

Homework No.2, 550.695, Due October 4, 2011.

1. This problem studies the local conservation laws of classical molecular fluids.

(a) Derive the local conservation of momentum

$$\partial_t \mathbf{j}(\mathbf{x}, t) + \nabla \cdot \mathbf{T}(\mathbf{x}, t) = \mathbf{0},$$

where \mathbf{T} is the stress-tensor given in class and $(\nabla \cdot \mathbf{T})_i = \partial_j T_{ij}$. *Hint:* Use Newton's third law, and also use the fundamental theorem of calculus to write

$$(\mathbf{r}_{nm} \cdot \nabla) \int_0^1 ds \delta^3(\mathbf{x} - \mathbf{r}_n + s\mathbf{r}_{nm}) = \delta^3(\mathbf{x} - \mathbf{r}_m) - \delta^3(\mathbf{x} - \mathbf{r}_n).$$

(b) Use a similar argument to derive the local conservation of energy

$$\partial_t e(\mathbf{x}, t) + \nabla \cdot \mathbf{s}(\mathbf{x}, t) = 0$$

where \mathbf{s} is the energy current given in class.

(c) Argue that, for a short-range potential, the operators $\mathbf{T}(\mathbf{x}, t)$ and $\mathbf{s}(\mathbf{x}, t)$ are truly local, i.e. depend upon the positions and momenta only of molecules near \mathbf{x} .

2. This problem studies another approach to space-scale resolution of functions via *orthonormal wavelet bases*. These are given by “mother wavelets” $\psi(x)$ whose discrete dilatations and translations

$$\psi_{m,n}(x) = 2^{m/2} \psi(2^m x - n), \quad m, n = 0, \pm 1, \pm 2, \dots$$

provide an orthonormal basis in the space of square-integrable functions. The wavelet $\psi_{m,n}$ has length-scale 2^{-m} and spatial location $2^{-m}n$.

(a) The simplest such basis is provided by the *Haar wavelet*:

$$\psi(x) = \begin{cases} +1 & 0 < x < 1/2 \\ -1 & 1/2 \leq x < 1 \\ 0 & \text{otherwise} \end{cases}$$

Prove the orthogonality property

$$\int_{-\infty}^{+\infty} dx \psi_{m,n}(x) \psi_{m',n'}(x) = \delta_{m,m'} \delta_{n,n'}.$$

Hint: Haar wavelets only overlap if they are at different scales. In that case, the smaller-scale wavelet with $m' > m$ is located where the other wavelet is constant.

(b) The expansion

$$f(x) = \sum_{m,n} c_{m,n} \psi_{m,n}(x)$$

with $c_{m,n} = \int_{-\infty}^{+\infty} f(x) \psi_{m,n}(x) dx$ converges for any square-integrable f and provides a *multiresolution analysis* of the function. For $x \in [0, 1]$ this expansion has the form

$$f(x) = \bar{c} + \sum_{m=0}^{\infty} \sum_{n=0}^{2^m-1} c_{m,n} \psi_{m,n}(x) \quad (*)$$

with $\bar{c} = \int_0^1 dx f(x)$. Use the latter form (*) to approximate the function $f(x) = e^x$ for $x \in [0, 1]$ by a low-pass filter approximation $f_M(x)$ obtained by keeping only the terms in the sum over m with $0 \leq m \leq M$. Plot the exact function $f(x)$ and the low-pass filter approximations $f_M(x)$ for $M = 1, 2, \dots, 8$.

(c) Although the Haar wavelet is compactly supported in physical space, it has very poor localization in wavenumber. Calculate the Fourier transform

$$\hat{\psi}(k) = \int_{-\infty}^{+\infty} dx e^{-ikx} \psi(x)$$

and determine its rate of decay for $|k| \rightarrow \infty$.

(d) EXTRA CREDIT: It is impossible to localize both $\psi(x)$ and $\hat{\psi}(k)$ arbitrarily well; for example, they cannot both decay exponentially rapidly. The proof of this result is based on showing the “vanishing-moments property” that

$$\hat{\psi}^{(m)}(0) = (-i)^m \int dx x^m \psi(x) = 0, \quad m = 0, 1, \dots, M-1 \quad (**)$$

if both $|\psi(x)| \leq C(1+|x|)^{-(M+1+\epsilon)}$ and $|\hat{\psi}(k)| \leq C(1+|k|)^{-(M+1+\epsilon)}$ for some positive constants C and ϵ . In that case, if ψ and $\hat{\psi}$ both decay exponentially, then *all* m th-derivatives $\hat{\psi}^{(m)}(0)$ vanish and thus the analytic function $\hat{\psi}(k)$ is identically zero.

You will develop here an argument for the vanishing moments property (**). Show that the orthogonality of ψ and $\psi_{m,n}$ is equivalent to $\int_{-\infty}^{+\infty} dk e^{-ika} \hat{\psi}(k)^* \hat{\psi}(2^{-m}k) = 0$ for all integers m and $a = 2^{-m}n$ with integer n . Then take m large and use a Taylor expansion of $\hat{\psi}(2^{-m}k)$ around 0 to derive the identity

$$0 = \sum_{p=0}^{M-1} \frac{i^p}{p!} \psi^{(p)}(a) \hat{\psi}^{(p)}(0) 2^{-pm} + O(2^{-Mm}).$$

By choosing a point a such that $\psi^{(p)}(a) \neq 0$ for all $p = 0, 1, \dots, M-1$ (if you can, prove that such an a exists!), show that (**) must hold.

3. This problem investigates the concept of formal closure.

(a) For the linear model problem discussed in class,

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{y} + \mathbf{f}(t), \\ \dot{\mathbf{y}} = \mathbf{C}\mathbf{x} + \mathbf{D}\mathbf{y} + \mathbf{g}(t), \end{cases}$$

derive the generalized Langevin equation

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \int_{-\infty}^t ds \mathbf{K}(t-s)\mathbf{x}(s) + \mathbf{f}^*(t) + \mathbf{f}(t),$$

with all notations as in the classnotes.

(b) A special case of the above is the linear system of ODE's

$$\begin{cases} \dot{x} = -2x + y, & x(0) = 2, \\ \dot{y} = -x - 2y, & y(0) = 2, \end{cases}$$

which yields the equation with memory

$$\dot{x} = -2x - \int_0^t d\tau e^{-2\tau} x(t-\tau) + 2e^{-2t}, \quad x(0) = 2.$$

If the integral is approximated by discretization and by imposing a finite memory $T = M\Delta t$, one obtains a delay-differential equation (DDE)

$$\dot{x} = -2x - \sum_{i=1}^M \Delta t e^{-2i\Delta t} x(t-i\Delta t) + 2e^{-2t}, \quad x(0) = 2.$$

Use numerical software, e.g. `dde23` in MATLAB, to compute the solution to the above DDE. Compare the solution, for accuracy and efficiency, with direct numerical solution of the original system of ODE's.