, we set $n = 3$ and 4 for the orientation-free models which could be thought of as introducing a kind of multiple scattering 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. Our preliminary results show that for $\theta \sim 0$ and/or $\theta = \pi/(2n)$, θ being a disorder parameter, there exist gaps of spectra for the corresponding periodic (wave-propagating) operator and possible (dynamical) localization (especially when the mean free path is of the same magnitude as the wavelength) which are similar to those reported in [2–8]. Our (discrete kinetic) approach, since it includes the non-uniform variation of those transport coefficients, like viscosity and thermal conductivity which are related to the mean free path of many particles (say, photons or electrons [5]) [9, 10] and cannot be handled by using the continuum mechanic or simple quantum mechanic approaches (e.g., that by Kirkpatrick in [5]), will thus give researchers more insights for similar problems.

2. Formulations

We assume that the (electron or photon) 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 is 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 require 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

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

where S is the effective collisional cross-section and the same order of magnitude as that (a, radius of hard-sphere scatters) used by Kirkpatrick in [1]. If all n ($p = 2n$) outputs are assumed to be equally probable, then $a_{ij}^{kl} = 1/n$ for all k and l, otherwise $a_{ij}^{kl} = 0$. $S|\boldsymbol{u}_i - \boldsymbol{u}_j|N_j$ is the number of j-molecules involved by the collision in unit time. Collisions which satisfy the conservation and reversibility conditions which have been stated above are defined as *admissible collisions*.

Thus, the model of discrete Boltzmann equation [9–12] is a system of $2n (= p)$ semilinear partial differential equations of the hyperbolic type:

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

where $N_i = N_{i+2n}$ (since we only consider head-on collisions during binary encounter and there are n different incident or scattered velocity directions) are unknown functions, and

$\boldsymbol{u}_i = c(\cos[\theta + (\mathrm{i} - 1)\pi/n], \sin[\theta + (\mathrm{i} - 1)\pi/n])$, c is a reference velocity modulus and the same order of magnitude as that (c, the sound speed in the absence of scatters) used by Kirkpatrick in [1], and 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 [3, 9–11]).

As passage of the sound wave will cause a small departure from equilibrium (Maxwellian type) which then results 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. The linearized version of the above equations is

$$\frac{\partial}{\partial t} P_m + \boldsymbol{u}_m \cdot \frac{\partial}{\partial \boldsymbol{x}} P_m + 2cSN_0(P_m + P_{m+n}) = \frac{2cSN_0}{n} \sum_{k=1}^{2n} P_k \qquad m = 1, \ldots, 2n \tag{4}$$

In these equations after replacing the index m with $m + n$ and using the identities $P_{m+2n} = P_m$, then we have

$$\frac{\partial}{\partial t} P_{m+n} - \boldsymbol{u}_m \cdot \frac{\partial}{\partial \boldsymbol{x}} P_{m+n} + 2cSN_0(P_m + P_{m+n}) = \frac{2cSN_0}{n} \sum_{k=1}^{2n} P_k. \tag{5}$$

Combining above two equations, firstly adding then subtracting, with $A_m = (P_m + P_{m+n})/2$ and $B_m = (P_m - P_{m+n})/2$, we obtain

$$\frac{\partial}{\partial t} A_m - c \cos\left[\frac{(m-1)\pi}{n} + \theta\right] \frac{\partial}{\partial x} B_m + 4cSN_0 A_m = \frac{4cSN_0}{n} \sum_{k=1}^{2n} A_k \tag{6}$$

$$\frac{\partial}{\partial t} B_m + c \cos\left[\frac{(m-1)\pi}{n} + \theta\right] \frac{\partial}{\partial x} A_m = 0 \qquad m = 1, \ldots, 2n. \tag{7}$$

From $P_{m+2n} = P_m$, and with $A_m = (P_m + P_{m+n})/2$ and $B_m = (P_m - P_{m+n})/2$, we have $A_{m+n} = A_m$, $B_{m+n} = -B_m$. After some manipulations [9–12], we

$$\left\{\frac{\partial^2}{\partial t^2} + c^2 \cos^2\left[\theta + \frac{(m-1)\pi}{n}\right] \frac{\partial^2}{\partial x^2} + 4cSN_0 \frac{\partial}{\partial t}\right\} D_m = \frac{4cSN_0}{n} \sum_{k=1}^{n} \frac{\partial}{\partial t} D_k \tag{8}$$

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 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 one-dimensional forced ultrasound propagation of the rarefied gases problem. Consequently, we have

$$\left\{1 + \mathrm{i}h - 2\lambda^2 \cos^2\left[\theta + \frac{(m-1)\pi}{n}\right]\right\} a_m - \frac{\mathrm{i}h}{n} \sum_{k=1}^{n} a_k = 0 \qquad m = 1, \ldots, n \tag{9}$$

with

$$\begin{aligned} \lambda &= kc/(\sqrt{2}\omega) \\ h &= 4cSN_0/\omega \qquad \propto 1/\mathrm{Kn} \end{aligned} \tag{10}$$

where h is the rarefaction parameter of the gas; Kn is the the Knudsen number defined as the ratio of the mean free path of particles to the wavelength of ultrasound [9–11].

