The D'yakov-Kontorovich Instability of Shock Waves in Real Gases

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In the 1950s, D'yakov and Kontorovich predicted that under certain conditions perturbed shock waves in nonideal gases can become unstable by emitting undamped sound and entropy-vortex waves. For the last 45 years, though, little progress has been made in the identification and numerical modeling of physical conditions for which this phenomenon might occur. Using a van der Waals equation of state, we present for the first time a dynamical simulation of a D'yakov-Kontorovich instability. The two-dimensional emission pattern of acoustic waves appearing in the simulation agrees with the prediction of a linearized theory.

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The stability of shock waves ranks as one of the fundamental problems of fluid dynamics. Along with the celebrated Rayleigh-Taylor [1] and Kelvin-Helmholtz [2] instabilities, the behavior of shocks subject to small perturbations is important in many hydrodynamic systems, including astrophysical environments [3] and inertial confinement fusion (ICF) targets [4]. D'yakov [5] was the first to investigate the stability of a plane shock wave with "corrugations" on its surface, and identified conditions under which such perturbations would grow exponentially in time. D'yakov's analysis (later corrected by Kontorovich [6]) also yielded a regime in which perturbations to the planarity of a shock front were apparently stationary. Because such cases correspond to the emission of undamped sound and entropy-vortex waves from the compressed gas side of the shock, this was termed "acoustic emission instability," although no true instability—in the conventional, temporally exponentiating sense of the word—occurs. Once created, perturbations on the shock front persist indefinitely and continue to radiate waves without being either damped or amplified.

In the analysis of shock wave stability, a crucial role is played by the Hugoniot curve [7] in the plane of specific volume V versus pressure p. This curve is the locus of all shocked or "downstream" states that can be connected by a single surface of discontinuity to a particular unshocked or "upstream" state. For an ideal gas, the Hugoniot curve has a smoothly varying, "regular" appearance, but for other materials, bumps, discontinuities, or changes in curvature are sometimes found. It is these "irregular" segments that can give rise to a variety of unusual dynamical features, including the formation of rarefactive shocks [8], and the splitting of shock fronts into more complex (but stable) wave structures [9].

For the D'yakov-Kontorovich instability to occur, it is not necessary for a Hugoniot curve to have any irregular features, only that its slope over some segment lies below a critical value. The criterion for this class of shock instabilities is most conveniently expressed in the form of an inequality involving the so-called "D'yakov parameter"

$$h = j^2 \left(\frac{dV}{dp}\right)_H , \qquad (1)$$

where $j^2 = (p_2 - p_1)/(V_1 - V_2)$ is the square of the mass flux density across the shock, and upstream and downstream states bear the subscripts "1" and "2," respectively. The derivative in Eq. (1) is taken along the Hugoniot curve and evaluated at the downstream state. The condition for instability to arise can be stated as [6,10]

$$h_c = \frac{1 - M_2^2(1 + V_1/V_2)}{1 - M_2^2(1 - V_1/V_2)} < h . \qquad (2)$$

Here, $M = |v/c|$ is a Mach number, where $v = jV$ and c are the fluid velocity and sound speed, respectively, in the frame of reference in which the shock is stationary. In an ideal gas, $h_c = (1 - 2M_1^2)^{-1}$ and $h = -1/M_1^2$, and so the above inequality can never be satisfied for $M_1 \geq 1$.

The inequality can be satisfied, though, for other materials possessing *nonideal* equations of state. Recently, Bates and Montgomery [11] showed that for a dissociation model of diatomic hydrogen at ICF-relevant conditions, a critical shock strength exists beyond which $h_c < h$ holds. Furthermore, Rutkevich, Zaretsky, and Mond have demonstrated that an emission instability is likely to occur for strong shocks in certain metals [12], as well as in inert gases undergoing ionization [13].

