Assignment 6 (Due Mar 11). Covers: pages 145-149 of text. Optional reading: pages 149-153, 184-196.

The questions marked "Optional" are more challenging, and will not count toward your final grade. They will however strengthen both your technical skills and your conceptual understanding of the material.

- Q1. Do Exercise 17 of Chapter 5 of the textbook.
- Q2. Do Exercise 5 of Chapter 6 of the textbook.
- Q3. (Optional) Do Exercise 7 of Chapter 6 of the textbook.
- Q4. Do Problem 7(a) in Section 7 of Chapter 6 of the textbook.
- Q5. Let $f(x)$ be a Schwartz function on $\mathbf{R}$, and let $u(x,t)$ be the solution to the one-dimensional heat equation

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t)$$

  as discussed in class (or in Section 2.1 of Chapter 5 of the textbook), defined for all $x \in \mathbf{R}$ and $t \geq 0$. Here we have set the thermal diffusivity κ to equal 1 for simplicity.

- Q5(a). Show that if $f(x)$ is non-negative for all $x \in \mathbf{R}$ (i.e. $f(x) \geq 0$ for all $x \in \mathbf{R}$), then $u(x,t)$ is also non-negative for all $x \in \mathbf{R}$. (Hint: use the heat kernel).
- Q5(b). Show that if there exist upper and lower bounds $M_1 < M_2$ such that $M_1 \leq f(x) \leq M_2$ for all $x \in \mathbf{R}$, then we also have $M_1 \leq u(x,t) \leq M_2$ for all $x \in \mathbf{R}$ and $t > 0$. Can you give a physical interpretation or explanation of this fact (which is sometimes referred to as the *maximum principle*)?
- Q6. The *Schrödinger equation*

$$i\frac{\partial \psi}{\partial t} + \frac{\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} = 0$$

  describes the evolution of a wave function $\psi(x,t)$ of a particle, which is a complex-valued function of one spatial variable $x \in \mathbf{R}$ and one time variable $t \in \mathbf{R}$. Here $\hbar$ and m are positive constants ($\hbar$ is Planck's constant, and m is the mass of the particle). This equation plays an important role in quantum physics. The purpose of this exercise is to illustrate the power of the Fourier transform in discovering important physical consequences of this equation.

- Q6(a). Suppose $\psi(x,t)$ is Schwartz for each t, and suppose we are given initial data $\psi(x,0) = f(x)$ for some Schwartz function f. By arguing as in class or in the textbook, derive the formulae

$$\hat{\psi}(\xi,t) = e^{2\pi^2 i\xi^2 t\hbar/m}\hat{f}(\xi)$$

and

$$\psi(x,t) = \int_{\mathbf{R}} e^{2\pi^2 i\xi^2 t\hbar/m} e^{-2\pi i x\xi}\hat{f}(\xi)\, d\xi.$$

Note: You may freely interchange time derivatives with spatial integrals without justification.

- Q6(b). Continuing part (a), suppose that we also know that $\int_{-\infty}^{\infty} |f(x)|^2\, dx = 1$. Conclude that $\int_{-\infty}^{\infty} |\psi(x,t)|^2\, dx = 1$ for all $t \in \mathbf{R}$. (This fact is sometimes referred to as *conservation of probability* in quantum physics).

- Q6(c). Continuing part (b), suppose that we also know that $\int_{-\infty}^{\infty} \frac{\hbar^2}{2m}|\frac{df}{dx}(x)|^2\, dx = \langle E\rangle$ for some non-negative real number $\langle E\rangle$ (this quantity is known as the *expected energy*). Conclude that $\int_{-\infty}^{\infty} \frac{\hbar^2}{2m}|\frac{\partial\psi}{\partial x}(x,t)|^2\, dx = \langle E\rangle$ for all $t \in \mathbf{R}$. (This fact is sometimes referred to as *conservation of energy* in quantum physics. Note that the factor $\frac{\hbar^2}{2m}$, while important for physics, will not play a major role in this mathematical problem. The presence of angled brackets around the E is for physical reasons; you can ignore them from a mathematical standpoint.).

- Q6(d). (Optional) Continuing part (c), suppose that we also know that $\int_{-\infty}^{\infty} \frac{\hbar}{i}\frac{df}{dx}(x)\overline{f(x)}\, dx = \langle p\rangle$ for some $\langle p\rangle \in \mathbf{R}$ (this quantity is known as the *expected momentum*). Conclude that that $\int_{-\infty}^{\infty} \frac{\hbar}{i}\frac{\partial\psi}{\partial x}(x,t)\overline{\psi(x,t)}\, dx = \langle p\rangle$ for all $t \in \mathbf{R}$. (This fact is sometimes referred to as *conservation of momentum* in quantum physics. Again, the factor $\frac{\hbar}{i}$ out the front do not play a major role in this question, although it is important for the next question). Is it possible for the expected momentum to be a complex number rather than a real number?

