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Partial differential equations

A generalization of the quantum Bohm identity: Hyperbolic CFL condition for Euler–Korteweg equations

Généralisation de l'identité de Bohm quantique : condition CFL hyperbolique pour équations d'Euler–Korteweg

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ABSTRACT

In this note, we propose a surprising and important generalization of the quantum Bohm potential identity. This formula allows us to design an original conservative extended formulation of Euler–Korteweg systems and the construction of a numerical scheme with entropy stability property under a hyperbolic CFL condition in the multi-dimensional setting. To the authors' knowledge, this generalization of the quantum Bohm identity strongly improves what is already known for simulation of such a dispersive system and is also important for theoretical studies on compressible Navier–Stokes equations with degenerate viscosities.

RÉSUMÉ

Dans cette note, on propose une importante généralisation de l'identité dite du potentiel de Bohm quantique. Cette dernière permet de définir une formulation augmentée des systèmes d'Euler–Korteweg, qui est sous forme conservative dans le cas multi-dimensionnel. Une conséquence très importante de cette formulation est la construction de schémas avec stabilité entropique sous condition CFL hyperbolique du système d'Euler–Korteweg. Cette généralisation de l'identité de Bohm évite donc le développement d'ondes parasites pour ces systèmes de type dispersif et est aussi importante, par exemple, dans l'étude des équations de Navier–Stokes compressibles à viscosités dégénérées.

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Dans cette note, nous présentons une généralisation importante de l'identité du potentiel quantique de Bohm. Nous montrons ensuite comment cette relation permet d'introduire de nouvelles formulations augmentées (sous forme conservative) du système d'Euler–Korteweg (2)–(4) en plusieurs dimensions d'espace. Selon le choix des coefficients de capillarité, ce type de système intervient dans la modélisation des mélanges de type liquide–vapeur, des super-fluides ou de l'hydrodynamique quantique par exemple. Ces nouvelles formulations permettent de construire un schéma numérique d'ordre 1 à stabilité entropique sous condition CFL hyperbolique alors que le système primal est dispersif. À titre d'illustration, nous présentons des résultats numériques pour des films minces avec tension de surface modélisés par les équations de Saint-Venant. Nous expliquons également rapidement comment cette généralisation de l'identité de Bohm peut être utilisée dans le cadre de résultats théoriques sur Navier–Stokes compressibles à viscosités dégénérées.

1. Introduction and generalization of the quantum potential Bohm identity

In this note, we present an important generalization of the quantum potential Bohm identity. Then we show how this relation allows us to introduce a new extended formulation of (2)–(3) by considering the conservative variables $\varrho\mathbf{u}$, $\varrho\mathbf{w}$ instead of $\mathbf{u}$, $\mathbf{w}$. It allows one to transform the Euler–Korteweg system into a hyperbolic system perturbed by a second-order skew symmetric term in a multi-dimensional setting. The main motivation is the construction of a numerical scheme that is easily proved "entropy" stable under a hyperbolic CFL condition. We present preliminary numerical results for thin films with surface tension modeled by the shallow water equations illustrating this important property. We then finish by a remark on the importance of the generalization of the quantum potential Bohm identity for the compressible Navier–Stokes system with degenerate viscosities.

1.1. Generalization of the quantum potential Bohm identity

Let us first present an extension of the quantum potential Bohm identity

$$2\varrho\operatorname{div}\big(\Delta\sqrt{\varrho}/\sqrt{\varrho}\big)=\operatorname{div}\Big(\varrho\nabla\nabla\log\varrho\Big)$$

strongly used in quantum fluid mechanics. More precisely, we can prove the following result.