Despite these predictions, the existence of an emission instability has never been confirmed in a dynamical computation. In this Letter, we present the first numerical evidence for the D'yakov-Kontorovich instability of a plane shock wave. Using a van der Waals equation of state as a paradigm for nonideal fluid behavior, we first show that real gases in the vicinity of a vapor-liquid phase transition

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can be susceptible to this type of instability. Then, the passage of a shock through a slightly narrowing two-dimensional channel filled with a uniform van der Waals gas at rest is modeled in a numerical simulation. (Physically, we imagine the shock as sustained by the motion of a piston far behind it.) The small constriction in the channel's cross section excites transverse perturbations to the one-dimensional flow [14], which in this case ultimately leads to the emission of undamped sound waves from the shock front; see Fig. 1. In agreement with the predictions of the linearized normal-mode analysis, the sound emanating from the shock appears in the simulation as pairs of plane acoustic waves, whose propagation vectors are discrete and directed upstream. (Transport due to the moving downstream fluid is what permits these waves to leave the shock's surface.) The numerical method employed is a two-dimensional "flux corrected transport" (FCT) algorithm [15], which ignores the effects of viscosity and thermal conductivity, and solves the Euler equations of compressible gas dynamics in a fixed coordinate system. FCT-based codes have been shown [16] to model accurately the passage of steep shocks through fluids without introducing spurious oscillations, but have the desirable property of not precluding the appearance of local extrema in the flow when they occur physically.

The equation of state for a van der Waals gas is $(p + a/V^2)(V - b) = NkT$, where N is the number of molecules per unit mass, k is Boltzmann's constant, T is the temperature, and a and b are constants. The van der Waals equation is a more accurate description of real fluid behavior than the ideal gas law, and is appropriate to use whenever the interactions between particles, a/V^2, and their finite volumes, b, become important. This equation can be cast in dimensionless form as

$$\left[p/p_0 + \frac{3}{(V/V_0)^2}\right](3\,V/V_0 - 1) = 8\,T/T_0\,, \qquad (3)$$

where $p_0 = a/(27b^2)$, $V_0 = 3b$, and $T_0 = 8\mu a/(27Rb)$ are convenient reference values. Here, $R = \mu Nk$ is the universal gas constant and μ is the gas molecular weight. In addition to Eq. (3), it is also necessary to have expressions for the entropy, s, and the specific internal energy per unit mass, ε. Ignoring unimportant additive constants, these are given by

$$s/s_0 = \log(T/T_0) + \frac{R}{\mu c_V}\log(3\,V/V_0 - 1)\,, \qquad (4)$$

$$\varepsilon/\varepsilon_0 = \frac{\mu c_V}{R}\,(T/T_0) - \frac{9}{8\,(V/V_0)}\,, \qquad (5)$$

where $s_0 = c_V$, $\varepsilon_0 = RT_0/\mu$, and $c_V =$ const is the specific heat per unit mass at constant volume. Equations (3) and (4) can be used to compute the speed of sound from the relation $c^2 = -V^2\,(\partial p/\partial V)_s$, which is needed in the evaluation of h_c in Eq. (2).

Using the above expressions in conjunction with the Rankine-Hugoniot relations [7,17], it is straightforward to compute Hugoniot curves for a van der Waals gas, an example of which is shown in Fig. 2. Note that the Hugoniot lies entirely outside of both the (liquid-vapor) coexistence region, and the so-called "anomalous" region [11,17,18] in which $(\partial^2 p/\partial V^2)_s < 0$. Figure 3 shows the difference $h_c - h$ versus upstream Mach number M_1 along the Hugoniot in Fig. 2. It is apparent that a region exists just beyond $M_1 \approx 1.2$ where $h_c - h < 0$, and the criterion for instability is satisfied. Accordingly, we choose $M_1 = 1.245$, which corresponds to the downstream state labeled "2" in Fig. 2. The value of h at this point is -0.542, and the entropy change from point "1" is $+0.037\%$. The downstream Mach number here is $M_2 = 0.745$, so that the conditions for the unperturbed flow to be evolutionary [7] are met.

