

## Homework No.2, 550.695, Due February 19, 2009.

1. This problem discusses the simultaneous localization of filter kernels in physical space and in Fourier space. For simplicity, we consider one space dimension.

(a) Show that the function  $\widehat{G}_0$  in Fourier space defined as

$$\widehat{G}_0(k) = \begin{cases} \exp\left(-\frac{k^2}{1/4-k^2}\right) & |k| < 1/2 \\ 0 & |k| \geq 1/2 \end{cases}$$

is infinitely differentiable or  $C^\infty$ . *Hint:* The key is to show that derivatives of all orders are zero at  $k = \pm 1/2$ , both from the left and the right.

(b) Explain why the above property implies that the inverse Fourier transform

$$G_0(x) = \int dk \widehat{G}_0(k) \cos(kx)$$

decays faster than any power  $|x|^{-p}$  as  $x \rightarrow \infty$ . Show also that  $G_0$  is real-analytic, i.e. has a convergent power series representation

$$G_0(x) = \sum_{n=0}^{\infty} c_{2n} x^{2n}.$$

*Hint:* Show that  $c_{2n} = \frac{(-1)^n}{(2n)!} \int dk \widehat{G}_0(k) k^{2n}$  and derive a bound on the growth in  $n$ .

(c) The function  $G_0(x)$  is not everywhere positive, but  $G(x) = [G_0(x)]^2$  is so. Show also that  $G(x)$  is  $C^\infty$  and decays faster than any power as  $|x| \rightarrow \infty$ .

(d) Show that

$$\widehat{G}(k) = \int dp \widehat{G}_0(p) \widehat{G}_0(k-p)$$

is positive,  $C^\infty$  and compactly supported in the  $k$ -interval  $[-1, 1]$ .

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

(a) Derive the local conservation of momentum

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

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  $\mathbf{x}$ .

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

$$\begin{cases} \dot{x} = -x + y, & x(0) = 4, \\ \dot{y} = x - y, & y(0) = 2, \end{cases}$$

which yields the equation with memory

$$\dot{x} = -x + \int_0^t d\tau e^{-\tau} x(t-\tau) + 2e^{-t}, \quad x(0) = 4.$$

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

$$\dot{x} = -x + \sum_{i=1}^M \Delta t e^{-i\Delta t} x(t - i\Delta t) + 2e^{-t}, \quad x(0) = 4.$$

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.