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The speed of sound in a hard disk gas: A computer simulation

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We discuss the simulation of a system consisting of a rectangular box that contains two identical hard disk gases with the same number of particles, separated by an internal movable piston. The piston exhibits a random oscillatory motion with a frequency that depends on the mass of the piston, the mass of the disks, the temperature, and the length of the box. The measurement of this frequency allows us to deduce the speed of sound in the gas. The result is compared with the speed of sound from the usual expression in terms of the isothermal compressibility. © 2002 American Association of

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I. INTRODUCTION

It is well known that the speed c_s of a sound wave in a gas is related to thermodynamic quantities by means of the following expression:^{1,2}

$$c_s = \sqrt{\frac{\gamma}{\rho \kappa_T}}, \quad (1)$$

where $\gamma = c_P/c_V$ is the ratio between the specific heats of the gas, ρ is the density, and $\kappa_T = -V^{-1}(\partial V/\partial P)_T$ is the isothermal compressibility. For an ideal gas, Eq. (1) becomes

$$c_s = \sqrt{\frac{\gamma k_B T}{m}}, \quad (2)$$

where T is the absolute temperature, k_B is Boltzmann's constant, and m is the mass of a particle.

Equation (2) allows γ to be obtained from experimental measurements of c_s and T . Clark and Katz developed a resonance method for measuring γ (see, for example, Ref. 1). A simplified version of this method was proposed by Smith.³ The resonance method is based on the measurement of the amplitude of vibration of a piston inside a closed cylindrical tube containing a gas. The piston is forced into horizontal oscillation at the center of the tube by an externally applied magnetic field. If we neglect friction, take the gas to be ideal, and assume that the piston oscillates so quickly that the changes of the pressure and volume may be considered to be adiabatic, the frequency of maximum amplitude (resonance frequency) is given by³

$$\nu = \frac{1}{2\pi} \sqrt{\frac{2\gamma P A^2}{M V}}, \quad (3)$$

where P is the mean gas pressure, A is the cross-sectional area of the tube, M is the mass of the piston, and V is the volume of the gas on one side of the piston. Equation (3) is the same as the relation for the natural frequency of the ball in Rüchardt's method of measuring γ ,¹ except for the factor of $\sqrt{2}$ due to the fact that there is gas on both sides of the piston.

Equation (3) allows γ to be calculated from experimental measurement of ν . To obtain accurate values of γ from this method requires corrections due to the finite mass of the

oscillating gas and the piston, the nonideal behavior of the gas, the friction between piston and cylinder, and the non-adiabaticity of the compressions to be taken into account.

Although the resonance method has been mainly used to calculate γ , it can also be used for measuring the speed of sound in the gas. In fact, using Eq. (2) and taking into account the equation of state of an ideal gas, $PV = Nk_B T$, in which N is the number of particles in each side, Eq. (3) becomes

$$\nu = \frac{c_s}{2\pi L_0} \sqrt{\frac{2Nm}{M}}, \quad (4)$$

where L_0 is half the length of the tube. An accurate calculation of c_s from this method requires taking into account the same corrections as those mentioned above for the calculation of γ .

The Clark and Katz experiment raises the following question: What kind of motion of the piston should be expected (in the absence of a magnetic field)? For a macroscopic system, like the one considered in the Clark and Katz experiment, the piston should be at rest at the center of the tube due to the large number of particles, the large mass of the piston relative to the mass of the disks, and the friction between the piston and the cylinder. However, in the absence of friction, if the mass of the piston and the mass of the disks are comparable, and if the system does not contain a very large number of particles, we expect the piston to fluctuate about the center of the tube due to random collisions of the gas particles with the piston. This fluctuating motion is illustrated in the demonstration by Prentis,⁴ who developed a pressure fluctuation apparatus that simulates the mechanical interaction between two gases separated by a movable piston.

The small fluctuations of the piston generate longitudinal sound waves that propagate through the tube. We expect the piston to exhibit a random oscillatory motion with a frequency distribution displaying a pronounced peak at the fundamental resonance frequency of the system. By measuring this frequency, we can obtain the speed of sound in the gas. This is the goal of our work.

We propose a simple computer experiment consisting of the analysis of the motion of an internal movable piston inside a rectangular box containing two identical hard disk

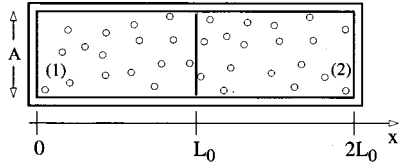


Fig. 1. Isolated rectangular box with a mechanical piston separating two identical hard disk gases.

gases separated by a piston. Using computer simulations we can do experiments without the presence of wall-piston friction and with adiabatic conditions. By doing a spectral analysis of the time evolution of the piston, we obtain the fundamental frequency and then calculate the speed of sound in a hard disk gas. The obtained simulation results can be compared with theoretical results that are obtained from the application of Eq. (1) to a hard disk gas.

The paper is structured as follows. In Sec. II we relate the resonance frequency of the oscillatory motion of the piston to the speed of sound in a gas and other parameters. In Sec. III we describe the details of the molecular dynamics simulations and compare our simulation results with theoretical predictions for the speed of sound in a hard disk gas. We conclude in Sec. IV with a brief summary.

II. THEORY

We consider the system depicted in Fig. 1. An isolated rectangular box contains a movable piston with no internal degrees of freedom, that initially divides the box into two regions of equal volume $V = AL_0$, where A is the cross-sectional area of the box and $L_0 \equiv L(0)$ is the initial length of each region. The left (1) and right (2) regions contain the same number of particles N of the same gas at the same mean temperature T , and thus the same mean pressure P is exerted on the piston. The piston exhibits fluctuations about the center position due to random collisions with gas particles from both regions. These fluctuations generate longitudinal sound waves that propagate in both regions and are described by the one-dimensional wave equations,

$$\frac{\partial^2 \xi_1}{\partial t^2} = c_s^2 \frac{\partial^2 \xi_1}{\partial x^2}, \quad (5)$$

$$\frac{\partial^2 \xi_2}{\partial t^2} = c_s^2 \frac{\partial^2 \xi_2}{\partial x^2}, \quad (6)$$

where $\xi_1 = \xi_1(x, t)$ and $\xi_2 = \xi_2(x, t)$ measure the displacement in the x direction of an infinitesimal slab of gas from its equilibrium position in the left and right regions, respectively, during the passage of the sound wave. The propagation speed of the sound wave, c_s , is the same in both regions and is given by Eq. (1). The boundary conditions of the system require that

$$\xi_1(0, t) = \xi_2(2L_0, t) = 0, \quad (7)$$

$$\xi_1(L_0, t) = \xi_2(L_0, t) = \xi(t), \quad (8)$$

where $\xi = \xi(t)$ measures the displacement of the piston with respect to its initial (equilibrium) position, that is, $\xi(t) = L(t) - L_0$.

If we take into account the boundary conditions (7), the general solutions of Eqs. (5) and (6) are, respectively,

$$\xi_1(x, t) = A_1 e^{i\omega t} \sin kx, \quad (9)$$

$$\xi_2(x, t) = A_2 e^{i\omega t} \sin k(x - 2L_0), \quad (10)$$

where A_1 and A_2 are the amplitudes of the corresponding sound waves, ω is the angular frequency, and $k = \omega/c_s$ is the wave number. By taking into account Eqs. (9) and (10), the first equality in Eq. (8) leads to

$$A_1 = -A_2. \quad (11)$$

On the other hand, the motion of the piston must be described by Newton's equation:

$$M \frac{\partial^2 \xi}{\partial t^2} = \left[-\tau \frac{\partial \xi_1}{\partial x} + \tau \frac{\partial \xi_2}{\partial x} \right]_{x=L_0}, \quad (12)$$

where the terms on the right-hand side are the forces acting on the piston arising from the sound pressure associated with the left and right sound waves, and the parameter τ (with the dimension of force) is given by²

$$\tau = \frac{Nm}{L_0} c_s^2 = \frac{Nm\omega^2}{k^2 L_0}. \quad (13)$$

From Eqs. (9) and (10), we obtain

$$\left(\frac{\partial \xi_1}{\partial x} \right)_{x=L_0} = A_1 k e^{i\omega t} \cos kL_0, \quad (14a)$$

$$\left(\frac{\partial \xi_2}{\partial x} \right)_{x=L_0} = A_2 k e^{i\omega t} \cos k(L_0 - 2L_0), \quad (14b)$$

and

$$\frac{\partial^2 \xi}{\partial t^2} = \frac{\partial^2 \xi_1(L_0, t)}{\partial t^2} = -\omega^2 A_1 e^{i\omega t} \sin kL_0. \quad (15)$$

