Numerical Survey on Hyperbolicity of the Homogenized Equation for Van Der Waals Gas in Eulerian Coordinates

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Abstract. We describe numerical methods for the location of the zero set of the periodic Evans function $D(\xi, \lambda)$ for λ, ξ sufficiently small, or equivalently the spectrum of a linearized operator L with periodic coefficients through the homogenization. We demonstrate these methods for an example system, van der Waals gas in eulerian coordinates. We observe the hyperbolicity of the system. The hyperbolicity is necessary to show asymptotic behavior of a multi-dimensional single periodic wave of systems of conservation laws with viscosity under small perturbation.

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1. Introduction

We consider van der Waals isentropic gas in eulerian coordinates

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p(\rho) = \mu_1 \triangle \mathbf{u} - \mu_2 \nabla \left(\triangle \frac{1}{\rho} \right)$$
(1)

where ρ denotes the density, $\mathbf{u} \in \mathbb{R}^2$ the velocity of the gas and the pressure $p(\rho) = \frac{RT\rho}{1-b\rho} - a\rho^2$ with the temperature T, the perfect gas constant R, and given positive numbers a, b. The van der Waals equation is a second order approximation of the equation of state of a gas that works even when the density of the gas is not low. The parameter a is related to intermolecular attractive force between the molecules and the parameter b is related to the size of each molecule. Here a and b are constants particular to a given gas. The net effect of the intermolecular attractive force is to reduce the pressure for a given volume and temperature. When the density of the gas is low the van der Waals

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equation reduces to that of the ideal gas law. One region where the van der Waals equation works well is for temperatures that are slightly above the critical temperature T of a substance. Note that μ_1 is viscosity coefficient and μ_2 is a capillarity coefficient. Let us rewrite (1) to connect the idea with the companion paper [2]:

$$\rho_t + \sum_j (\rho \mathbf{u} \cdot \mathbf{e}_j)_{x_j} = 0$$

$$(\rho \mathbf{u})_t + \sum_j \left(\rho \mathbf{u} \mathbf{u}^T \mathbf{e}_j + p(\rho) \mathbf{e}_j\right)_{x_j} = \sum_{j,k} \left(\mu_1 B^{jk} \mathbf{u}_{x_k} - \mu_2 \mathbf{e}_j \left(\frac{1}{\rho}\right)_{x_k x_k}\right)_{x_j}$$
(2)

where $B^{jk} \in \mathbb{R}^{2 \times 2}$ with $B^{jj} = I$, $B^{jk} = 0$, $j \neq k$, and e_j is the standard basis vector. Let $\frac{1}{\rho} = V$, volume. Since the properties of the coefficient matrices we can simplify (2) as

$$\rho_t + \sum_j (\rho \mathbf{u} \cdot \mathbf{e}_j)_{x_j} = 0$$

$$(\rho \mathbf{u})_t + \sum_j \left(\rho \mathbf{u} \mathbf{u}^T \mathbf{e}_j + p(\rho) \mathbf{e}_j\right)_{x_j} = \sum_j \left(\mu_1 \mathbf{u}_{x_j} - \mu_2 \sum_k \mathbf{e}_j V_{x_k x_k}\right)_{x_j}$$
(3)

Let $x \in \mathbb{R}^2$, and $(\rho, \mathbf{u}) = w$. A periodic solution $w = w(x \cdot \nu - st)$ of period X of (1) and (2) satisfies the traveling wave ordinary differential equations

$$-s\rho' + \sum_{j} \nu_{j}(\rho \mathbf{u} \cdot \mathbf{e}_{j})' = 0$$

$$-s(\rho \mathbf{u})' + \sum_{j} \nu_{j} \left(\rho \mathbf{u} \mathbf{u}^{T} \mathbf{e}_{j} + p(\rho) \mathbf{e}_{j}\right)' = \sum_{j} \nu_{j} \left(\mu_{1} \nu_{j} \mathbf{u}' - \mu_{2} \sum_{k} \nu_{k} \nu_{k} \mathbf{e}_{j} V''\right)'.$$
(4)

Note that ν is the direction of the wave and a unit vector, i.e. $\nu \in S^1$. Integrating (4), we reduce to a first order profile equation

$$0 = \sum_{j} \nu_{j} (\rho \mathbf{u} \cdot \mathbf{e}_{j}) - s\rho - q_{1}$$
$$\sum_{j} \nu_{j} \left(\mu_{1} \nu_{j} \mathbf{u}' - \mu_{2} \sum_{k} \nu_{k} \nu_{k} \mathbf{e}_{j} V'' \right) = \sum_{j} \nu_{j} \left(\rho \mathbf{u} \mathbf{u}^{T} \mathbf{e}_{j} + p(\rho) \mathbf{e}_{j} \right) - s(\rho \mathbf{u}) - \mathbf{q}$$
⁽⁵⁾

where $q = (q_1, \mathbf{q})$ is a constant of motion.

