Lecture 1

Spectral Theory I — Spring 2012

Prerequisite: basic course in functional analysis & Hilbert space

References

(1) Volumes I → IV, Methods of Modern Mathematical Physics, M. Reed and B. Simon

(2) Perturbation Theory for Linear Operators, T. Kato.

In this semester, and next semester, we will study the spectral theory of self-adjoint operators A in a (separable) Hilbert space $\mathcal{H}$.

Such operators, and their spectra, are of interest in many areas of mathematics, applied mathematics and mathematical physics. A key example is quantum mechanics, where many of the results and techniques that we will study originated

Recall that in classical mechanics a particle is described by a point $(x, p) =$ (position, momentum) in phase space, $\mathbb{R}^6 = \mathbb{R}^3 \times \mathbb{R}^3$, and the dynamics is given by Hamilton's equations

$$\dot{x}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial x_k}, \quad k = 1, \dots, n$$

where $H = H(x, p)$ is the <u>Hamiltonian</u> for the system.

In quantum mechanics, particles are described by unit vectors in a (separable) Hilbert space $\mathcal{H}$. Corresponding to each <u>unit</u> vector, there is a <u>physical state</u>: vectors differing by a phase

$$\varphi \to e^{i\alpha} \varphi \qquad \alpha \in \mathbb{R}$$

describe the same state. Observables correspond to self-adjoint operators A acting in $\mathcal{H}$. Associated to any self-adjoint operator A there is (see later) a <u>projection</u>

valued measure is a family of projections $\{P_\Omega,$ Ω a Borel set in $\mathbb{R}\}$ such that

(3.1) (a) for each Borel set Ω, P_Ω is an orthogonal projection

(b) $P_\phi = 0$, $P_{\mathbb{R}} = 1$

(c) If $\Omega = \bigcup_{n=1}^{\infty} \Omega_n$, $\Omega_n \cap \Omega_m = \phi$ for $n \neq m$,

then $P_\Omega = \operatorname{s-lim}_{N \to \infty} \left(\sum_{n=1}^{N} P_{\Omega_n} \right)$

(d) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$

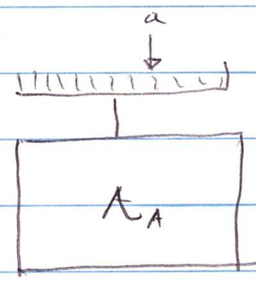
The nomenclature "measure" reflects the following:

If $\phi \in \mathcal{H}$, then $\Omega \to (\phi, P_\Omega \phi)$ is an ordinary (finite) measure on $\mathbb{R}$, $(\phi, P_{\mathbb{R}} \phi) = \|\phi\|^2$. Denoting integration with respect to this measure by the symbol $d(\phi, P_\lambda \phi)$ we have the basic relation

(3.2) $$A = \int \lambda \, dP_\lambda \quad \text{i.e.} \quad (\phi, A\phi) = \int \lambda \, d(\phi, P_\lambda \phi)$$

for all ϕ in the domain of A (see later).

Associated to an observable A, we imagine an apparatus, $\mathcal{A}_A$, say with a scale to read the output



The particle in state ϕ is inserted into $\mathcal{A}_A$; the dial then reads off an expected value

$$a = (\phi, A\phi)$$

Moreover, the probability that the dial will read off a value between a_1 and a_2, $a_1 < a_2$, is given by

$$(\phi, P_{[a_1, a_2]}\phi)$$

This is called the "Copenhagen" interpretation of quantum mechanics.

The dynamics of the quantum system is given by a group of unitary operators $U(t)$,

- $t \mapsto U(t)$ is strongly continuous
- $U(t+s) = U(t)\, U(s)$, $t, s \in \mathbb{R}$
- $U(0) = 1$

If the system is in state φ at time $t=0$, then the system is in a state $\varphi(t_0) = U(t_0)\,\varphi$ at time $t = t_0$.

As $U(t)$ is unitary for each t

(5.1) $$\|\varphi(t_0)\| = \|U(t_0)\varphi\| = \|\varphi\| = 1$$

so that $\varphi(t_0)$ is indeed a state.