Lemma 1.1. *Let φ, K and F be three smooth functions from $R^+\to R^+$ such that*

$$\sqrt{\varrho}\varphi'(\varrho)=\sqrt{K(\varrho)},\qquad F'(\varrho)=\sqrt{K(\varrho)\,\varrho}.$$

Then

$$\varrho\nabla\Big(\sqrt{K(\varrho)}\,\Delta\Big(\int_0^{\varrho}\sqrt{K(s)}\,\mathrm{d}s\Big)\Big)=\operatorname{div}\Big(F(\varrho)\nabla\nabla\varphi(\varrho)\Big)-\nabla\Big(\big(F(\varrho)-F'(\varrho)\varrho\big)\Delta\varphi(\varrho)\Big)\tag{1}$$

This relation is a non-trivial extension of the quantum Bohm identity, which corresponds to the case $K(\varrho)=c/\varrho$. Its proof relies on some algebraic calculations.

2. Euler–Korteweg system

Using the new generalization of the quantum potential Bohm identity, let us now introduce (new) extended formulations of the so-called Euler–Korteweg system, which, in several space dimensions, reads

$$\partial_t\varrho+\operatorname{div}(\varrho\mathbf{u})=0,\tag{2}$$

$$\partial_t(\varrho\mathbf{u})+\operatorname{div}(\varrho\mathbf{u}\otimes\mathbf{u})+\nabla p(\varrho)=\operatorname{div}(\mathbf{K}),\tag{3}$$

where ϱ denotes the fluid density, $\mathbf{u}$ the fluid velocity, $p(\varrho)$ the fluid pressure and $\mathbf{K}$ the Korteweg stress tensor defined as

$$\mathbf{K}=\left(\varrho\operatorname{div}(K(\varrho)\nabla\varrho)+\frac{1}{2}(K(\varrho)-\varrho K'(\varrho))|\nabla\varrho|^2\right)\mathbf{I}_{\mathbb{R}^n}-K(\varrho)\nabla\varrho\otimes\nabla\varrho.\tag{4}$$

with $K(\varrho)$ the capillary coefficient. Then we show the importance of such formulations from a numerical point of view, allowing to control numerical instabilities. These models comprise a liquid–vapor mixture (for instance highly pressurized and hot water in nuclear reactors cooling system) [8], superfluids (helium near the absolute zero) [7] or even regular fluids at sufficiently small scales (think of ripples on shallow waters) [9]. In quantum hydrodynamics, the capillary coefficient

is chosen so that $\varrho K(\varrho) = constant$: in this case, the Euler–Korteweg equations correspond to the nonlinear Schrödinger equation after Madelung transform. In classical fluid mechanics, the capillary coefficient $K(\varrho)$ is chosen constant.

The system (2)–(3) admits two additional conservations laws. One conservation law is satisfied by the fluid velocity

$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla(\delta\mathcal{E}) = 0, \tag{5}$$

with $\mathcal{E}$ the potential energy and $\delta\mathcal{E}$ its *variational* gradient

$$\mathcal{E}(\varrho,\nabla\varrho) = F_0(\varrho) + \frac{1}{2}K(\varrho)|\nabla\varrho|^2, \quad \delta\mathcal{E} = F_0'(\varrho) - \frac{1}{2}K'(\varrho)|\nabla\varrho|^2 - K(\varrho)\Delta\varrho. \tag{6}$$

The local existence of strong solution to (2), (5) is proved in [1]. For that purpose, the authors introduced an extended formulation by considering an additional velocity $\mathbf{w} = \nabla\varphi(\varrho)$ with $\sqrt{\varrho}\varphi'(\varrho) = \sqrt{K(\varrho)}$:

$$\partial_t\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla\left(F_0'(\varrho) - \frac{|\mathbf{w}|^2}{2}\right) = \nabla\left(a(\varrho)\mathrm{div}(\mathbf{w})\right), \quad \partial_t\mathbf{w} + \nabla\left(\mathbf{u}^{\mathrm{T}}\mathbf{w}\right) = -\nabla\left(a(\varrho)\mathrm{div}(\mathbf{u})\right), \tag{7}$$

where $a(\varrho) = \sqrt{K(\varrho)\varrho}$. This formulation is particularly adapted to the derivation of a priori estimates, the very first one being a conservation law on the total (kinematic + potential) energy:

$$\begin{aligned}\partial_t\left(\frac{\varrho}{2}|\mathbf{u}|^2 + \mathcal{E}(\varrho,\nabla\varrho)\right) + \mathrm{div}\left(\mathbf{u}\left(\frac{\varrho}{2}|\mathbf{u}|^2 + \mathcal{E}(\varrho,\nabla\varrho) + p(\varrho)\right)\right) &= \mathrm{div}\Big(F(\varrho)(\nabla\mathbf{w}\,\mathbf{u} - \nabla\mathbf{u}\,\mathbf{w})\Big)\\ - \mathrm{div}\Big((F(\varrho) - \varrho F'(\varrho))(\mathrm{div}(\mathbf{w})\mathbf{u} - \mathrm{div}(\mathbf{u})\mathbf{w})\Big).\end{aligned} \tag{8}$$

with $F'(\varrho) = \varrho\varphi'(\varrho)$. Remark that the left-hand side of (1) corresponds to the Euler–Lagrange quantity from the capillarity term $\int K(\varrho)|\nabla\varrho|^2/2$. It suffices to observe that

$$K(\varrho)|\nabla\varrho|^2 = |\nabla(\int_0^\varrho \sqrt{K(s)}\,\mathrm{d}s)|^2$$

and thus as observed in [3] the variational gradient of the potential energy may be written

$$\delta\mathcal{E} = F_0'(\varrho) - \left(\sqrt{K(\varrho)}\,\Delta(\int_0^\varrho \sqrt{K(s)}\,\mathrm{d}s)\right).$$

This explains the importance of the generalization of the quantum Bohm potential. Following now the strategy of [1], we introduce a "good" additional unknown, homogeneous to a velocity. We denote this additional velocity $\mathbf{w} = \nabla\varphi(\varrho)$ with $\sqrt{\varrho}\varphi'(\varrho) = \sqrt{K(\varrho)}$. In order to write a suitable extended formulation of the Euler–Korteweg model, we also define $F(\varrho)$ so that $F'(\varrho) = \sqrt{K(\varrho)\varrho}$. Using the generalization of the quantum Bohm potential (1), the Euler–Korteweg system admits the extended formulation:

$$\begin{cases}\partial_t\varrho + \mathrm{div}(\varrho\,\mathbf{u}) = 0,\\ \partial_t(\varrho\,\mathbf{u}) + \mathrm{div}(\varrho\mathbf{u}\otimes\mathbf{u}) + \nabla p(\varrho) = \mathrm{div}(F(\varrho)\nabla\mathbf{w}^{\mathrm{T}}) - \nabla\left((F(\varrho) - \varrho F'(\varrho))\mathrm{div}(\mathbf{w})\right),\\ \partial_t(\varrho\,\mathbf{w}) + \mathrm{div}(\varrho\mathbf{w}\otimes\mathbf{u}) = -\mathrm{div}(F(\varrho)\nabla\mathbf{u}^{\mathrm{T}}) + \nabla\left((F(\varrho) - \varrho F'(\varrho))\mathrm{div}(\mathbf{u})\right).\end{cases} \tag{9}$$

The total energy is then transformed into a classical entropy of the first-order part of (9)

$$\frac{\varrho}{2}\|\mathbf{u}\|^2 + \mathcal{E}(\varrho,\nabla\varrho) = \frac{\varrho}{2}\left(\|\mathbf{u}\|^2 + \|\mathbf{w}\|^2\right) + F_0(\varrho) := \bar{\mathcal{E}}(\varrho,\mathbf{u},\mathbf{w}),$$

whereas the second-order part is skew symmetric. As a consequence, the energy conservation law (8) is obtained through a computation similar to that used in the first-order case.