2. Homogenization

Now we carry out a multi-dimensional version of the slow modulation expansion. Rescale $(x, t) \mapsto (\epsilon x, \epsilon t)$ in (3) to obtain

$$\rho_t + \sum_j (\rho \mathbf{u} \cdot \mathbf{e}_j)_{x_j} = 0$$

$$(\rho \mathbf{u})_t + \sum_j \left(\rho \mathbf{u} \mathbf{u}^T \mathbf{e}_j + p(\rho) \mathbf{e}_j \right)_{x_j} = \sum_j \epsilon \left(\mu_1 \mathbf{u}_{x_j} - \epsilon \mu_2 \sum_k \mathbf{e}_j V_{x_k x_k} \right)_{x_j}.$$
(6)

Let

$$w^{\epsilon}(x,t) = w^{0}\left(x,t,\frac{\phi(x,t)}{\epsilon}\right) + \epsilon w^{1}\left(x,t,\frac{\phi(x,t)}{\epsilon}\right) + \cdots,$$
(7)

where $y \mapsto w^0(x, t, y)$ is a periodic function with $\partial_x \phi \neq 0$. We plug (7) into (6) and consider the equations obtained by equating coefficients at successive powers of ϵ . At order ϵ^{-1} , we have

$$-s\omega\partial_{y}\rho^{0} + \sum_{j}\omega\nu_{j}\partial_{y}(\rho^{0}\mathbf{u}^{0}\cdot\mathbf{e}_{j}) = 0$$

$$-s\omega\partial_{y}(\rho^{0}\mathbf{u}^{0}) + \sum_{j}\omega\nu_{j}\partial_{y}(\rho^{0}\mathbf{u}^{0}(\mathbf{u}^{0})^{T}\mathbf{e}_{j} + p(\rho^{0})\mathbf{e}_{j}) = \omega^{2}\sum_{j}\nu_{j}\partial_{y}\left(\mu_{1}\nu_{j}\partial_{y}\mathbf{u}^{0} - \mu_{2}\omega\sum_{k}\nu_{k}\nu_{k}\mathbf{e}_{j}\partial_{yy}V^{0}\right)$$

with

$$s := -\frac{\partial_t \phi}{|\partial_x \phi|}, \quad \nu := \frac{\partial_x \phi}{|\partial_x \phi|}, \quad \omega := |\partial_x \phi|,$$

which may be recognized as the traveling-profile equation after rescaling $y \to \omega y$. That is, $w^0(y) = w(\omega y)$ for a periodic profile of period $X = \omega^{-1}$, hence w^0 is periodic of *period one*, as described in [2]. The quantities $\omega(x,t)$, s(x,t), $\nu(x,t)$ are the local frequency, speed, and direction of the modulated wave. At order ϵ^0 , we have

$$\partial_t \rho^0 + \sum_j \partial_{x_j} (\rho^0 \mathbf{u}^0 \cdot \mathbf{e}_j) = \partial_y (\dots)$$
$$\partial_t (\rho^0 \mathbf{u}^0) + \sum_j \partial_{x_j} \left[\rho^0 \mathbf{u}^0 (\mathbf{u}^0)^T \mathbf{e}_j + p(\rho^0) \mathbf{e}_j - \left(\mu_1 \omega \nu_j \partial_y \mathbf{u}^0 - \mu_2 \sum_k \omega^2 \nu_k \nu_k \mathbf{e}_j \partial_{yy} V^0 \right) \right] = \partial_y (\dots).$$

Taking the average with repect to y, and rescaling with $y := \omega y$, we obtain

$$\partial_t \langle \rho^0 \mathbf{u}^0 \rangle + \sum_j \partial_{x_j} \langle \rho^0 \mathbf{u}^0 \cdot \mathbf{e}_j \rangle = 0$$
$$\partial_t \langle \rho^0 \mathbf{u}^0 \rangle + \sum_j \partial_{x_j} \left\langle \rho^0 \mathbf{u}^0 (\mathbf{u}^0)^T \mathbf{e}_j + p(\rho^0) \mathbf{e}_j - \left(\mu_1 \omega \nu_j \partial_y \mathbf{u}^0 - \mu_2 \sum_k \omega^2 \nu_k \nu_k \mathbf{e}_j \partial_{yy} V^0 \right) \right\rangle = 0,$$

where we define the average

$$\langle f \rangle = \frac{1}{X} \int_0^X f(y) dy,$$

for an arbitrary X periodic function f. We introduce variables:

$$M_{1} = \langle \rho^{0} \rangle, \quad M_{2} = \langle \rho^{0} \mathbf{u}^{0} \rangle, \quad F_{1}^{j} = \langle \rho^{0} \mathbf{u}^{0} \cdot \mathbf{e}_{j} \rangle$$
$$F_{2}^{j} = \left\langle \rho^{0} \mathbf{u}^{0} (\mathbf{u}^{0})^{T} \mathbf{e}_{j} + p(\rho^{0}) \mathbf{e}_{j} - \left(\mu_{1} \omega \nu_{j} \partial_{y} \mathbf{u}^{0} - \mu_{2} \sum_{k} \omega^{2} \nu_{k} \nu_{k} \mathbf{e}_{j} \partial_{yy} V^{0} \right) \right\rangle.$$
(8)

Since these quantities are translation invariant, we consider the set P of periodic functions w that are solutions of (5) for some triple (s, ν, q) , and construct the quotient set $\mathcal{P} := P/\mathcal{R}$ under the relation

$$(u \mathcal{R} v) \iff (\exists h \in \mathbb{R}; v = u(\cdot - h)).$$

We thus have class functions: $X = X(\dot{u}), \omega = \Omega(\dot{u}), s = S(\dot{u}), \nu = N(\dot{u}), q = Q(\dot{u}), M_k = M_k(\dot{u}), F_k^j = F_k^j(\dot{u})$, where \dot{u} is the equivalence class of translates of different periodic functions. Note that $\sum_j \nu_j F_k^j$ is the averaged flux along orbit w^0 with

$$\sum_{j} \nu_{j} F_{1}^{j} = (SM_{1} + Q_{1})(w^{0}), \qquad \sum_{j} \nu_{j} F_{2}^{j} = (SM_{2} + \mathbf{Q})(w^{0})$$

by the profile equation. We have an additional two equations

$$\partial_t(\Omega N)(w^0) + \partial_x(\Omega S(w^0)) = 0$$

from the Schwarz identity $\partial_t \partial_x \phi = \partial_x \partial_t \phi$, where 2 is the dimension of the spatial variable x. (Note: (Ω, N) may be regarded as polar coordinates for ΩN .) Combining, we obtain finally the closed homogenized system

$$\partial_t(M_1, M_2, \Omega N) + \sum_j \partial_{x_j}(F_1^j, F_2^j, \Omega S e_j)$$

consisting of five equations in five unknowns.

Proposition 2.1. With the nondegeneracy condition

$$\det\left(\frac{\partial(M_1, M_2, \Omega N)}{\partial \dot{w}}(\bar{w})\right) \neq 0,$$

then for λ, ξ sufficiently small, the zero-set of the Evans function $D(\cdot, \cdot)$, corresponding to spectra of L, consists of four characteristic surfaces:

$$\lambda_j(\xi) = -ia_j(\xi) + o(\xi), \quad j = 1, \dots, 4,$$

where $a_j(\xi)$ denote the eigenvalues of

$$\mathcal{A} := \sum_{j} \xi_{j} \frac{\partial(F_{1}^{j}, F_{2}^{j}, S\Omega \mathbf{e}_{j})}{\partial(M_{1}, M_{2}, \Omega N)},$$

excluding one identically zero eigenvalues associated with modes not satisfying constraint curl $\Omega N \neq 0$.

Proof. The proof follows one in [2] with n = 3 and d = 2.

Remark 2.2. The result of [2] is equivalent to low-frequency spectral stability, hence necessary for stability of the background periodic wave. It also corresponds to well-posedness of the modulated system. But it is not clear from [2] whether hyperbolicity could ever be satisfied in multi-dimensional case. We will investigate that numerically in the next section.

3. Numerics

We determine the hyperbolicity of the averaged system of the model considered by numerics. The hyperbolicity in the sense that it possesses a full set of real characteristics $\hat{\lambda}_j(\xi)$ for each $\xi \in \mathbb{R}^d$, i.e., the eigenvalues of \mathcal{A} are real and distinct. The real advantage of the numerical approach is that it is applicable to general models. The basic strategy for numerical verification of hyperbolicity is a construction of 5×5 matrix of \mathcal{A} . Note that

$$\Omega N = \langle (\partial_{x_1} \phi, \partial_{x_2} \phi)^T \rangle, \qquad S \Omega = \langle \partial_t \phi \rangle. \tag{9}$$

Together with (9) we recall the averages (8) and $\dot{w} = (\rho, u, v, \phi_{x_1}, \phi_{x_2})$. We shall compute

$$\frac{\partial(M_1, M_2, \Omega N)}{\partial \dot{w}}(\bar{w}), \qquad \sum_j \frac{\partial(F_1^j, F_2^j, S\Omega e_j)}{\partial \dot{w}}(\bar{w}),$$

and eventually

$$\sum_{j} \xi_{j} \left(\frac{\partial (M_{1}, M_{2}, \Omega N)}{\partial \dot{w}} (\bar{w}) \right)^{-1} \frac{\partial (F_{1}^{j}, F_{2}^{j}, S \Omega e_{j})}{\partial \dot{w}} (\bar{w}).$$

To simplify the problem, without loss of generality, assume $\nu = e_1$. Then we obtain $\rho u - s\rho - q_1 = 0$ for $\mathbf{u} = (u, v)$ from the first equation of (5) and thus $u = \frac{q_1}{\rho} + s$. The second equation of (5) becomes

$$\mu_1 u' - \mu_2 \left(\frac{1}{\rho}\right)'' = \rho u^2 + p(\rho) - s\rho u - q_2 = (\rho u - s\rho)u + p(\rho) - q_2 \qquad (10)$$
$$\mu_1 v' = \rho uv - s\rho v - q_3.$$

Plugging in u into (10), we have

$$\mu_1 \left(\frac{q_1}{\rho} + s\right)' - \mu_2 \left(\frac{1}{\rho}\right)'' = q_1(\frac{q_1}{\rho} + s) + p(\rho) - q_2$$

$$\mu_1 v' = \rho(\frac{q_1}{\rho} + s)v - s\rho v - q_3 = q_1 v - q_3.$$
(11)

The first equation of (11) becomes

$$\rho'' = \frac{1}{\mu_2} \left[q_1^2 \rho + q_1 s \rho^2 + p(\rho) \rho^2 - q_2 \rho^2 + \mu_1 q_1 \rho' \right] + 2 \frac{(\rho')^2}{\rho}$$

hence we have the first order system

$$\begin{pmatrix} \rho \\ \rho' \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ \frac{1}{\mu_2} \left[q_1^2 + q_1 s \rho + \frac{RT\rho^2}{1 - b\rho} - a\rho^3 - q_2\rho \right] \qquad \frac{\mu_1 q_1}{\mu_2} + 2\frac{\rho'}{\rho} \end{pmatrix} \begin{pmatrix} \rho \\ \rho' \end{pmatrix}$$

where $\mu_1, \mu_2, a, b, q_1, q_2, s, R, T$ are all constants. We determine the values of ρ numerically by using a fourth order Runge-Kutta method, for which analytical error estimates may be found, for example, in [3]. Once we determine the values of ρ , we determine the values of u, respectively. The second equation of (11) is independent of u and ρ , and v can be determined by solving the linear first order differential equation. The values of v can be determined analytically but here we use the fourth order Runge-Kutta method again. About averages, we use the mean value theorem for integration. We obtain the values of (ρ, u, v) and the values of their derivatives with some fixed constants and a fixed given function $\phi(x, t)$. Then we compute the eigenvalues of

$$\sum_{j} \xi_{j} \frac{\partial(F_{1}^{j}, F_{2}^{j}, \Omega S e_{j})}{\partial(M_{1}, M_{2}, \Omega N)}$$

with "eig" function in MATLAB. Note that we use "rand" function for ξ_j for each j. These eigenvalues determine the hyperbolicity of the homogenized system. The table below shows some van der Waals constants:

Substance	a(J. m3/mole2)	b(m3/mole)	Pc(MPa)	Tc(K)
Air	.1358	3.64x10-5	3.77	133
Carbon Dioxide (CO2)	.3643	4.27x10-5	7.39	304.2
Nitrogen (N2)	.1361	3.85x10-5	3.39	126.2
Hydrogen (H2)	.0247	2.65x10-5	1.30	33.2
Water (H2O)	.5507	3.04x10-5	22.09	647.3
Ammonia (NH3)	.4233	3.73x10-5	11.28	406
Helium (He)	.00341	2.34x10-5	0.23	5.2
Freon (CCl2F2)	1.078	9.98x10-5	4.12	385

We obtain three different real eigenvalues and two zero eigenvalue for each substance. As we mentioned above, one zero eigenvalue corresponds to the constraint curl $(\Omega N) = 0$ as explained in [2].

4. Discussion

The figures show that only eigenvalues different from zero with varying ξ . We conclude that the van der Waals gas model has the hyperbolicity. Our study justifies that hyperbolicity indeed can hold for interesting systems. In [1], assuming hyperbolicity (= low-frequency stability) and full spectral stability, we show the asymptotic behavior of a multi-dimensional single periodic wave of systems of conservation laws with viscosity under small perturbation.



Figure 1: Eigenvalues of \mathcal{A} : Air



Figure 2: Eigenvalues of \mathcal{A} : Water



Figure 3: Eigenvalues of \mathcal{A} : Freon

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