Week 14

Topics: time–dependent and time–independent Schrödinger equations

Review from Week 13:

- **Eigenvalues and Spectrum:** If $T : D_T \to \mathcal{H}$ is a linear operator with domain $D_T \subset \mathcal{H}$ we say that $0 \neq \phi \in D_T$ is an eigenvector of T with eigenvalue $\lambda \in \mathbb{C}$ if and only if $T\phi = \lambda\phi$. Notice that there are two subtle details in this definition: $\phi \neq 0$ is not the zero vector and $\phi \in D_T$ must be in the domain of T. The spectrum $\sigma(T)$ is defined as

$$\sigma(T) = \{\lambda \in \mathbb{C} : \lambda \text{ is an eigenvalue of T } \} \subset \mathbb{C}.$$

- **Symmetric operators:** An operator $T : D_T \to \mathcal{H}$ is called symmetric if and only if

$$\langle \psi, T\phi \rangle_{\mathcal{H}} = \langle T\psi, \phi \rangle_{\mathcal{H}} \qquad \forall\ \psi, \phi \in D_T.$$

- **Self-adjoint operators:** An operator $T : D_T \to \mathcal{H}$ is called self-adjoint if and only if $T = T^*$ and $D_T = D_{T^*}$, where $T^* : D_{T^*} \to \mathcal{H}$ denotes the adjoint of T. It is defined through

$$\langle T\psi, \phi \rangle_{\mathcal{H}} = \langle \psi, T^*\phi \rangle_{\mathcal{H}} \qquad \forall\ \psi \in D_T, \phi \in D_{T^*}$$

  and we always have that $D_T \subset D_{T^*}$. If T is symmetric, then T^* is an extension of T. The spectral theorem holds true for self-adjoint operators.

- **Hermite's operator:** Hermite's operator $\ell(y) = -e^{x^2/2}\partial_x\big(e^{-x^2/2}\partial_x y\big)$ is defined on a suitable domain $D_\ell \subset L^2(\mathbb{R}, e^{-x^2/2}dx)$. We have seen that $\sigma(\ell) = \mathbb{N}_0$ and that each eigenvalue is simple

- **Hermite polynomials:** The eigenfunctions of Hermite's operator are the Hermite polynomials H_n. The n–th eigenfunction H_n is a polynomial of degree n that is even if n is even and odd if n is odd. It is normalized in the sense that $H_n = x^n + p(x)$ for some polynomial p of degree strictly less than n. The norm of H_n in $L^2(\mathbb{R}, e^{-x^2/2}dx)$ is $\langle H_n, H_n \rangle = \sqrt{2\pi}\, n!$. The Hermite polynomials, once normalized in $L^2(\mathbb{R}, e^{-x^2/2}dx)$, form a complete orthonormal basis in $L^2(\mathbb{R}; e^{-x^2/2}dx)$.

1. **The free, time–independent Schrödinger equation.** In this problem, we discuss the general solution of the time–independent Schrödinger equation of a quantum particle moving in a box $\Lambda = [0;L]^3$ with zero–boundary conditions. The time evolution is modeled by

$$\begin{cases} i\partial_t \psi = -\left(\partial_{x_1}^2 + \partial_{x_2}^2 + \partial_{x_3}^2\right)\psi, \\ \psi_{|t=0} = \psi_0 \in L^2(\Lambda; dx). \end{cases} \tag{1}$$

where $(x,t) \mapsto \psi(t,x)$ is the wave function of the system, for $t \in \mathbb{R}$ and $x \in [0;L]^3 \subset \mathbb{R}^3$. The differential operator on the right hand side is called the (three–dimensional) Laplace operator and we abbreviate it from now on by $-\Delta = -\partial_{x_1}^2 - \partial_{x_2}^2 - \partial_{x_3}^2$. $-\Delta$ is self-adjoint with domain

$$\mathcal{D} = \left\{\psi \in H^2(\Lambda; dx) : \psi_{|\partial\Lambda} \equiv 0\right\}.$$

Equation (1) describes a particle that moves freely in $\Lambda = [0;L]^3$ without external forces. Before solving the equation (1) by the Hilbert space method, let's first make some interesting physical observations. Recall that $x \mapsto |\psi_0(x)|^2$ is interpreted in quantum mechanics as a probability density function and that we only consider $\psi_0 \in L^2(\Lambda; dx)$ with $\|\psi_0\|_2 = 1$.

(a) Show that if $t \mapsto \psi_t$ solves the Schrödinger equation (1), then $\|\psi_t\|_2 = 1$ for all $t \in \mathbb{R}$. This means that $x \mapsto |\psi_t(x)|^2$ defines a probability density for all times $t \in \mathbb{R}$, if this is the case initially at time $t = 0$.

(b) The energy of a particle with normalized wave function $\psi_0 \in L^2(\Lambda; dx)$ is $\langle \psi_0, -\Delta\psi_0\rangle$. Suppose $t \mapsto \psi_t$ solves the Schrödinger equation (1). Then $t \mapsto \psi_t$ describes a particle moving in Λ without external forces, in particular the particle should not lose any energy. Prove that this is the case by showing that $t \mapsto \langle \psi_t, -\Delta\psi_t\rangle$ is constant in time $t \in \mathbb{R}$.

Our next goal is to derive the solution of the initial value problem (1) in the Hilbert space framework. To do so, we interpret (1) as a vector–valued ordinary differential equation in time with time–dependent $L^2([0;L]^3, dx)$ valued map $t \mapsto \psi_t \in \mathcal{D}$ for all $t \in \mathbb{R}$. That is, for every fixed time $t \in \mathbb{R}$, we have that the wave function at time t lies in $\psi_t \in \mathcal{D}$.

(a) Find an orthonormal eigenbasis of the self-adjoint operator $-\Delta$ and determine $\sigma(\ell) \subset \mathbb{R}$. *Hint: What are the eigenfunctions of $\ell(y) = y''$ in one dimension? Having this in mind, construct a suitable product eigenbasis for $-\Delta$, similarly as on problem set 9.*

(b) Given a fixed time $t \in \mathbb{R}$, describe the general form of $\psi_t \in \mathcal{D}$, the wave function at time $t \in \mathbb{R}$.

(c) Using the Schrödinger equation (1), derive an equation for the time-dependent coefficients in the basis expansion of $\psi_t \in \mathcal{D}$. Find the general form of the coefficients by solving a sequence of linear, first order ODE.

(d) Plug in the initial condition $x \mapsto \psi_0$ and determine the unique solution to the free Schrödinger equation (1) with initial data ψ_0.

2. The Harmonic Oscillator. As explained in the lecture, the time–independent Schrödinger equation refers to the eigenvalue equation of the Hamilton operator $H = -\Delta + V(x)$, where V denotes the potential energy. Let's consider in this problem the setting of $L^2(\mathbb{R}; dx)$, describing a particle in $\mathbb{R}$. For a general potential V, the time–independent Schrödinger equation is almost surely ;) not solvable. A remarkable model which, however, can be solved explicitly is the harmonic oscillator. This is the model where H is given by

$$H\psi = -\partial_x^2 \psi + \frac{x^2}{4}\psi,$$

defined as a self-adjoint operator on a suitable subspace $D_H \subset L^2(\mathbb{R}; dx)$. We want to find the energy levels of H, that is, its spectrum $\sigma(H) \subset \mathbb{R}$.

(a) As a preparation, consider $\psi \in L^2(\mathbb{R}; dx)$. Show that $\psi \in L^2(\mathbb{R}; dx)$ if and only if the associated function $x \mapsto \varphi(x) = \psi(x)e^{x^2/4} \in L^2(\mathbb{R}; e^{-x^2/2}dx)$: more precisely that $\|\psi\|_{L^2(\mathbb{R};dx)} = \|\varphi\|_{L^2(\mathbb{R};e^{-x^2/2}dx)}$. We say that the map Φ, that sends ψ to φ, is an *isometry*. In fact, it turns out that Φ is a unitary map and we can therefore work equivalently in the Hilbert space $L^2(\mathbb{R}; e^{-x^2/2}dx)$.

(b) What is the inverse map of Φ, i.e. $\Phi^{-1} : L^2(\mathbb{R}; e^{-x^2/2}dx) \to L^2(\mathbb{R}; dx)$? As a linear operator, H is unitarily equivalent to the operator $\Phi\, H\, \Phi^{-1}$ acting on $L^2(\mathbb{R}; e^{-x^2/2}dx)$. As in the finite dimensional case, the spectrum is preserved under unitary conjugation. Compute its action in $L^2(\mathbb{R}; e^{-x^2/2}dx)$.

(c) Consider the eigenvalue equation for $\Phi\, H\, \Phi^{-1}$ and determine $\sigma(\Phi\, H\, \Phi^{-1}) = \sigma(H)$. In addition to that, determine the eigenfunctions of H.