2.1. Application: stable schemes under hyperbolic CFL condition

In this section, we introduce a numerical scheme for the important extended formulation (9). This strongly improves what has been done in [10]. The numerical domain is a rectangle defined by $0 \le x \le L_x$ and $0 \le y \le L_y$, which is divided into $N = n_x \times n_y$ rectangular cells. For the sake of simplicity, we consider uniform grid with constant spatial steps δx and δy. We focus on the spatial discretization of the second-order terms: they are written as $\partial_\alpha(f(\varrho)\partial_\beta u)$ with $(\alpha,\beta) \in \{x,y\}$ and $f(\varrho) = F(\varrho), \varrho F'(\varrho), F(\varrho) - \varrho F'(\varrho)$. For that purpose, we introduce the following finite difference operators:

$$(d_1 u)_{i,j} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{\delta x}, \quad (d_1^+ u)_{i+1/2,j} = \frac{u_{i+1,j} - u_{i,j}}{\delta x}, \quad (\bar{d}_1 u)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2\delta x},$$
$$(d_2 u)_{i,j} = \frac{u_{i,j+1/2} - u_{i,j-1/2}}{\delta y}, \quad (d_2^+ u)_{i,j+1/2} = \frac{u_{i,j+1} - u_{i,j}}{\delta y}, \quad (\bar{d}_2 u)_{i,j} = \frac{u_{i,j+1} - u_{i,j-1}}{2\delta y}. \tag{10}$$

As a result, the differential operator $\mathcal{T}(\varrho)\mathbf{u} = \mathrm{div}(F(\varrho)\nabla\mathbf{u}^{\mathrm{T}}) + \nabla\left((\varrho F'(\varrho) - F(\varrho))\mathrm{div}(\mathbf{u})\right)$ is approximated by $\mathcal{T}_h(\varrho)$ defined as

$$\mathcal{T}_h(\varrho)\mathbf{u}_{i,j} = \begin{cases} d_1\left(\varrho\, F'(\varrho) d_1^+ \mathbf{u}_1\right)_{i,j} + \bar{d}_2\left(F(\varrho)\bar{d}_1\mathbf{u}_2\right)_{i,j} + \bar{d}_1\left((\varrho F'(\varrho) - F(\varrho))\bar{d}_2\mathbf{u}_2\right)_{i,j}, \\ \bar{d}_1\left(F(\varrho)\bar{d}_2\mathbf{u}_1\right)_{i,j} + \bar{d}_2\left((\varrho F'(\varrho) - F(\varrho))\bar{d}_1\mathbf{u}_1\right)_{i,j} + d_2\left(\varrho F'(\varrho) d_2^+\mathbf{u}_2\right)_{i,j} \end{cases}$$

We discretize (9) as follows:

$$\begin{cases} \dfrac{\varrho_{i,j}^{n+1} - \varrho_{i,j}^n}{\delta t} + d_1(\mathcal{F}_{\varrho,1}^n)_{i,j} + d_2(\mathcal{F}_{\varrho,2}^n)_{i,j} = 0, \\ \dfrac{(\varrho\,\mathbf{u})_{i,j}^{n+1} - (\varrho\mathbf{u})_{i,j}^n}{\delta t} + d_1(\boldsymbol{\mathcal{F}}_{\mathbf{u},1}^n)_{i,j} + d_2(\boldsymbol{\mathcal{F}}_{\mathbf{u},2}^n)_{i,j} = \mathcal{T}_h(\varrho^{n+1})\mathbf{w}_{i,j}^{n+1}, \\ \dfrac{(\varrho\mathbf{w})_{i,j}^{n+1} - (\varrho\mathbf{w})_{i,j}^n}{\delta t} + d_1(\boldsymbol{\mathcal{F}}_{\mathbf{w},1}^n)_{i,j} + d_2(\boldsymbol{\mathcal{F}}_{\mathbf{w},2}^n)_{i,j} = -\mathcal{T}_h(\varrho^{n+1})\mathbf{u}_{i,j}^{n+1}, \end{cases} \tag{11}$$

where $\mathcal{F}_{\varrho,k}^n$, $\boldsymbol{\mathcal{F}}_{\mathbf{u},k}^n$, $\boldsymbol{\mathcal{F}}_{\mathbf{w},k}^n$ $(k = 1, 2)$ are classical Rusanov fluxes evaluated at ϱ^n, $\mathbf{u}^n$, $\mathbf{w}^n$. More precisely, the convection part is treated explicitly, whereas the capillary terms are treated implicitly. Remark that there are no capillary terms in the mass conservation law so that the implicit step amounts to solve a *linear* sparse system and is easily proved entropy stable. As a consequence, one can prove, by using discrete duality properties of the discrete second-order operators, the following entropy stability result.