Let us investigate the response of this shock to small disturbances. Before presenting the results of our numerical simulation, we first review the theory of perturbed shocks for general equations of state. This analysis usually proceeds from a linearized normal-mode approach, as discussed in Ref. [7]. Following that discussion, we transform to a coordinate frame in which the shock is at rest and aligned with the y axis at $x = 0$. Contrary to the convention of Ref. [7], though, our unperturbed flow is from right to left so that v_1, $v_2 < 0$.

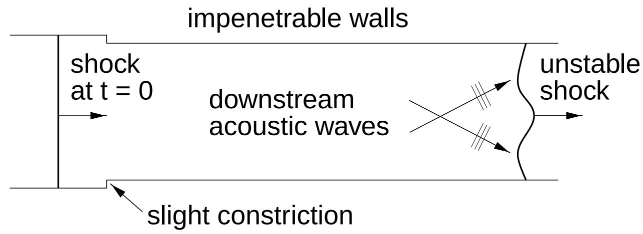

FIG. 1. The passage of a shock through a van der Waals gas in a channel with a slight constriction is modeled. The size of the constriction is exaggerated here for clarity.

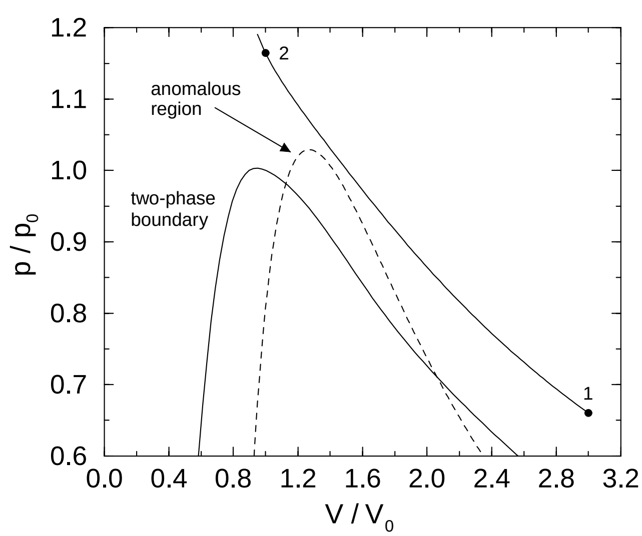

FIG. 2. Hugoniot for a van der Waals gas with $\mu c_V/R = 30$ (not an uncommon value). Initial and final states are $(V_1, p_1) = (3\,V_0, 0.66\,p_0)$ and $(V_2, p_2) = (V_0, 1.165\,p_0)$, respectively.

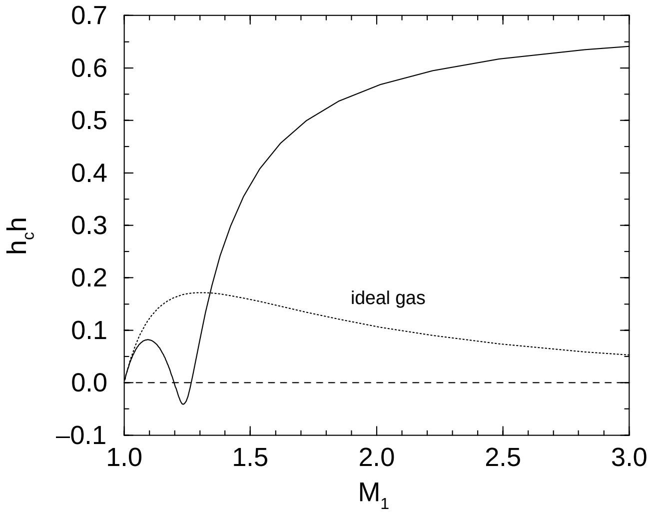

FIG. 3. Plot of the difference $h_c - h$ versus M_1 for the Hugoniot in Fig. 2.

We now give the planar shock front a corrugation of the form $\exp[i\,(k_y\,y - \omega\,t)]$, where k_y and ω are a transverse wave number and eigenfrequency, respectively, and t is the time. This perturbation affects the downstream flow ($x < 0$) only, where, in general, both entropy-vortex and sound waves are produced. Each type of linear wave is represented by a factor $\exp[i\,(k_x\,x + k_y\,y - \omega\,t)]$, with the same values of k_y and ω as the original disturbance, but differing by the value of their longitudinal wave number k_x. In the entropy-vortex wave, which has no pressure variation, k_x is simply given by ω/v_2, expressing the fact that small disturbances of this type are swept along with the downstream flow. For the sound wave, though, k_x is determined from

$$\omega_0^2 = (\omega - v_2 k_x)^2 = c_2^2\left(k_x^2 + k_y^2\right), \qquad (6)$$

where ω_0 is the sound frequency in a coordinate frame moving with the downstream fluid. Equation (6) can be solved to give k_x as a function of ω and k_y. In general, k_x and ω are complex-valued quantities, whereas k_y is real. (Of course, if k_y is present in the Fourier decomposition, so must be $-k_y$.)

The next step is to determine all possible eigenmodes of oscillation for the system. By linearizing the perturbed Euler equations and Rankine-Hugoniot jump conditions at the shock's surface, a dispersion relation for ω can be derived. We refer the reader to Refs. [7] and [19] for details. The result is

$$\frac{2\,\omega\,v_2}{v_1}\left(k_y^2 + \frac{\omega^2}{v_2^2}\right) - \left(\frac{\omega^2}{v_1 v_2} + k_y^2\right)(\omega - v_2 k_x)(1 + h) = 0\,, \qquad (7)$$

where k_x is the acoustic wave number appearing in Eq. (6). Roots of Eq. (7) with purely real values of ω and k_x correspond to the emission of undamped waves from the shock (i.e., the D'yakov-Kontorovich "instability"). This equation can be cast in a more useful form by introducing the angle θ between the sound propagation vector (k_x, k_y) and the positive x axis. With the transformation $c_2 k_x = \omega_0 \cos\theta$ and $c_2 k_y = \omega_0 \sin\theta$, Eq. (6) can be written as $\omega = \omega_0(1 + M_2 \cos\theta)$. Then, substituting these three expressions into Eq. (7) yields

$$A\cos^2\theta - B\cos\theta + C = 0\,, \qquad (8)$$

where

$$A = M_2^2\left(\frac{4}{1+h} + \frac{V_1}{V_2} - 1\right),$$

$$B = 2M_2\left(\frac{3 + M_2^2}{1+h} - 1\right),$$

$$C = \frac{2(1 + M_2^2)}{1+h} - \left(1 + M_2^2\frac{V_1}{V_2}\right).$$

For our parameters, we find that the two roots of Eq. (8) are $\cos\theta = 0.996$ and 0.696. These values specify a longitudinal component of the sound propagation direction, but not a transverse one, which could have either sign since $\sin\theta = \pm\sqrt{1 - \cos^2\theta}$. In other words, each root is associated with two waves running in opposite directions along the y axis.

In order for a sound wave to leave the shock's surface, though, it must have an overall propagation velocity in the negative x direction such that $v_2 + c_2\cos\theta < 0$. Said another way, the emission of undamped sound waves can occur if $-1 < \cos\theta < M_2$, a condition that is satisfied for $\cos\theta = 0.696$ only. This root corresponds to a case in which the emission is in the upstream direction, but transport due to the moving gas makes it still a wave that leaves the surface of discontinuity. (For a discussion of the distinction between the direction of the propagation vector and the direction of energy flow, see Whitham [20].) Thus, in the event of a D'yakov-Kontorovich instability of the van der Waals shock depicted in Fig. 2, we should expect to see *pairs* of plane acoustic waves emanating from the downstream side of the shock at approximately $\pm\cos^{-1}(0.696) = \pm 46°$ about the x axis.