We then substitute Eqs. (14a)–(15) into Eq. (12), take into account Eq. (11), and find

$$-M\omega^2 A_1 e^{i\omega t} \sin kL_0 = -2A_1 \tau k e^{i\omega t} \cos kL_0, \quad (16)$$

and thus

$$\cot K = \frac{M\omega^2}{2\tau k} = \frac{M}{2Nm} K, \quad (17)$$

where $K = kL_0$ and Eq. (13) has been used. Therefore, the resonance frequencies of the piston are given by

$$\nu = \frac{\omega}{2\pi} = \frac{c_s}{2\pi L_0} K, \quad (18)$$

with K given by the solutions of the transcendental equation (17). Equations (17) and (18) are the main theoretical results that we will use to obtain c_s from the measurement of the fundamental resonance frequency of the position of the piston.

The transcendental equation (17) can be solved numerically or graphically, as shown in Fig. 2. For the limiting cases $M \gg 2Nm$ and $M \ll 2Nm$, we can derive suitable asymptotic approximations. For $M \gg 2Nm$, $\cot K \approx 1/K$ for $K \ll 1$, and the first root behaves as $K \approx \sqrt{2Nm/M}$. If we substitute this result into Eq. (18), we obtain

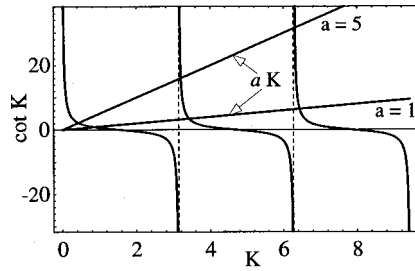


Fig. 2. Graphical solution of $\cot K = aK$ for $a = 1$ and $a = 5$.

$$\nu_1 \approx \frac{c_s}{2\pi L_0} \sqrt{\frac{2Nm}{M}}, \quad (19)$$

for the fundamental resonance frequency, in agreement with Eq. (4). The remaining roots approach the values $K \approx n\pi$ with $n = 2, 3, 4, \dots$, and the corresponding resonance frequencies approach the values

$$\nu_n \approx \frac{nc_s}{2L_0} \quad (n = 2, 3, 4, \dots), \quad (20)$$

which coincide with the harmonic frequencies of a tube of length L_0 closed at both ends. For $M \ll 2Nm$, the roots of Eq. (17) approach the values $K \approx n\pi/2$ with $n = 1, 3, 5, \dots$. From Eq. (18) the corresponding resonance frequencies are

$$\nu_n \approx \frac{nc_s}{4L_0} \quad (n = 1, 3, 5, \dots), \quad (21)$$

which coincide with the odd standing frequencies of a tube of length $2L_0$ closed at both ends. The reason why the even standing frequencies do not appear is that the corresponding sound waves have a node at the center of the box, where the piston is located.

III. COMPUTER SIMULATION AND RESULTS

The simulated system consists of $N_0 = 100$ hard disks of diameter σ and mass m , confined in a rectangular box of length $2L_0$ and cross-sectional area A . The box is divided by a piston of mass M and zero width. The collisions of the particles with the piston and walls and between particles are perfectly elastic, and there is no friction between the piston and the box, so the total energy $E_0 = N_0 k_B T$ is conserved. After the piston is released, the total energy will be $E_0 = N_0 k_B T' + E_{\text{piston}}$. Because the piston only has one degree of freedom, its mean kinetic energy is $k_B T'/2$, and thus its energy can be neglected with respect to the total energy E_0 and $T = T' + O(1/N_0) \approx T'$. For simplicity, we have chosen $\sigma = 1$ and $m = 1$. This choice is equivalent to scaling distances by σ and masses by m . Energies are scaled by $k_B T$, and time is scaled by $(m\sigma^2/k_B T)^{1/2}$.