Every unitary group $U(t)$ can be expressed uniquely in the form (Stone's Theorem)

(5.2) $$U(t) = e^{-itH}$$

for some unique self-adjoint operator H, and conversely. If $\varphi(t) = U(t)\varphi = e^{-itH}\varphi$, then $\varphi(t)$ solves the Schrödinger equation

(5.3) $$i\,\partial\varphi/\partial t = H\varphi(t), \qquad \varphi(0) = \varphi$$

H is the Hamiltonian for the quantum system

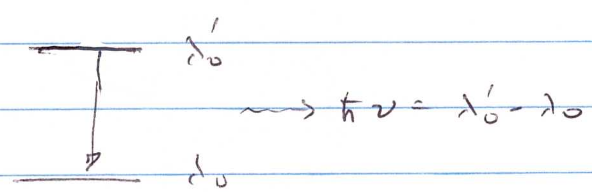
The <u>point spectrum</u> $\{\lambda_0\}$ (see later) of H

$$H\varphi_0 = \lambda_0 \varphi_0 \quad , \quad 0 \neq \varphi_0 \in \mathcal{H} ,$$

is of special interest. The λ_0's are necessarily real, and hence

$$\varphi(t) = e^{-itH}\varphi_0 = e^{-it\lambda_0}\varphi_0$$

gives rise to a stationary solution of the Schrödinger equation (recall that vectors differing by a phase describe the same state) The typical reaction of the system to outside stimulae is to move from one stationary state to another



emitting light whose frequency ν is proportional to the difference between the corresponding point spectra.

In mathematical quantum mechanics, 3 general types of problems arise

(i) <u>Self-adjointness</u>

In most cases, physical reasoning gives a <u>formal</u> expression for the Hamiltonian and other observables as operators on $\mathcal{H}$. The word "formal" is used because the <u>domains</u> of the operators are not specified. It is usually easy to find a domain on which a given formal expression (e.g. a differential operator on $C_0^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$, say) is a <u>symmetric</u> operator. The <u>first</u> mathematical problem is to determine domains on which the operator is self-adjoint, or failing that, to prove that the operator on the given domain is <u>essentially self-adjoint</u> (<u>e.s.a</u>) (i.e. its <u>closure</u> is self-adjoint) (see later). If the operator is not e.s.a., one must examine various self-adjoint extensions of the operator and determine which is the "right" one for the observable: the "right" one is determined by the physics of the problem, typically through a choice of boundary conditions. Note that only self-adjoint operators H give rise to unitary groups e^{-itH} (and hence dynamics, if H is the putative Hamiltonian): operators B which are not s.adjoint, or e.s.a., cannot be exponentiated to form unitary groups e^{-itB}: This is true in particular if B is only symmetric, but not s.adj. or e.s.a.

(2) Spectral analysis

The 2^{nd} problem is to investigate the spectrum of observables, and in particular, the Hamiltonian H, and to estimate, in particular, the number and positions of the point spectra of H.

But there is far more to the spectral analysis of H. Recall the <u>spectral theorem</u> (more later) for s.adj. op's on a (separable) Hilbert space $\mathcal{H}$: Let A be s.adj. on $\mathcal{H}$. Then $\exists$ measures $\{\mu_n\}_{n=1}^{N}$, $1 \le N \le \infty$, on the spectrum of A, $\sigma(A)$, and a unitary operator

(9.1) $$U : \mathcal{H} \to \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$$

so that

(9.2) $$(UAU^{-1}\psi)(\lambda, n) = \lambda\, \psi(\lambda, n)$$

where we write an element $\psi \in \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$ as an N-tuple $\psi = \{\psi(\lambda, 1), \psi(\lambda, 2), \dots\}$,

(9.3) $$\|\psi\|^2 = \Sigma_{n=1}^{N} \int |\psi(\lambda, n)|^2 d\mu_n(\lambda) < \infty$$

The domain of A is given by

(10.1) $$\operatorname{dom} A = D(A) = \left\{ U^{-1}\psi : \sum_{n=1}^{\infty} \int_{\mathbb{R}_n} \lambda^2 |\psi(\lambda, n)|^2 d\mu_n(\lambda) < \infty \right\}$$

Note: (9.1)(9.2) $\Rightarrow$ the $\exists^{ce}$ of the p.v.m $\{P_\Omega\}$ above (see later)

Now any measure $d\mu$ on $\mathbb{R}$ can be decomposed uniquely as a sum of 3 mutually singular measures (i.e. supported on disjoint sets)

(10.2) $$d\mu = d\mu_{pp} + d\mu_{ac} + d\mu_{sing}$$

where μ_{pp} is a pure point measure,

$$d\mu_{pp} = \sum_i a_i \, \delta_{\lambda_i}, \quad a_i > 0.$$

μ_{ac} is abs. cont. with respect to Lebesgue measure, and $d\mu_{sing}$ is singular wrt Lebesgue measure but has no points.