Theorem 2.1. *Suppose (11) is completed with periodic boundary conditions. Assume the hyperbolic scheme (system (11) with $F = 0$) is entropy stable then the fully hyperbolic/capillary scheme (11) is entropy stable:*

$$\sum_{i=0}^{n_x}\sum_{j=0}^{n_y} \bar{\mathcal{E}}(\varrho_{i,j}^{n+1}, \mathbf{u}_{i,j}^{n+1}, \mathbf{w}_{i,j}^{n+1}) \le \sum_{i=0}^{n_x}\sum_{j=0}^{n_y} \bar{\mathcal{E}}(\varrho_{i,j}^{n}, \mathbf{u}_{i,j}^{n}, \mathbf{w}_{i,j}^{n}).$$

This means that the numerical scheme (11) is entropy stable under a classical hyperbolic Courant–Friedrichs–Lewy condition. As an application, we carried out a numerical simulation of a thin film falling down an inclined plane. A consistent shallow water model [2] is given by

$$\partial_t h + \mathrm{div}\,(h\mathbf{u}) = 0, \tag{12}$$

$$\partial_t(h\mathbf{u}) + \mathrm{div}\,(h\,\mathbf{u}\otimes\mathbf{u}) + \nabla(p(h)) + \left(\frac{g\sin(\theta)}{\nu}\right)^2 \partial_x\left(\frac{2h^5}{225}\right)\mathbf{e}_1 = S(h,\mathbf{u}) + \frac{\sigma h}{\rho}\nabla(\Delta h). \tag{13}$$

with $p(h) = g\cos(\theta)h^2/2$ and $S(h,\mathbf{u}) = gh\sin(\theta)\mathbf{e}_1 - 3\nu\mathbf{u}/h$ and $\mathbf{e}_1$ the first vector of the canonical base directed downstream. Here $g = 9.8$ is the gravity constant, ρ, ν, σ are respectively the fluid density, the kinematic viscosity, and the surface tension, whereas θ is the inclination of the plane. We picked the values found in [9] for a solution with 31% glycerin by weight: $\rho = 1.07\times10^3$ kg m^{-3}, $\nu = 2.3\times10^{-6}$ m^2 s^{-1} and $\sigma = 67\times10^{-3}$ kg s^{-2}. The source term is treated implicitly: since the source term is only in the equation for $\mathbf{u}$ and is linear with respect to $\mathbf{u}$, the implicit step remains linear. We first carry out a numerical simulation of the original experience in [9], but imposed periodic boundary conditions in both directions (see Fig. 1).

In order to test the robustness of the scheme, we also carried various numerical experiments of a drop falling down a plane in order to deal with wet/dry fronts. For that purpose, we introduced a precursor film with a thickness of 1.0×10^{-5} mm (see Fig. 2).

We will deal the problems of considering physical boundary conditions, deriving higher order schemes and considering wet/dry fronts in a forthcoming paper [5]. This will be useful to compute instabilities in moving contact lines.

3. Compressible Navier–Stokes equations with degenerate viscosities

Note that our formulation (mainly the generalization of the quantum Bohm potential) may be coupled with the result recently obtained in [6], allowing one to write an augmented formulation to the following compressible Navier–Stokes system with drag and capillary terms