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 the different $2n$-velocity model reduces to $F_n(\lambda) = 0$, or

$$1 - \frac{\mathrm{i}h}{n} \sum_{m=1}^{n} \frac{1}{1 + \mathrm{i}h - 2\lambda^2 \cos^2\left[\theta + \frac{(m-1)\pi}{n}\right]} = 0. \tag{11}$$

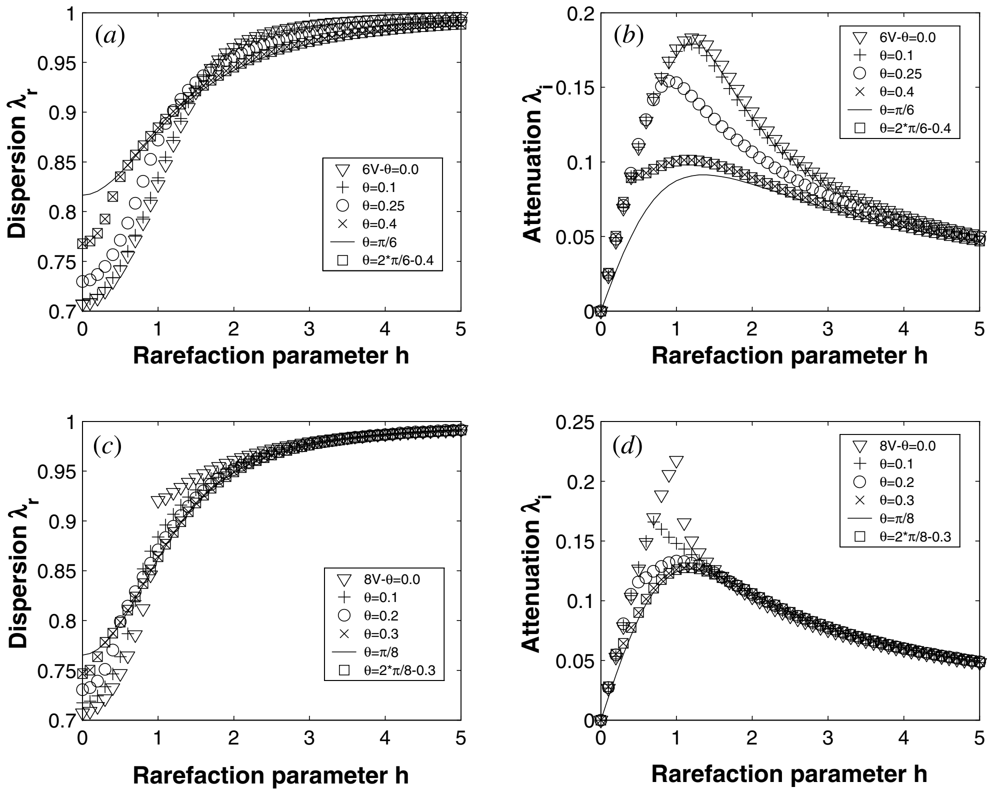

Figure 1. Comparison of $2n$-velocity orientational effects ($\theta = 0, 0.1, 0.25, 0.4, \pi/6, 2 \times \pi/6 - 0.4$) on: ($a$) the dispersion λ_r, $h = 4cSN_0/\omega$, S is the effective collisional cross-section, $n = 3$; (b) the attenuation λ_i, $n = 3$; (c) the dispersion λ_r, $n = 4$; (d) the attenuation λ_i, $n = 4$.

We only solve $n = 3, 4$, i.e. the 6- and 8-velocity cases, here. The corresponding eigenvalue equations become of algebraic polynomial-form with the complex roots being the results of λ [3]. As a continuous investigation of our previous works ($n = 2$) [3] and a similar study to the localization of classical (acoustic) waves (the primary interest only relates to the spectra of the relevant operator) [3, 4, 6, 8], we examine only the eigenvalues of the above equations for two cases ($n = 3, 4$) which means the possible (incident or scattered) direction of discrete velocities on binary encounter for head-on collisions could be three and four instead of two.

3. Results and discussions

As $\theta \neq 0$ and n increases, 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 the $\theta = 0$ results [9, 10] from equation (11), we then solve step by step equation (11) to get the complete (complex) spectra from $\theta = 0$ up to $\theta = \pi/2$. We only present those of θ up to $\pi/(2n)$ as spectra of orientation effects are symmetric w.r.t. $\theta = \pi/(2n)$ after our checking [11, 12]. They are shown in figures 1 and 2.