And that is indeed what appears in the numerical simulation. Figure 4(a) shows a gray scale plot of pressure at $t/t_0 = 1001$ for a shock that has traveled down the "numerical shock tube" sketched in Fig. 1, and is now far to the right of the constriction. Here, t_0 is a reference time defined by $\sqrt{\varepsilon_0} = L/t_0$, where L is an arbitrary reference length. In this figure, two crossed sets of plane acoustic waves leaving the downstream face of the shock are clearly visible, as is the persistence of a perturbation to the planarity of the shock's surface. The effect is somewhat reminiscent of the sound generated by supersonic flow past a corrugated wall [21], but in that case only plane waves at a single angle of emission are produced. Our simulation was initiated at $t/t_0 = 0$ by first establishing a steady planar shock at $x/L = 20$ with upstream and downstream equilibrium values of pressure, specific volume, and x component of velocity chosen to correspond to the states labeled "1" and "2," respectively, in Fig. 2. The planarity

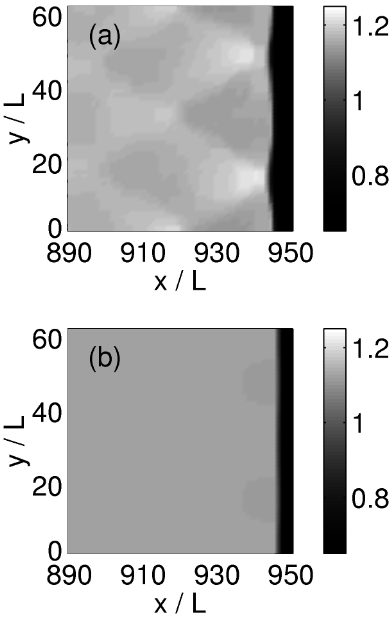

FIG. 4. Pressure near the shock front in (a) an unstable van der Waals gas and (b) a stable ideal gas. The waves visible behind the shock in (a) are linear sound waves with rms pressure fluctuations of about 1.5%; fluctuations in (b) are an order of magnitude smaller. In additional runs performed for a van der Waals gas with $h < h_c$ (stable case), the emission phenomenon was not observed.

of this shock was then disturbed upon passage through the slight constriction in the shock tube's cross section, which had a width of one cell and was located at $x/L = 32$. The entire computational grid was 1024×64 cells with $\Delta x/L = \Delta y/L = 1$. The walls of the shock tube were modeled as ideal solid boundaries where "free-slip" conditions apply, while inflow and outflow conditions were imposed at the left and right ends, respectively, of the computational domain. The maximum dimensionless time step allowed here was $\Delta t/t_0 = 0.005$.

For comparison, Fig. 4(b) shows a run at $t/t_0 = 409$ using a monatomic ideal-gas equation of state. This shock has the same Mach number and upstream values of specific volume and pressure as that in Fig. 4(a), but now the roots of Eq. (8) do not satisfy $-1 < \cos\theta < M_2$. Consequently, sound waves cannot escape from the downstream surface of the discontinuity and the system is not susceptible to the D'yakov-Kontorovich instability. This result was to be expected since planar shocks in ideal gases are known [22] to be inherently stable, and to ultimately regain their uniform shape when subject to small disturbances.

In summary, we have observed in a gas-dynamical computation that sound waves can be emitted from the surface of a shock when the criterion for spontaneous emission is satisfied. This result agrees with predictions made over 40 years ago [5,6]. Although the molecular processes ultimately responsible for this special class of shock wave instabilities have never been entirely amenable to theoretical explanation, they are likely related to the thermodynamic proximity of regions characterized by increasingly easier adiabatic compression, and the relative ease of exciting sound waves in those regimes. In the future, it would be desirable to investigate these underlying microscopic phenomena by utilizing a numerical scheme capable of resolving the kinetic structure of the shock front.

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