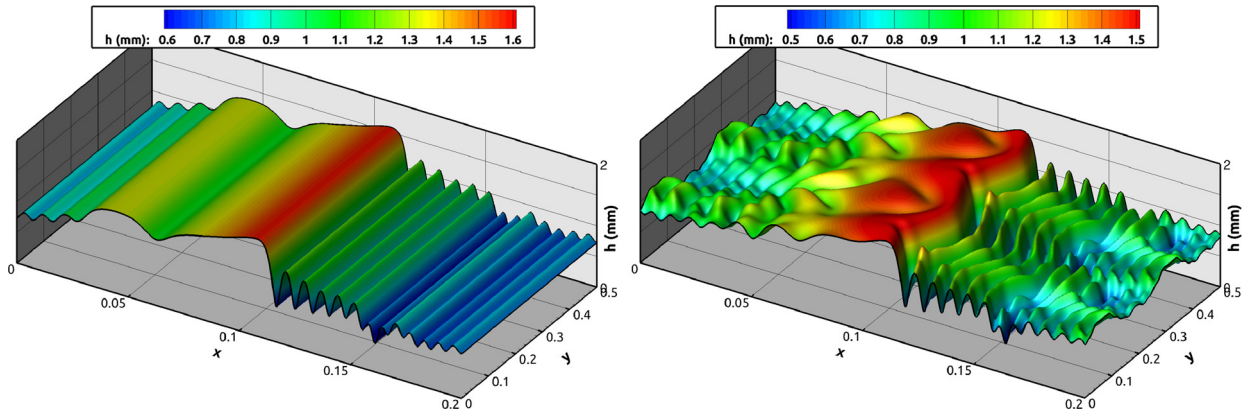

Fig. 1. (Color online.) Numerical simulation of a roll-wave in presence of surface tension. On the left: one-dimensional roll-wave without transverse perturbations. On the right: a two-dimensional roll-wave.

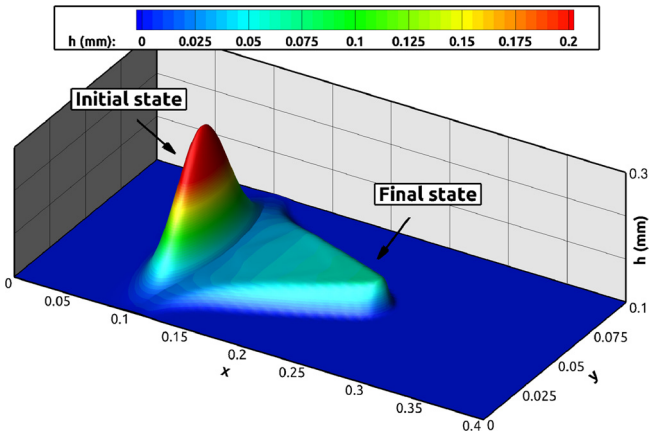

Fig. 2. (Color online.) Drop falling down an incline plane ($\theta = 60°$) at time $t = 0$ and $t = 1$ s. The fluid density, kinematic viscosity and surface tension are respectively $\rho = 1.0 \times 10^3$ kg m^{-3}, $\nu = 1.0 \times 10^{-6}$ m^2 s^{-1} and $\sigma = 67 \times 10^{-3}$ kg s^{-2}.

$$\partial_t \varrho + \operatorname{div}(\varrho \mathbf{u}) = 0, \tag{14}$$

$$\partial_t(\varrho \mathbf{u}) + \operatorname{div}(\varrho \mathbf{u} \otimes \mathbf{u}) - 2\operatorname{div}(\mu(\varrho) D(\mathbf{u}) - \nabla(\lambda(\varrho)\operatorname{div}\mathbf{u}) + \nabla p(\varrho) + r_1 \varrho |u|^\alpha u = \operatorname{div}(\mathbf{K}), \tag{15}$$

with $\lambda(\varrho) = 2(\mu'(\varrho)\varrho - \mu(\varrho))$ and $K(\varrho) = c(\mu'(\varrho))^2/\varrho$. Such a compatible system may be used to prove the global existence of weak solutions to the compressible Navier–Stokes equations with degenerate viscosities without capillary and drag terms, see [4]. This gives a generalization of the result in [11] where they consider the case $\mu(\varrho) = \mu\varrho$ and $\lambda(\varrho) = 0$ and where they strongly use the usual quantum Bohm identity in the approximate system.

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