These 3 pieces give rise to an orthogonal decomposition

(10.3) $$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{pp}) \oplus L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sing})$$

It is easy to see that, via the spectral Th^m, this leads to an orthogonal decomposition of $\mathcal{H}$ into subspaces

(11.1) $$\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sing}$$

Each of these subspaces is <u>invariant</u> under A. $A \upharpoonright \mathcal{H}_{pp}$ has a complete set of eigenvectors (i.e. all its spectral measures $d\mu_\psi(\lambda ; A \upharpoonright \mathcal{H}_{pp})$ are pure point); $A \upharpoonright \mathcal{H}_{ac}$ has only absolutely continuous spectral measures and $A \upharpoonright \mathcal{H}_{sing}$ has only continuous singular spectral measures. The dynamical behavior of the system $e^{-itA}\psi$, is different, depending on whether $\psi \in \mathcal{H}_{pp}$, $\mathcal{H}_{ac}$ or $\mathcal{H}_{sing}$. The determination of the decomposition (11.1) for A is of fundamental interest. Vectors $\mathcal{H}_{pp}$ give rise to <u>stationary states</u>, vectors in $\mathcal{H}_{ac}$ give rise to <u>scattering states</u>, and vectors in $\mathcal{H}_{sing}$ give rise to anomalous behavior. In many physical problems, we show that $\mathcal{H}_{sing} = \{0\}$.

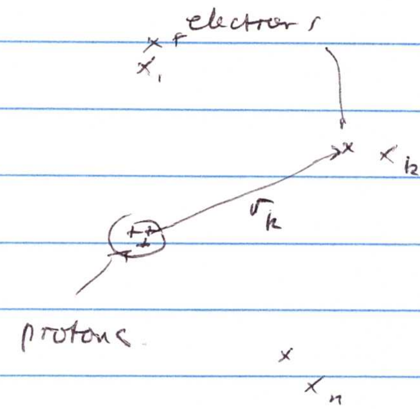
(3) <u>Scattering Theory</u>

The <u>third</u> problem is to describe in some way the behavior of the system for large t ie given $\psi = \psi(t=0)$, describe

$$\psi(t) = e^{-itA}\psi$$

in some explicit way as $t \to \pm\infty$. As noted above, whereas the point spectrum is associated with $\mathcal{H}_{pp}$, this <u>scattering problem</u> is naturally associated with $\mathcal{H}_{ac}$.

As an example, we consider the n-electron model in the field of n fixed protons in the nucleus at the origin of the system



The classical Hamiltonian for the system is

$$h = \sum_{k=1}^{n} \frac{(p_x^k)^2 + (p_y^k)^2 + (p_z^k)^2}{2m} \qquad (13.1)$$

$$- \sum_{k=1}^{n} \frac{ne^2}{|r_k|} + \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \frac{e^2}{|r_k - r_l|}$$

where p_x^k, p_y^k, p_z^k are the x, y, z components of the momentum of the k^{th} electron, $r_k = (x_k, y_k, z_k)$ its position, m and e its mass and charge respectively. The term $-ne^2/|r_k|$ is the potential energy of the k^{th} electron due to the attraction of the protons in the nucleus; the term $e^2/|r_k - r_l|$ describes the repulsion between the k^{th} and l^{th} electrons.

We take as our Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{3n}, dx^{3n})$ and make the following ~~classical~~ correspondence between the classical variables $x_k, \ldots, p_x^k, \ldots$ and operators on $\mathcal{H}$ (we choose units so that Planck's constant $\hbar = 1$)

(14.1) $$p_x^k \to \frac{1}{i}\frac{\partial}{\partial x_k}, \quad p_y^k \to \frac{1}{i}\frac{\partial}{\partial y_k}, \quad p_z^k \to \frac{1}{i}\frac{\partial}{\partial z_k}$$

and

$$x_k, y_k, z_k \to \text{multiplication } X_k, Y_k, Z_k$$
by x_k, y_k, z_k resp.

ie $X_k f(x) = x_k f(x)$ etc.

