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Spectral Theory in QM

1 Introduction

An important aspect of quantum mechanics is finding solutions $|\Psi\rangle$ to the time-independent Schrodinger equation. For an arbitrary Hamiltonian $\hat{H}$, it states in its full generality

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle\,.$$

Physically, E corresponds to energy, but mathematically E just appears to be an eigenvalue of $\hat{H}$. Rearranging the Schrodinger equation, $(\hat{H} - E\hat{I})\,|\Psi\rangle = 0$; thus, the problem boils down to computing what *seems* to be the null-space of a new operator $\hat{H} - E\hat{I}$ where $\hat{I}$ is the identity operator and E varies in $\mathbb{R}$. The set of E such that $\hat{H} - E\hat{I}$ is "pathological" has a special name, called the *spectrum* $\sigma(\hat{H})$. In the next section we will define exactly what we mean by "pathological," and shed more light on the subtleties of this problem.

2 What exactly is the spectrum?

Let T be a linear operator $T : X \to X$, where X is a complex Banach space. For any $\lambda \in \mathbb{C}$, define the *resolvent* mapping $R_\lambda(T) : X \to X$ of T as $R_\lambda(T) = (T - \lambda I)^{-1}$. If $R_\lambda(T)$ is single-valued, is bounded, and is defined on a domain that's dense in X, then $\lambda \in \rho(T)$. Here, $\rho(T)$ is called the *resolvent set* of T and λ is called a *regular value* of T. Otherwise, $\lambda \in \sigma(T)$, whereby $\sigma(T)$ is called the *spectrum* of T and λ is a *spectral value* of T. Depending on which of the conditions for $\lambda \in \rho(T)$ were violated, λ falls into one of three sets:

- *Point spectrum:* If $R_\lambda(T)$ is multi-valued (i.e., $T - \lambda I$ is not injective), then $\lambda \in \sigma_p(T)$.
- *Continuous spectrum:* If $R_\lambda(T)$ is single-valued and has a dense domain, but $R_\lambda(T)$ is unbounded, then $\lambda \in \sigma_c(T)$.
- *Residual spectrum:* If $R_\lambda(T)$ exists but doesn't have a dense domain, then $\lambda \in \sigma_r(T)$.

These three cases are disjoint and account for all $\lambda \in \sigma(T)$, so $\sigma(T) = \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T)$. Furthermore, $\rho(T)$ and $\sigma(T)$ are disjoint and account for all $\lambda \in \mathbb{C}$, so together the three spectra and the resolvent set partition $\mathbb{C}$:

$$\mathbb{C} = \rho(T) \cup \sigma_p(T) \cup \sigma_c(T) \cup \sigma_r(T).$$

In the case that $T = \hat{H}$ and $X = H$ where $\hat{H}$ is a self-adjoint Hamiltonian and H is a Hilbert space, it turns out that there is no residual spectrum. There are non-self-adjoint Hamiltonians that do admit a residual spectrum[1], but these are beyond the scope of this discussion; thus, we limit ourselves to point spectra and continuous spectra.

2.1 Point spectra

Let $\lambda \in \sigma_p(T)$. By definition, $R_\lambda(T) = (T - \lambda I)^{-1}$ doesn't exist. This implies that $T - \lambda I$ is not injective and has a non-trivial null-space. So, there is some $v \in \text{null}(T - \lambda I), v \neq 0$ such that $(T - \lambda I)v = Tv - \lambda v = 0$. This is a familiar situation from linear algebra: $Tv = \lambda v$. Indeed, λ is called *eigenvalue* of T and v is called an *eigenvector* of T. For this specific v, T behaves like scalar multiplication by λ.

Sometimes T only has a point spectrum. For instance, this happens in the Hamiltonians for the quantum harmonic oscillator and the hydrogen atom. These examples illuminate why the point spectrum has its name: it typically consists of countably many discrete points.

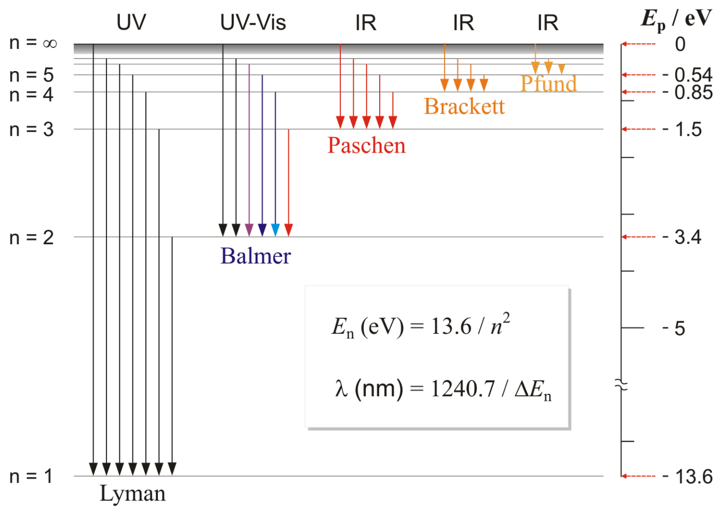

Figure 1: The spectrum of the Hamiltonian for the hydrogen atom corresponds to its emission spectrum[2]

To instantiate T concretely, let $\hat{H}$ be a Hamiltonian with a countably infinite point spectrum

$$\sigma(\hat{H}) = \{E_n \mid n \in \mathbb{Z}^+ \cup \{0\}\}.$$

Furthermore, let $|\psi_n\rangle$ be the normalized energy eigenvector associated with E_n. It turns out that eigenvectors corresponding to different eigenvalues are orthogonal, even in this abstract setting. Indeed, let $|\psi_i\rangle$ and $|\psi_j\rangle$ be distinct eigenvectors. Then,

$$\langle\psi_i| \hat{H} |\psi_j\rangle = E_j \langle\psi_i \mid \psi_j\rangle .$$

But also

$$\langle\psi_i| \hat{H} |\psi_j\rangle = \left(\langle\psi_j| \hat{H} |\psi_i\rangle\right)^\dagger = E_i \left(\langle\psi_j \mid \psi_i\rangle\right)^\dagger = E_i \langle\psi_i \mid \psi_j\rangle .$$

Since E_i and E_j are distinct, $\langle\psi_i \mid \psi_j\rangle = 0$. Now, this along with the assumption that each E_n corresponds only to one eigenvector allows us to write $|\Psi\rangle$, the general normalized solution to the time-independent Schrodinger equation, in the following form:

$$|\Psi\rangle = \sum_{n=0}^{\infty} c_n |\psi_n\rangle ,$$

$$\sum_{n=0}^{\infty} |c_n|^2 = 1, \quad \langle \psi_i \mid \psi_j \rangle = \delta_{ij}.$$

Here, δ_{ij} is the Kronecker delta (not to be confused with the Dirac delta function). The representation follows because the eigenvectors $|\psi_n\rangle$ are dense in H, so they form a (complete) orthonormal basis. Ultimately, the upshot of it is that we can derive a new representation

$$\hat{H} = \sum_{n=0}^{\infty} E_n |\psi_n\rangle \langle \psi_n| \, .$$

Each outer product $|\psi_n\rangle \langle \psi_n|$ corresponds to a projection operator onto the null-space of $\hat{H} - E_n \hat{I}$. This is fundamentally what the spectral theorem, the highlight of spectral theory, is about.

2.2 Continuous spectra

Let $\lambda \in \sigma_c(T)$. Recall that this means that $R_\lambda(T)$ is unbounded. Formally, there exists a sequence of vectors (x_n) such that $\|x_n\| = 1$, which maps to an image sequence (y_n) whereby $y_n = R_\lambda(T) x_n$ and

$$\lim_{n \to \infty} \|y_n\| = \infty.$$

But since $(T - \lambda I) R_\lambda(T) = I$, $\|x_n\| = \|(T - \lambda I) y_n\|$ and

$$\lim_{n \to \infty} \|(T - \lambda I) y_n\| = 1.$$

Hopefully, this makes the issue clear. $T - \lambda I$ sends the divergent sequence (y_n) to something convergent. By linearity, this is equivalent to saying that $T - \lambda I$ sends $(y_n / \|y_n\|)$ to an arbitrarily small vector. Thus, $(y_n / \|y_n\|)$ gives a sequence of normalized *approximate eigenvectors*, because having an image with norm ≈ 0 *almost* puts them in the null-space of the operator $T - \lambda I$. Sometimes λ is also called an *approximate eigenvalue*.

It's possible for T to only have a continuous spectrum. For instance, the Hamiltonian corresponding to the free particle, a particle that isn't bound by any potential, has a purely continuous spectrum.

To illustrate the properties of continuous spectra, let $\hat{p}$ be the momentum operator, given by the following formula:

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}.$$

Spectral Theory in QM

If we let $\psi(x)$ be a solution to the equation $\hat{p}\psi(x) = p\psi(x)$, then

$$\psi(x) = Ce^{ipx/\hbar}, \quad C \in \mathbb{C}.$$

The issue is that $\psi(x)$ is not localized, so it's not a well-defined wave-function. But, if we pretend that $\psi(x)$ exists, something interesting happens. Let $\psi_p(x)$ and $\psi_{p'}(x)$ be eigenfunctions of $\hat{p}$ corresponding to eigenvalues p and p', respectively. Then, it turns out that

$$\langle \psi_p \mid \psi_{p'} \rangle = \delta(p - p')$$

where $\delta(\cdot)$ is the Dirac delta function. The twisted version of orthonormality we've recovered here is called *Dirac orthonormality*[5]. Moreover, $\psi_p(x)$ is exactly the divergent limit of vectors (y_n). In fact, Dirac orthonormality tells us

$$\|\psi_p\| = \langle \psi_p \mid \psi_p \rangle = \delta(0) = \infty.$$

3 Applied to Quantum Mechanics

There are two theorems of significant practical importance from spectral theory. The first is called the *spectral theorem*. Just like in the example in the point spectrum section, it allows us to decompose an arbitrary self-adjoint operator into projection operators. The exact details are somewhat complicated because of continuous spectra, which requires Riemann-Stieltjes integration, but the following example will embody the idea behind theorem.

Let $\hat{H}$ be the Hamiltonian from the point spectrum section and suppose we want to compute $\hat{H}^p$ where $p \in \mathbb{Z}^+$. Using the definition

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

we would have to solve a differential equation of order $2p$. *Yuck!* Luckily, we can use the other representation

$$\hat{H} = \sum_{n=0}^{\infty} E_n \left|\psi_n\right\rangle \left\langle\psi_n\right|.$$

To illustrate, expand $\hat{H}^2$ as

$$\begin{aligned}\hat{H}^2 = \left(\sum_{n=0}^{\infty} E_n \left|\psi_n\right\rangle \left\langle\psi_n\right|\right)^2 &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} E_m E_n \left|\psi_m\right\rangle \left\langle\psi_m \mid \psi_n\right\rangle \left\langle\psi_n\right| \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \delta_{mn} E_m E_n \left|\psi_m\right\rangle \left\langle\psi_n\right| \\ &= \sum_{n=0}^{\infty} E_n^2 \left|\psi_n\right\rangle \left\langle\psi_n\right|.\end{aligned}$$

By induction, it follows that $\hat{H}^p = \sum_{n=0}^{\infty} E_n^p \left|\psi_n\right\rangle \left\langle\psi_n\right|$. Using the fact that polynomials are dense in the set of continuous functions on bounded domains, an even more general result follows for a continuous function f:

$$f(\hat{H}) = \sum_{n=0}^{\infty} f(E_n) \left|\psi_n\right\rangle \left\langle\psi_n\right|.$$

These are the two main elements of the spectral theorem, decomposing $\hat{H}$ into projection operators and extending polynomials of $\hat{H}$ to arbitrary continuous functions f.

There is a second theorem of practical importance, called the *spectral mapping theorem*. To illustrate it, consider the following example. Let $\hat{H}$ be an arbitrary Hamiltonian. This describes a quantum system under unitary evolution $U(t)$, where

$$U(t) = e^{-i\hat{H}t/\hbar}.$$

Naively, computing the spectrum of $U(t)$ would involve explicitly the operator $e^{-i\hat{H}t/\hbar}$. But, it's too cumbersome and seems to depend strongly on $\hat{H}$. This is where the spectral mapping theorem comes in, also known as the *continuous functional calculus*[4] in the context of C^* algebras, which states that for a continuous function f and operator T,

$$\sigma(f(T)) = f(\sigma(T)).$$

Instantiating $f(x) = e^{-ixt/\hbar}$,

$$\sigma(U(t)) = \sigma(f(\hat{H})) = f(\sigma(\hat{H})) = \{e^{-i\lambda t/\hbar} \mid \lambda \in \sigma(\hat{H})\}.$$

It seems like we could have solved the problem by expanding the matrix exponential as a Maclaurin series, but note that this strategy fails to account for the continuous spectrum. Thus, we have both achieved a more elegant and more general result.

4 References

1. https://en.wikipedia.org/wiki/Non-Hermitian_quantum_mechanics.

2. https://glossary.periodni.com/glossary.php?en=Balmer+series.

3. *Introductory Functional Analysis and Applications* by Kreyszig.

4. *C^*-Algebras by Example* by Kenneth B. Davidson.

5. *Introduction to Quantum Mechanics Second Edititon* by David J. Griffiths.