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(a), (c) and figures 1(b), (d) for $n = 3, 4$,

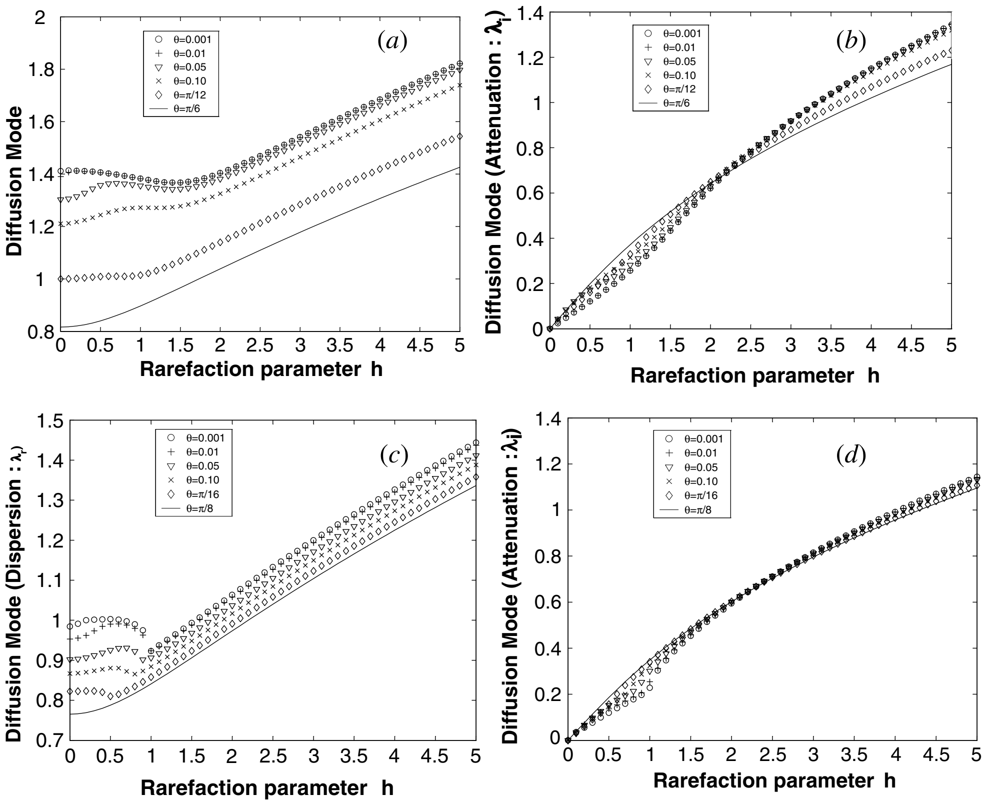

Figure 2. Orientational effects (θ) on the diffusion mode: (a) dispersion λ_r, $n = 3$ case; (b) attenuation λ_i; (c) dispersion λ_r, $n = 4$ case; (d) attenuation λ_i.

respectively) shows a continuous trend as θ increases toward $\pi/(2n)$. 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. This result provides a good verification for our previous works mentioned in [3, 11] even though n now increases from 2 to 3 and 4 which are related to the multiple scattering cases. We also notice that around $h \sim 1$ as shown in figures 1(b) ($n = 3$) and 1(d) ($n = 4$), there exists a trend for the absence of diffusion (λ_i starts decreasing rapidly). The latter trend ($n = 4$) is sharp enough which seems to be enhanced by the multiple scattering (cf page 34 of [5] for the case of $h \sim 1$ where a transition from extended to localized normal modes takes place as discussed by John). In fact, there are gaps of spectra (both λ_r and λ_i) for the corresponding operator (which resembles that reported by Figotin [6] or Figotin and Klein [8]) when $n = 4$ as shown in figures 1(c) and (d) for the case of $\theta = 0$ where $h \sim 1$.

Meanwhile, for the larger (absolute values of λ) branch (the anomalous one which is similar to those for propagation of the diffusion mode or entropy wave reported in [9, 10]) or higher values of both real and imaginary roots (figures 2(a), (c) and figures 2(b), (d) for $n = 3, 4$ respectively), there is no discontinuity near $\theta = 0$ compared to the case of $n = 2$ [3, 11]. Once θ increases from zero, there also exists no gap compared to the case of $n = 2$ [3, 11]. Spectra (both the dispersion λ_r and the absorption or attenuation λ_i) will span only for a limited range (after starting from $\theta = 0$ which means there is no disorder) and then approach to the asymptotic case $\pi/(2n)$ which accounts for the propagation of the diffusion mode or entropy wave as verified in [9, 10]. Interestingly, there exist gaps or sudden transitions (resembling of figures 4 and 5 in [5] presented by John; the Rayleigh scattering at low frequencies resembles our diffusion mode) for this kind of diffusion mode when $h \sim 1$ in the dispersion relation for both the $n = 3$ (a sudden transitions near $h = 1$) and $n = 4$ (gaps near $h = 1$) cases as shown in figures 2(*a*), (*c*) and 2(*b*), (*d*) respectively. The observed gap for $n = 4$ ($h \sim 1$) is orientation or disorder dependent as shown in figures 2(*c*) and (*d*). Note that from the definition of h or Kn, $h = f_{\text{collision}}/f_{\text{sound}}$, where f_{sound} (cf that used by Kirkpatrick in [5]) 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 in [5] by Kirkpatrick 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 thus related to the inverse of h that we used. In fact, Kirkpatrick obtained the expression of ξ by setting $\omega \to 0$ in [5] (cf equation (5.1*b*) 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 figures 1(*b*) and (*d*); 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 [5] by Kirkpatrick) is qualitatively similar to that reported by Kirkpatrick in [5]. Note that the spectrum associated with a periodic medium has a bandgap structure and that the most significant manifestation of coherent multiple scattering is the rise of a gap in the spectrum (cf Figotin [6] or Figotin and Klein [8]). Here, as n increases to 4, for $h \sim 1$, gaps of spectra occur as shown in figures 2(*c*) and (*d*).

To conclude in brief, our calculations here, as they are either orientation dependent or related to the multiple scattering, may also give more clues to the reconstruction of the time-reversed acoustic field (via the angular spectrum), the experimental set-up for ultrasound transducers or the understanding of sound propagation in microscopically random, disordered or granular media [13, 14]. The mode of diffusion resembles the Rayleigh scattering which takes place in light scattering due to density fluctuations (at low frequencies, cf page 36 of [5] as discussed by John). The possible localized behaviour of the spectra (for larger values) near $\theta = 0$ and $\pi/(2n)$ for different branches of the spectra seems to be the same as the acoustical analogue of the *localization* found elsewhere [3, 5–8] 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 is similar to that mentioned in [8] by Figotin and Klein, show that when a periodic medium with a gap (in resulting spectra) is (slightly) randomized (like our orientation-free 6- and 8-velocity cases), possible (Anderson) localization occurs in a vicinity of the edges of the gap (like that of $\pi/(2n)$ here) [15]. The localization behaviour for $n = 3$ or 4, however, is not exactly the same as that reported before for $n = 2$ [3, 11]. This may be due to multiple scattering [1, 5] and/or dynamical localization [4]. As we only consider plane waves propagating in a hard-sphere gas, which are a kind of hard (Neumann) scatters [15], then it is interesting that our results for the dispersion relation [12] resemble those of the Neumann cases (especially figure 9 in [15]) by Condat and Kirkpatrick.

Acknowledgments

This research is partially supported by the China Post-Dr Science Foundation. The author would like to thank Q Y Jie (Shanghai) for his valuable comments.

References

[1] Foldy L L 1945 *Phys. Rev.* **67** 107
Lax M 1951 *Rev. Mod. Phys.* **23** 287
[2] Stockman M I, Faleev S V and Bergman D J 2001 *Phys. Rev. Lett.* **87** 167401
[3] Chu K-H W 2001 *J. Phys. A: Math. Gen.* **34** L673
[4] Damanik D and Stollmann P 2001 *Geom. Funct. Anal.* **11** 11
[5] John S 1991 *Phys. Today* **44** 32
Kirkpatrick T R 1985 *Phys. Rev.* B **31** 5746
[6] Figotin A 1993 *J Stat. Phys.* **73** 571
Ishimann A 1978 *Wave Propagation and Scattering in a Random Media* (New York: Academic)
[7] Maynard J D 2001 *Rev. Mod. Phys.* **73** 401
Sheng P 1995 *Introduction to Wave Scattering, Localization, and Mesoscopic Phenomena* (New York: Academic)
[8] Anderson P W 1958 *Phys. Rev.* **109** 1492
Figotin A and Klein A 1996 *Commun. Math. Phys.* **180** 439
[9] Chu A K-H 1999 *Meccanica* **34** 59
Chu A K-H 1999 *Eur. Phys. J.* B **10** 1
[10] Chu Kwang-Hua 1998 *PhD Thesis* HKUST, Hong Kong/PRC
[11] Chu W K-H 2001 *Appl. Math. Lett.* **14** 275
[12] Chu K-H W 2002 *Preprint*
[13] Tourin A, Derode A and Fink M 1999 *Eur. Phys. Lett.* **47** 175
[14] Chu K-H W 2001 *Phys. Scr.* **63** 357
[15] Condat C A and Kirkpatrick T R 1987 *Phys. Rev.* B **36** 6782