TU Wien WS 2016
Institute for Analysis and Scientific Computing
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10. Exercise sheet for the course "Modeling with PDEs"
(Collision operators, energy-transport model, Madelung equations)

Exercise 1. Consider the so-called *elastic collision operator* (in the parabolic band approximation):

$$Q_{el}(f)(x,k) = \int_{\{|k'|=|k|\}} \sigma(x,k,k')(f(x,k') - f(x,k))\frac{dS(k')}{|k'|} \qquad x,k \in \mathbb{R}^3,$$

where $dS(k')$ is the boundary element and $\sigma(x,k,k')$ is the cross-section, which is positive and symmetric with respect to (k,k'), that is $\sigma(x,k,k') = \sigma(x,k',k) > 0$ for $x,k,k' \in \mathbb{R}^3$. Show that, for any distribution function $f = f(x,k)$,

(i) $\int_{\mathbb{R}^3} Q_{el}(f)dk = \int_{\mathbb{R}^3} Q_{el}(f)|k|^2 dk = 0$;

(ii) $\int_{\mathbb{R}^3} Q_{el}(f)f dk \le 0$;

(iii) $Q_{el}(f) = 0$ if and only if $f(x,k) = \tilde{f}(x,|k|)$ for some function $\tilde{f} : \mathbb{R}^3 \times [0,\infty) \to \mathbb{R}$.

Hint. The proof of point (ii) can be of help in showing point (iii).

Exercise 2. Consider the scaled energy-transport equations:

$$\partial_t n = \operatorname{div} J_0, \qquad \partial_t\left(\frac{3}{2}nT\right) = \operatorname{div} J_1 - J_0 \cdot \nabla V, \tag{1}$$

$$J_0 = \nabla n - \frac{n}{T}\nabla V, \qquad J_1 = \frac{3}{2}(\nabla(nT) - n\nabla V), \tag{2}$$

where $V = V(x)$ is a given function (electrostatic potential).

(i) Let $u_0 = \log(nT^{-3/2})$, $u_1 = -1/T$. Express n, $\mathcal{E} \equiv \frac{3}{2}nT$ in terms of u_0, u_1, and rewrite the fluxes J_0, J_1 explicitly as

$$J_0 = D_{00}\nabla u_0 + D_{01}\nabla u_1 + D_{00}u_1\nabla V, \quad J_1 = D_{10}\nabla u_0 + D_{11}\nabla u_1 + D_{10}u_1\nabla V \tag{3}$$

where $D_{01} = D_{10}$.

(ii) Define $w_0 = u_0 + Vu_1$, $w_1 = u_1$, $\rho_0 = n$, $\rho_1 = \frac{3}{2}nT - nV$. Keeping in mind (1), (3), derive the equations

$$\partial_t\rho_0 = \operatorname{div}(L_{00}\nabla w_0 + L_{01}\nabla w_1), \qquad \partial_t\rho_1 = \operatorname{div}(L_{10}\nabla w_0 + L_{11}\nabla w_1),$$

with $L_{00} = D_{00}$, $L_{01} = L_{10} = D_{01} - D_{00}V$, $L_{11} = D_{11} - 2VD_{01} + D_{00}V^2$.

Exercise 3. Referring to the framework of Exercise 2, consider (1), (2) in a bounded domain $\Omega \subset \mathbb{R}^3$. Assume that the following homogeneous Neumann boundary conditions are satisfied:

$$\nu \cdot \nabla n = \nu \cdot \nabla(nT) = 0, \qquad \text{on } \partial\Omega,$$

where ν is the outward normal to $\partial\Omega$. Define the (mathematical) entropy functional $S = \int_\Omega n \log(nT^{-3/2}) dx$. Prove that, for any (smooth enough, positive) solution (n, T) to (1), (2), it holds $S(t_1) \geq S(t_2)$ for $0 < t_1 < t_2$.

Hint. Use points (i), (ii) of the previous exercise. Write $n \log(nT^{-3/2})$ as function of $(n, \mathcal{E})$ to differentiate S. Keeping in mind the boundary conditions, use integration by parts. Prove that the matrix $L = (L_{ij})_{i,j=0,1}$ in point (ii) of Ex. 2 is related to $D = (D_{ij})_{i,j=0,1}$ in point (i) by $L = P^\top D P$ with $P = \begin{pmatrix} 1 & \varphi \\ 0 & 1 \end{pmatrix}$ and $\varphi(x)$ a suitable scalar function.

Remark. *It is possible to show that, if n, T are uniformely positive and bounded in $\Omega \times (0, \infty)$, and V is bounded in Ω, the entropy dissipation inequality*

$$\frac{dS}{dt} + c \int_\Omega \left| \nabla \left(\log(nT^{-3/2}) - \frac{V}{T} \right) \right|^2 + \left| \nabla \left(\frac{1}{T} \right) \right|^2 dx \leq 0, \quad t > 0,$$

holds, where $c > 0$ is a suitable constant.

Exercise 4. A single electron with mass m and charge q in a vacuum subject to an electric potential V is described by a *wavefunction* $\psi = \psi(x, t)$, $\psi : \mathbb{R}^3 \times [0, \infty) \to \mathbb{C}$, which obeys to the *Schrödinger equation*

$$i\hbar \partial_t \psi = -\frac{\hbar^2}{2m} \Delta \psi + qV\psi, \quad t > 0.$$

In the above equation, i is the imaginary unit, while $\hbar$ is the so-called Dirac constant. The WKB form of the wavefunction ψ is the decomposition

$$\psi(x, t) = \sqrt{n(x, t)} e^{iS(x,t)/\hbar},$$

where $S : \mathbb{R}^3 \times [0, \infty) \to \mathbb{R}$ is the phase of the wavefunction, while $n : \mathbb{R}^3 \times [0, \infty) \to [0, \infty)$ is the "electron density" (to be precise, the probability density associated to the electron). Define the current J as $J = \frac{\hbar}{m} \Im(\overline{\psi} \nabla \psi)$. Prove that n, J satisfy the *Madelung equations*:

$$\partial_t n + \operatorname{div} J = 0, \quad \partial_t J + \operatorname{div} \left(\frac{J \otimes J}{n} \right) + \frac{q}{m} n \nabla V - n \frac{\hbar^2}{2m^2} \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0. \tag{4}$$

Hint. Insert the WKB ansatz into the Schrödinger equation, then take real and imaginary part of the resulting equation. Write J in term of n, S.

The exercises will be reviewed in class on January 25, 2017.