The piston is initially ($t = 0$) fixed at the center of the box. Before the piston is released, a large number of collisions per particle ($\sim 10^4$) is performed to guarantee a Maxwellian velocity distribution for the gas particles. We have performed molecular dynamics simulations for $A = 10$ and $L_0 = 7.5, 10, 15, 20, 25, 30$, and 35 . For each value of L_0 , we considered several values of the mass of the piston, ranging from $M = 20$ to $M = 1000$.

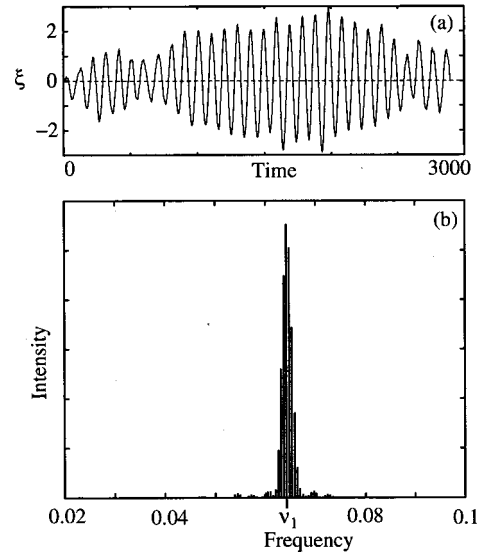


Fig. 3. (a) Plot of the displacement of the piston $\xi(t) = L(t) - L_0$ for $L_0 = 20$, $N = N_0/2 = 50$, $M = 200$, $A = 10$, and $k_B T = 1$. (b) The power spectrum of the time series displayed in part (a).

The molecular dynamics simulations were performed using a standard method for hard disks.^{5,6} This method is based on the fact that the dynamics of a hard disk system with periodic boundary conditions can be described by a sequence of collisions between elastic disks. When a collision occurs between two disks, i and j , their velocities \mathbf{v}_i and \mathbf{v}_j are instantaneously modified to the new values \mathbf{v}'_i and \mathbf{v}'_j . Between two consecutive collisions the motion of every disk i in the system is characterized by a constant velocity \mathbf{v}_i . The simulation consists in finding the next collision time, moving forward all the disks until the collision takes place, and calculating the new velocities for the colliding pair. More details on the molecular dynamics simulation of the hard disk fluid and sample computer code can be found in Ref. 6. For the simulations considered in this paper, we need to take into account collisions of the disks with the hard walls of the box and the movable piston (which moves in the x direction with constant speed between collisions). Thus in our case the dynamics of the hard disk system is a sequence of three different collision events: disk-disk, disk-wall, and disk-piston. For a disk-wall collision, the component of the velocity perpendicular to the wall changes its sign. In a disk-piston collision the new x component of the disk velocity and the new piston velocity are

$$v'_{x,i} = \frac{v_{x,i}(m - M) + 2Mv_p}{M + m} \quad (22)$$

and

$$v'_p = \frac{2mv_{x,i} + v_p(M - m)}{M + m}, \quad (23)$$

respectively. The position of the piston is measured at fixed time intervals.

An example of the displacement of the piston ξ as a function of time is plotted in Fig. 3(a) for $L_0 = 20$, $M = 200$, and $k_B T = 1$. The piston exhibits a fluctuating motion about the center of the box with a well-defined characteristic frequency. This frequency can be obtained from the time-

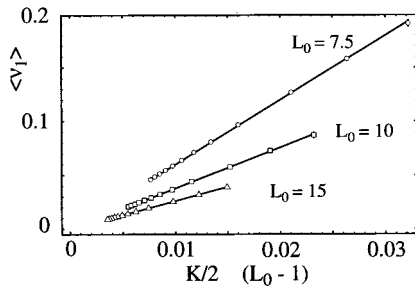


Fig. 4. The measured fundamental frequency $\langle \nu_1 \rangle$ vs $K/2\pi(L_0 - 1)$, where K is the lowest root of the transcendental equation (17) with $N=50$ and $M=20, 50, 100, 200, 300, 400, 500, 600, 700, 800, 900$, and 1000 , for $k_B T=1$ and $L_0=7.5$ (\circ), 10 (\square), and 15 (\triangle). The lines are the best fit through the obtained points. Note that most error bars are smaller than the size of the symbols.

domain data by measuring the period of the waveform. A more efficient way is to use a standard fast Fourier transform (FFT) method⁷ to obtain the power spectrum of the displacement $\xi(t)$. Figure 3(b) shows the power spectrum of the time series displayed in Fig. 3(a). We measure the nonzero value of the frequency corresponding to the maximum peak in the spectrum. To obtain a more accurate value of the fundamental frequency ν_1 , we have performed 100 trajectories for each case. Then, we take the average and the standard deviation for the 100 values of the maximum peak frequency of the spectrum. The values of $\langle \nu_1 \rangle$, with the corresponding errors for $L_0=7.5, 10$, and 15 are plotted versus $K/2\pi(L_0 - 1)$ in Fig. 4, where K is the lowest root of the transcendental equation (17). The appearance of the factor $1/(L_0 - 1)$, instead of $1/L_0$ in Eq. (18), is due to the fact that the effective length of one region for a hard disk is $L_0 - \sigma$ instead of L_0 . Similar plots (not shown) are obtained for the other values of L_0 . For each length, the corresponding speed of sound was obtained from the slope of the least squares fit to the data. The obtained values are given in the third column of Table I, with the corresponding uncertainties calculated by standard methods.

The speed of sound can be calculated theoretically using Eq. (1). For a hard disk gas, $c_P=2k_B T$ and $c_V=k_B T$, and hence $\gamma=2$. The isothermal compressibility κ_T can be obtained from the expression

$$\frac{V}{N\kappa_T} = k_B T \frac{\partial}{\partial \eta} [\eta Z(\eta)], \quad (24)$$

Table I. Speed of sound of a hard disk gas. The columns show L_0 , the half length of the rectangular box, the packing fraction η , the velocity of sound c_s determined from the motion of the piston, the velocity of sound obtained by using the scaled particle theory equation of state, $c_s^{(SPT)}$, and the velocity of sound obtained from the Henderson equation of state, $c_s^{(H)}$, respectively.

L_0	η	c_s	$c_s^{(SPT)}$	$c_s^{(H)}$
7.5	0.524	5.99 ± 0.09	5.31	5.45
10	0.393	3.78 ± 0.08	3.53	3.59
15	0.262	2.61 ± 0.03	2.50	2.53
20	0.196	2.20 ± 0.02	2.15	2.16
25	0.157	2.01 ± 0.02	1.97	1.97
30	0.131	1.89 ± 0.02	1.86	1.86
35	0.112	1.81 ± 0.02	1.78	1.79

where η is the packing fraction of the gas and $Z(\eta) = PV/Nk_B T$ is its compressibility factor. The packing fraction is the ratio of the volume occupied by the particles to the total volume V , and thus for a hard disk gas $\eta = \pi\sigma^2 N/4V$. No exact analytical expressions of $Z(\eta)$ are available for a hard disk gas, but several approximations have been proposed. The simplest one has the form⁸

$$Z(\eta) = \frac{1 + a\eta^2}{(1 - \eta)^2}, \quad (25)$$

where a is a constant. The value $a=0$ gives the scaled particle theory (SPT) equation of state, while the value $a=0.125$ corresponds to the Henderson equation of state. The substitution of Eqs. (24) and (25) into Eq. (1) yields

$$c_s = \sqrt{\frac{2k_B T}{m} \frac{(1 + \eta + 3a\eta^2 - a\eta^3)}{(1 - \eta)^3}}. \quad (26)$$

The values of the packing fraction η for $N=50$ and $A=10$ and length L_0 are given in the second column of Table I. The values of the corresponding speed of sound obtained from Eq. (26) with $m=1$, $k_B T=1$, and $a=0$ and $a=0.125$ are given, respectively, in the fourth and fifth columns of Table I. There is no significant difference between the values obtained from the SPT and Henderson's equations.

A comparison between the third (simulation results) and fifth (theoretical results) columns of Table I shows that the values of the speed of sound obtained from the computer simulation are slightly larger than those obtained from Eq. (26), and the difference increases as the packing fraction η increases, that is, as the gas becomes more dense. These discrepancies could be ascribed to the fact that Eq. (26) is strictly applicable in the thermodynamic limit while the simulations have a finite number of particles confined to a finite volume, where surface effects can be important.

We next consider finite size effects on the calculation of the speed of sound. However, the algorithm used in the simulations is order N for each collision event,⁶ and the number of collisions per unit time is proportional to N which makes the method order N^2 . Because large runs are required for measuring a piston trajectory ($\sim 7 \times 10^6$ collisions per particle), the number of disks that can be handled by a typical personal computer with the present algorithm is limited to $N \sim 50$. Larger systems can be studied with a more efficient algorithm⁹ that reduces the calculation to order $N \log N$. The details of the algorithm and the computer code for a hard particle system can be found in Ref. 9. The impressive performance of the algorithm is achieved by the combined effect of the following changes to the standard method: (i) the system is divided into cells that only hold a few particles so that one has to check only for collision events with particles in the same and adjacent cells; (ii) each particle has its own local time variable that is updated only when required, that is, in a collision or cell crossing events in which the particle is involved; and (iii) a very efficient event calendar is used to obtain the next event and to remove scheduled events that are no longer relevant. It is not difficult to modify the code of Ref. 9 to incorporate the piston as an additional special particle that only moves in the x direction and belongs to an entire column of cells.

The results of the study of size effects on the speed of sound are presented in Table II for systems with $N=N_0/2 = 64, 256, 1024$, and 4096 disks in boxes with the same

Table II. Influence of the size of the system on the speed of sound of a hard disk gas with packing fraction $\eta=0.393$.

N	L_0	c_s
64	$8\sqrt{2}$	3.81
256	$16\sqrt{2}$	3.78
1024	$32\sqrt{2}$	3.76
4096	$64\sqrt{2}$	3.75

aspect ratio ($A=L_0$) at fixed $\eta=0.393$. For the sake of comparison (and to reduce the computational effort) the simulations have been done at constant $K=1.07687$, that is, with a piston mass $M=Nm$. As it is shown in Table II, finite size effects are present, but are not significant. Thus, increasing the number of particles and extrapolating to the infinite-size system does not modify the results significantly (the extrapolated value of the velocity of sound is $c_s=3.74$). This result implies that other effects not considered in our simple model can influence the calculation of the speed of sound, specially at high densities. In particular, we note that our model considers a one-dimensional standing wave in a two-dimensional system so that coupling with other modes could affect the results.

IV. SUMMARY

We have presented a computer simulation of a system designed to calculate the speed of sound in a hard disk gas. The system consists of a rigid piston that divides an isolated rectangular box into two equal parts. If the piston can move freely, it will have a fluctuating motion about the center of the box induced by collisions with the hard disks. In this manner, the piston can be considered as a vibrating object that couples to the hard disk gas and excites sound waves. Therefore, the piston exhibits an oscillatory behavior driven

by the fundamental standing sound wave of the system. We have used a FFT method to calculate the power spectrum of the time evolution of the piston. The maximum peak of this spectrum corresponds to the frequency of the fundamental standing sound wave of the system. The speed of sound in the hard disk gas is calculated from this frequency. The results are compared with theoretical values calculated from the isothermal compressibility of a hard disk gas in the thermodynamic limit. There is good agreement between simulation and theoretical results for systems at low density, with increasing discrepancies as the density increases.

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THE EXTENT OF THE UNIVERSE

I recall being stumped as a child on the question of the extent of the universe. It seemed absurd that the universe be infinite, how could it just go on and on forever? It also seemed absurd that it be finite, for then there would be a wall, and one could wonder about what was beyond it. When one has a question like this, perhaps the only hope is that someone will someday imagine a third option, which gets us out of the paradox. This is exactly what Einstein did, when he turned his attention to what his new general theory of relativity might have to say about cosmology. He found that his theory could describe a universe that was finite, but closed, exactly like the surface of a globe that has finite area but no boundary. In this way, general relativity can resolve, at least for space, the great paradox of whether the universe is finite or infinite. Had Einstein imagined only this he still would be one of the great natural philosophers of our century.

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