- Q6(e). (Optional) Continuing part (d), for each time $t \in \mathbf{R}$, let $\langle x(t) \rangle$ denote the quantity

$$\langle x(t) \rangle := \int_{-\infty}^{\infty} x |\psi(x,t)|^2 \, dx;$$

this quantity is known as the *expected position at time t*. Suppose also that the expected momentum $\langle p \rangle$ is equal to $\langle p \rangle = m \langle v \rangle$ for some real number $\langle v \rangle$ (this quantity is known as the *expected velocity*). Show that

$$\langle x(t) \rangle = \langle x(0) \rangle + t \langle v \rangle$$

(this is sometimes referred to as *Newton's first law* for the Schrödinger equation).

- Q7. Let $v = (v_1, v_2, v_3)$ and $w = (w_1, w_2, w_3)$ be two vectors in $\mathbf{R}^3$. Recall that the *dot product* $v \cdot w$ and *cross product* $v \times w$ are defined as

$$v \cdot w = v_1 w_1 + v_2 w_2 + v_3 w_3$$

and

$$v \times w = (v_2 w_3 - v_3 w_2, v_3 w_1 - v_1 w_3, v_1 w_2 - v_2 w_1).$$

Let $\vec{f}(x_1, x_2, x_3) = (f_1(x_1, x_2, x_3), f_2(x_1, x_2, x_3), f_3(x_1, x_2, x_3)$ be a vector-valued function on $\mathbf{R}^3$, i.e. a function from $\mathbf{R}^3$ to $\mathbf{R}^3$. (The component functions f_1, f_2, f_3 are thus scalar valued functions, i.e. functions from $\mathbf{R}^3$ to $\mathbf{R}$. If $\vec{f}$ is differentiable (i.e. each of the components f_1, f_2, f_3 are differentiable, we define the *divergence* $\mathrm{div}\vec{f}$ of $\vec{f}$ to be the scalar-valued function

$$\mathrm{div}\vec{f} = \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} + \frac{\partial f_3}{\partial x_3}$$

and the *curl* $\mathrm{curl}\vec{f}$ of $\vec{f}$ to be the vector-valued function

$$\mathrm{curl}\vec{f} = (\frac{\partial f_3}{\partial x_2} - \frac{\partial f_2}{\partial x_3}, \frac{\partial f_1}{\partial x_3} - \frac{\partial f_3}{\partial x_1}, \frac{\partial f_2}{\partial x_1} - \frac{\partial f_1}{\partial x_2}).$$

If $\vec{f}$ is Schwartz (i.e. each of the components f_1, f_2, f_3 is Schwartz, we define the vector-valued Fourier transform $\widehat{\vec{f}}(\xi)$ by the formula

$$\widehat{\vec{f}}(\xi) := \int_{\mathbf{R}^3} e^{-2\pi i x \cdot \xi} \vec{f}(\xi) \, d\xi.$$

- Q7(a) If $\vec{f}$ is Schwartz, show that $\widehat{\vec{f}} = (\hat{f}_1, \hat{f}_2, \hat{f}_3)$.
- Q7(b) If $\vec{f}$ is Schwartz, show that

  $$\widehat{\mathrm{div}\vec{f}}(\xi) = 2\pi i \xi \cdot \widehat{\vec{f}}(\xi)$$

  and

  $$\widehat{\mathrm{curl}\vec{f}}(\xi) = 2\pi i \xi \times \widehat{\vec{f}}(\xi)$$

  (recall that $\xi = (\xi_1, \xi_2, \xi_3)$ is a vector in $\mathbf{R}^3$). In a similar spirit, show that for any scalar-valued Schwartz function $F(x)$, we have

  $$\widehat{\mathrm{grad}F}(\xi) = 2\pi i \xi \hat{F}(\xi)$$

  where the gradient $\mathrm{grad}F$ of F is defined as $\mathrm{grad}F = (\frac{\partial F}{\partial x_1}, \frac{\partial F}{\partial x_2}, \frac{\partial F}{\partial x_3})$.
- Q7(c) Suppose we define the Laplacian $\Delta\vec{f}$ of $\vec{f}$ by the formula

  $$\Delta\vec{f} = \frac{\partial^2}{\partial x_1^2}\vec{f} + \frac{\partial^2}{\partial x_2^2}\vec{f} + \frac{\partial^2}{\partial x_3^2}\vec{f} = (\Delta f_1, \Delta f_2, \Delta f_3).$$

  Show that

  $$\widehat{\Delta\vec{f}}(\xi) = -4\pi^2|\xi|^2\widehat{\vec{f}}(\xi).$$
- Q7(d) For any two vectors v and w in $\mathbf{R}^3$, verify the identity

  $$|v|^2 w = v(v \cdot w) + v \times (v \times w).$$

  (Note: while this can be done algebraically, the geometric proof may be more clear conceptually).
- Q7(e) Using Q7(bcd), verify the *Hodge identity*

  $$\Delta\vec{f} = \mathrm{graddiv}\vec{f} + \mathrm{curlcurl}\vec{f}.$$