Under this correspondence

(14.2) $$h \to H = -\sum_{k=1}^{n} \frac{1}{2m} \Delta_k + V(r_1, \ldots, r_n)$$

where $\Delta_k = \partial^2/\partial x_k^2 + \partial^2/\partial y_k^2 + \partial^2/\partial z_k^2$ and

V denotes the operator of multiplication by the function

$$- \sum_{k=1}^{n} \frac{ne^2}{|r_k|} + \sum_{\substack{k,l=1 \\ k \neq l}}^{n} \frac{e^2}{|r_k - r_l|}$$

All of these formal operators are symmetric on Schwartz space $\mathcal{S}(\mathbb{R}^{3n}) \subset L^2(\mathbb{R}^{3n})$ i.e.

$$(\varphi, H\varphi) = (H\varphi, \varphi)$$

where $(\varphi, \psi) = \int \overline{\varphi(x)}\, \psi(x)\, d^{3n}x$ is the standard inner product on $\mathbb{R}^{3n}$ (integrate by parts!). What is not at all obvious, but nevertheless true (see later), is that they are e.s.a. on $\mathcal{S}(\mathbb{R}^n)$, and in fact also on $C_0^\infty(\mathbb{R}^{3n}) \subset \mathcal{S}(\mathbb{R}^{3n})$. Thus $e^{-it\overline{H}}$ gives the unitary dynamics, where $\overline{H}$ is the <u>closure</u> of H.

In this course we will proceed as follows:

In the present spring semester, we will introduce the basic objects of spectral analysis — viz closed operators, symmetric operators, s. adj. operators, deficiency indices, min-max principal, quadratic forms, limit point - limit circle theory, ~~etc~~ — and analyze their properties, illustrating the theory mostly with ordinary differential operators. In the coming fall semester, we will consider Schrödinger operators of type (14.2) above and address the 3 basic questions – s. adjointness, spectral analysis and scattering theory — for these operators.

In finite dimensions, symmetric (or Hermitian) matrices A

(16.1) $$(Ax, y) = (x, Ay) \quad , x, y \in \mathbb{C}^n$$

play a distinctive role. Not only do they have real spectrum (all eigenvalues) but they have a spectral representation

$$A = U \Lambda U^* \tag{17.1}$$

where U is a unitary matrix, $UU^* = I$,

and $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$. $u_j = Ue_j$, $e_j = (0, \ldots, 1, 0, \ldots, 0)^T$
↑
j^{th} position

is the eigenvector corresp. to λ_j, $Au_j = \lambda_j u_j$.

The representation (17.1) can be rewritten in form

(9.1) (9.2) as follows: assume first that the λ_i's

are distinct. Set $\mu = \sum_{i=1}^{n} \delta(\lambda - \lambda_i)$

Then $f \in L^2(\mathbb{R}, d\mu) \iff \int |f(\lambda)|^2 d\mu(\lambda) = \sum_i^n |f(\lambda_i)|^2 < \infty$

Thus $L^2(\mathbb{R}, d\mu)$ is $\cong \mathbb{C}^n$. Define $U : \mathbb{C}^n \to L^2(d\mu)$

as follows

$$(Ux)(\lambda) = (u_j, x) \quad \text{if } \lambda = \lambda_j$$
$$= 0 \quad \lambda \in \mathbb{R} \setminus \{\lambda_1, \ldots, \lambda_n\}$$

Then $\|Ux\|_{L^2(d\mu)} = \sum_i^n |(u_i, x)|^2 = \|x\|^2$

so U is unitary. Also

$$(UAx)(\lambda) = \Big(U\big(\textstyle\sum \lambda_i (u_i, x) u_i\big)\Big)(\lambda)$$

$$= \lambda_i (u_i, x) \qquad \text{if } \lambda = \lambda_i$$

$$= 0 \qquad \text{otherwise.}$$

ie $\quad (UAU^{-1}f)(\lambda) = \lambda f(\lambda)$.

<u>Exercise</u> Describe U when A has repeated eigenvalues. $\square$

Instead of $\mu = \sum_{i=1}^{n} \delta(\lambda - \lambda_i)$ we could have chosen $\tilde{\mu} = \sum_{i=1}^{n} a_i \delta(\lambda - \lambda_i)$ for <u>any</u> $a_1, \ldots, a_n > 0$. This would have led to a unitary op. $\tilde{U} : \mathbb{C}^n \to L^2(\mathbb{R}, d\tilde{\mu})$ and again $(\tilde{U}A\tilde{U}^{-1}f)(\lambda) = \lambda f(\lambda)$

So we see that spectral reps of form (9.1)(9.2) are not unique: but we also see how they may differ!

<u>Lecture 2</u>

In infinite dimensions the situation is complicated by the following 2 observations: