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Determining spectra in quantum theory, by Michael Demuth and M. Krishna, Progress in Mathematical Physics, vol. 44, Birkhäuser, Boston, 2005, x+219 pp., US$99.00, ISBN 978-0-8176-4366-9

The mathematical theory of quantum mechanics traces its roots to the seminal work of John von Neumann in 1929, *The Mathematical Theory of Quantum Mechanics* [18]. At that time, theoretical physicists had developed two competing computational formalisms for describing the behavior of atoms and molecules: one was the matrix mechanics of W. Heisenberg [12], and the other was the partial differential equation approach of E. Schrödinger [22]. von Neumann formulated the theory in terms of linear operators on Hilbert space, then a recent invention, and showed that the two approaches are simply equivalent representations. He proved that all infinite-dimensional, separable, complex Hilbert spaces are isometrically isomorphic, a fact anticipated by Schrödinger in [22]. This, and related results in [18], provided the mathematical foundations for quantum mechanics and some key results in the new field of functional analysis. Eventually, the linear differential operator approach to quantum mechanics became widely accepted. Partially because of this, the spectral theory of linear operators developed in parallel with the mathematical theory of quantum mechanics during the middle of the twentieth century. Research in quantum mechanics also stimulated work in related fields of mathematics, especially group representation theory. The role of symmetries and group representations in quantum mechanics was clarified with the publication of treatises such as *The Theory of Groups and Quantum Mechanics* by Hermann Weyl [29].

The next major impetus to the development of mathematical quantum mechanics came with an improved understanding of dynamics. Stone [28] and Kato [16] recognized the importance of the self-adjointness of Schrödinger operators in proving the existence of a unitary time evolution, an essential component of quantum mechanics, and much effort was directed towards proving the self-adjointness of various Schrödinger operators. Finally, scattering theory, a technique for understanding the relationship between the continuous spectra of two self-adjoint operators, based on collision processes between quantum particles, was widely developed in the 1950's, 1960's, and 1970's. The latter part of the twentieth century saw major progress in understanding complex N-body quantum systems, the stability of matter, quantum resonances, the semiclassical approximation, and models of disordered media.

The basic partial differential equation of nonrelativistic quantum mechanics is the Schrödinger equation. The state of a quantum mechanical system is represented by a function $\psi(x,t)$, with the interpretation that $|\psi(x,t)|^2$ is a probability density on $\mathbb{R}^d$ at each time t. Thus, the function must be square integrable and $\int_{\mathbb{R}^d} |\psi(x,t)|^2\, dx = 1$ for each time. This means that the description of the system should take place on the Hilbert space $L^2(\mathbb{R}^d)$, where the dimension d depends on the spatial dimension and on the number of particles in the system (neglecting spin). Furthermore, the square-integrability condition means that the probability is preserved under the time evolution of an initial state. The Schrödinger equation

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is the equation for that time evolution having the form

$$i\frac{\partial \psi}{\partial t} = H\psi, \tag{1}$$

with the initial condition $\psi(x, t = 0) = \psi_0(x) \in L^2(\mathbb{R}^d)$. The formal solution to the first-order equation in time (1) is

$$\psi(x,t) = U(t)\psi_0(x) = e^{-itH}\psi_0(x). \tag{2}$$

In order to make sense of this equation on the Hilbert space $L^2(\mathbb{R}^d)$, it is necessary and sufficient that the generator H of the time evolution $U(t)$ be a self-adjoint operator. In this case, the evolution operator $U(t)$ is a strongly continuous, one-parameter unitary group.

The specific quantum system is modeled by the choice of the Schrödinger operator. The Schrödinger operator, or Hamiltonian, H_V, is an unbounded linear transformation on the Hilbert space $L^2(\mathbb{R}^d)$ of the form

$$H_V = H_0 + V, \tag{3}$$

where H_0 is called the unperturbed operator, describing a simple system, and the real-valued function $V(x)$, acting as a multiplication operator, is called the potential. The potential V represents the interaction among the particles and the interaction of the particles with their environment. Typically, the unperturbed operator H_0 is taken to be the Laplacian on $\mathbb{R}^d$ and is given in Cartesian coordinates by $H_0 = -\Delta = -\sum_{j=1}^{d} \partial^2/\partial x_j^2$. This choice of H_0 describes the kinetic energy of free quantum particles, such as noninteracting electrons. One of the achievements of nonrelativistic quantum mechanics is the description of the simplest atom, the hydrogen atom. In the approximation that the proton is infinitely more massive than the electron, the operator H_V has the form

$$H_V = -\Delta - 1/\|x\|, \text{ on } L^2(\mathbb{R}^3), \tag{4}$$

where $V(x) = -1/\|x\|$ is the Coulomb potential. We have set Planck's constant $h = 2\pi$, the electric charge $e = 1$, and the mass $m = 1/2$. The corresponding Schrödinger equation is completely solvable. The prediction of the energy levels of hydrogen, easily observed in the laboratory, is one of the remarkable successes of the theory.

More complicated atoms and molecules are described by more complicated self-adjoint operators H_V and these are no longer exactly solvable. An essential tool for understanding these more complicated Schrödinger operators is the spectrum of the operator. The spectrum of a self-adjoint operator A on a Hilbert space $\mathcal{H}$ is the closed, nonempty subset of real numbers $\lambda \in \mathbb{R}$ for which the operator $(A - \lambda I)$ does not have a bounded inverse. The spectrum divides naturally into two disjoint subsets of the real numbers: the discrete values E, called eigenvalues, for which there is a function $\psi_E \in \mathcal{H}$ satisfying $A\psi_E = E\psi_E$, and the rest. The fact that the complement in the spectrum of A of the set of eigenvalues of A may be nonempty is a consequence of the infinite dimensionality of the Hilbert space.

The eigenvalues of a Schrödinger operator H_V lie on the negative real axis. They describe the stationary or bound states of the system. It follows from (1) that the time evolution of such a state is trivial: $U(t)\psi_E = e^{-itE}\psi_E$. Many approximation techniques have been developed for computing eigenvalues. One of the most useful tools is perturbation theory in which eigenvalues of a complicated system are approximated by those of simpler systems. Typically, one considers a Hamiltonian

$H_\lambda = H_0 + \lambda V$ and assumes that the eigenvalues $E_j(\lambda)$ have an expansion in λ about $\lambda = 0$. Perturbation theory provides formulas for the coefficients in the expansion $E_j(\lambda) = e_0 + \lambda e_1 + \cdots$, where e_0 is the corresponding eigenvalue of H_0. Perturbation theory was raised to an art form by K. Friedrichs [10], F. Rellich [21], and T. Kato [16], among others. T. Kato's book *Perturbation Theory for Linear Operators* [16] is a classic in the field.

The nature of the rest of the spectrum, which is called the essential spectrum (more precisely, the complement of the set of isolated eigenvalues of finite multiplicity), is more complicated. However, it is also robust. The essential spectrum is the component of the spectrum that is stable under relatively compact perturbations. To describe it further, we note that in its simplest form, the Spectral Theorem for a self-adjoint operator A states that A determines a measure μ^A on the real line. This measure has a Lebesgue decomposition into a point measure μ_p^A and a continuous measure μ_c^A. The continuous measure, in turn, can be decomposed as $\mu_c^A = \mu_{ac}^A + \mu_{sc}^A$, where the measure μ_{ac}^A, respectively μ_{sc}^A, is absolutely continuous, respectively singular continuous, with respect to Lebesgue measure. Roughly speaking, the supports of these measures correspond to the another decomposition of the spectrum of A into pure point, absolutely continuous, and singular continuous parts. The essential spectrum of A contains the absolutely continuous and singular continuous components of the spectrum, along with any limit points of eigenvalues and eigenvalues of infinite multiplicity.

The absolutely continuous component of the spectrum is described by scattering theory. Extensive treatments of scattering theory can be found in M. Reed and B. Simon's volume 3 of the *Methods of Modern Mathematical Physics* [20], and in D. Yafaev's text *Mathematical Scattering Theory* [30]. Classical and quantum scattering theory for N-body systems is the main topic of the text *Scattering Theory of Classical and Quantum N-Particle Systems* by J. Dereziński and Ch. Gérard [8]. The basic idea of scattering theory is that the description of the long-time asymptotics of a quantum system with Hamiltonian H_V, given by $\psi(x,t)$ in (2), can be described by the asymptotics of a simpler system with Hamiltonian H_0, provided the perturbation $V \equiv H - H_0$ is sufficiently weak. Rather than comparing the operators directly, as in usual eigenvalue perturbation theory, one studies the unitary evolution groups, defined in (2), associated with the Hamiltonians H_0 and H_V. Let us assume that H_0 and H_V have no singular continuous spectra. The central objects in the study of the time evolution are the wave operators defined, in the simplest case, by the following limits in the strong operator topology

$$\Omega_\pm(H_V, H_0) \equiv s - \lim_{t \to \pm\infty} e^{itH_V} e^{-itH_0} P_{ac}(H_0), \tag{5}$$

when they exist. Here, $P_{ac}(A)$ is the orthogonal projection onto the absolutely continuous subspace of A which is the subspace of the Hilbert space orthogonal to the span of all of the eigenfunctions of A. One basic result is that the existence of both of the wave operators $\Omega_+(H, H_0)$ and $\Omega_+(H_0, H)$ implies that the absolutely continuous components of H_0 and H_V, defined as the restriction of each operator to its absolutely continuous subspace, are unitarily equivalent.

As the above discussion illustrates, the spectral analysis of self-adjoint operators is one of the prime tasks of mathematical quantum mechanics. The book by Demuth and Krishna is a very nice account of some recent developments. The authors concentrate on the spectral problem for mainly self-adjoint linear operators on

Hilbert spaces. They describe some recently developed tools that help with the understanding of the spectral properties of these operators. The foundations are presented in Chapter 1, Measures and Transforms. This chapter describes the basic relations between linear operators, measures, and transforms. As a first example, let us consider the Borel-Stieltjes transform. If H is a possibly unbounded linear operator on a separable Hilbert space $\mathcal{H}$ with a cyclic vector $\phi \in \mathcal{H}$, there is a naturally associated measure μ_ϕ^H defined by using the resolvent $R_H(z) = (H-z)^{-1}$, which exists for $\Im z \neq 0$, by

$$F_H(z) \equiv \langle \phi, R_H(z)\phi \rangle = \int_{\mathbb{R}} \frac{d\mu_\phi^H(\lambda)}{\lambda - z}. \tag{6}$$

In other words, the matrix element of the resolvent is the Borel-Stieltjes transform of the measure μ_ϕ^H. The spectral properties of H are encoded in the behavior of the boundary values of the function $F_H(E + i\epsilon)$, as $\epsilon \to 0$. When H does not have a cyclic vector such measures still exist, but one has to consider a family of such measures for sufficiently many vectors. The authors present two other transforms on measures that play an important role in spectral analysis of linear operators: the Fourier transform and the Wavelet transform. These will be described in more detail below.

Chapter 2, Selfadjointness and Spectrum, contains traditional material on self-adjointness and the spectra of linear operators. This is a well-written and concise chapter. The chapter contains a clear presentation of the Spectral Theorem for self-adjoint operators (although the authors assume the existence of a spectral family). A more expanded version of this material can be found in the treatise of Reed and Simon [20]; specifically, general spectral theory is described in volume 1, self-adjointness in volume 2, and applications to Schrödinger operators, in volume 4.

In Chapter 3, Criteria for Identifying the Spectrum, the authors begin an approach that brings together many techniques that have been very helpful in spectral analysis. They concentrate their study of self-adjoint operators on the Borel, Fourier, and Wavelet transforms of the measures associated with a self-adjoint operator and vectors in the Hilbert space (see (6) and (11)). The Borel transform of the measure μ_ϕ^A associated with a self-adjoint operator A and the state ϕ was defined in (6). The Borel transform plays a key role in the Aronszajn-Donoghue theory [2, 9] of rank one perturbations. Let $K = P_\psi$ be a rank one self-adjoint operator whose range is the one-dimensional subspace spanned by ψ. Let us assume that ψ is cyclic for A. We consider the perturbation $A(\lambda) = A + \lambda K$. If $F_\lambda(z)$ is the Borel transform of the spectral measure of $A(\lambda)$ and the state ψ, one easily derives the rather amazing formula

$$F_\lambda(z)(1 + \lambda F_0(z)) = F_0(z), \ \Im z > 0. \tag{7}$$

This equation allows us to study the boundary values of the Herglotz function $F_\lambda(z)$, and hence the spectral properties of $A(\lambda)$, in terms of those of the Herglotz function $F_0(z)$ for the unperturbed operator. For example, one can easily identify the supports of the various components of the Lebesgue decomposition of the spectral measure by applying classical theorems, like Fatou's Theorem and the de la Vallée Poussin Theorem (see section I.3 of [4]). Among mathematical physicists working on localization, the use of the Borel transform had a renaissance in the 1980's with the work of Kotani (see, for example, [17]) and with the Simon-Wolff proof of localization for the Anderson model [26]. With the aid of

the Aronszajn-Donoghue theory, these authors proved the absence of singular continuous spectrum with probability one for various families of random Schrödinger operators. The book by Demuth and Krishna presents the classical Aronszajn-Donoghue theory for rank one perturbations. They then present the applications to random Schrödinger operators due to Simon-Wolff [26], on the almost sure absence of singular continuous spectrum, and due to Jaksić-Last [14], on the almost sure purity of the absolutely continuous spectrum. Another presentation of this material can be found in the new edition of Barry Simon's book on trace ideals [24], in which his 1993 Vancouver lectures are reprinted.

The use of the Fourier transform to study self-adjoint operators is somewhat more classical. The Fourier transform of a measure μ is formally defined by

$$\hat{\mu}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikt} \, d\mu(t). \tag{8}$$

Wiener (cf. [5]) proved a beautiful result on the Fourier transform $\hat{\mu}$ of a finite measure μ. If $\mathcal{A}(\mu)$ is the set of atoms of μ, then

$$\lim_{T\to\infty} \frac{1}{2T} \int_{-T}^{T} |\hat{\mu}(t)|^2 \, dt = \frac{1}{2\pi} \sum_{x\in\mathcal{A}(\mu)} |\mu(\{x\})|^2. \tag{9}$$

It follows immediately that if the limit on the left in (9) is zero, then the measure μ is purely continuous.

This result has applications to quantum mechanical scattering theory. Stone's representation of a one-parameter, strongly continuous unitary group $U(t)$ as the exponential of a unique self-adjoint operator $U(t) = e^{-itA}$ allows us to construct a functional calculus based on the Fourier transform. For a Schwartz class function f and a Hilbert space vector ϕ, one can define an operator $f(A)$ by

$$\langle \phi, f(A)\phi \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(t) \, \langle \phi, U(-t)\phi \rangle \, dt. \tag{10}$$

This is a bounded linear functional and the Riesz-Markov Theorem (cf. [20]) implies that there exists a measure μ_ϕ^A on the real line so that

$$\langle \phi, f(A)\phi \rangle = \int_{-\infty}^{\infty} f(t) \, d\mu_\phi^A(t). \tag{11}$$

This is the same measure occurring in (6) where $f(x) = (x - z)^{-1}$. We will refer to these measures as spectral measures for A.

Returning to scattering theory, the matrix element of the unitary time-evolution group $U(t)$ in (2) is the Fourier transform of this measure μ_ϕ^H for the generator H:

$$\langle \phi, U(t)\phi \rangle = \int_{-\infty}^{\infty} e^{-it\lambda} \, d\mu_\phi^H(\lambda) = \hat{\mu}_\phi^H(t). \tag{12}$$

Hence, the large time asymptotic behavior of the time-averaged absolute square of the matrix element evolution group $U(t)$ is related to the Fourier transform of the spectral measure and, by Wiener's Theorem, to the presence or not of point spectrum for the generator H.

The third transform discussed by the authors is the Wavelet transform, a new tool in the spectral analysis of self-adjoint operators. Let $\psi \in L^1(\mathbb{R})$ be a mother

wavelet. The continuous wavelet transform of a function $g \in L^p(\mathbb{R})$, for $1 \le p \le \infty$, with respect to ψ, is a function of $(x_1, x_2) \in \mathbb{R}^+ \times \mathbb{R}$ representing dilations and translations. It is given by

$$(T_\psi g)(x_1, x_2) = \int_{\mathbb{R}} \psi(x_1^{-1}(y - x_2))g(y)\, dy. \tag{13}$$

The fundamental paper of Jensen and Krishna [15] describes how the measure and its components can be obtained from its wavelet transform. Applied to a self-adjoint operator A, the authors show how to recover spectral properties of A from matrix elements of its wavelet transform, defined as

$$\langle \phi, \psi(a^{-1}(A - \lambda))\phi \rangle, \tag{14}$$

and various averages of this function over λ, as $a \to 0^+$. For example, if for all $\lambda \in (a, b)$, one has

$$\sup_{a>0} a^{-1} \langle \phi, \psi(a^{-1}(A - \lambda))\phi \rangle < \infty, \tag{15}$$

for some ϕ, then A has no singular spectrum in the interval (a, b).

Chapter 4, Operators of Interest, is devoted to a careful treatment of Schrödinger operators of the type (3). The techniques introduced in the previous chapters are used to study first the unperturbed operators and then various perturbations. The issues here are twofold: determine classes of potentials for which the perturbed operator (3) is self-adjoint, given a self-adjoint, unperturbed operator H_0; and, second, determine the spectral properties of the perturbed operator H_V, assuming some knowledge of the spectrum of H_0. As examples of H_0, the authors treat fractional powers of the Laplacian on $L^2(\mathbb{R}^d)$ via the Fourier transform. They also discuss the discrete finite-difference Laplacian on $\ell^2(\mathbb{Z}^d)$ and give several properties of the Green's function. Using methods of stochastic analysis, they study the semigroups generated by these unperturbed operators and the corresponding kernels. There is a nice section on Dirichlet forms and their relation to Hunt processes, but without proofs. A much more complete version of this material can be found, for example, in the book of Demuth and van Casteren [7]. Next, the authors discuss perturbations by real-valued potentials and distinguish permissible sets of deterministic potentials and of random potential. The outlook is dominated by the relationship between the semigroups associated to H_V and various stochastic processes. The discussion of perturbations by random potentials is standard, emphasizing the families of ergodic random potentials and the corresponding deterministic spectrum of the family of randomly perturbed operators. Stochastic analysis takes the foreground again in the discussion of singular perturbations. The authors consider singular perturbations that are perturbations by boundary conditions, or, equivalently, perturbations by potentials that take the value plus infinity on some closed subset of $\mathbb{R}^d$.

The last chapter, Applications, has two main components. In the first, the authors discuss the spectral theory of random Schrödinger operators on the lattice. The basic Anderson model is the family of Schrödinger operators having the form

$$H_\omega = \Delta + V_\omega, \text{ on } \ell^2(\mathbb{Z}^d), \tag{16}$$

where Δ is the discrete, finite-difference Laplacian, and V_ω is the multiplication operator $(V_\omega f)(n) = \omega_n f(n)$, for $n \in \mathbb{Z}^d$. The family $\{\omega_n\}$ is a family of independent, identically distributed random variables. These operators are fascinating from the spectral theory point of view as they exhibit unexpected spectral properties. Chief

among these unusual properties is Anderson localization. This property means the existence of an interval of dense, pure point spectrum with exponentially decaying eigenfunctions, almost surely. The authors present the method of Aizenman and Molchanov [1] that is used to obtain estimates on the expectation of fractional powers of the Green's function. Another interesting model described in detail in the present book is the Anderson model on the Bethe lattice, a rooted tree with constant branching number greater than or equal to two. For this model, it is known that there is both absolutely continuous spectrum and dense pure point spectrum with probability one in disjoint intervals. This section provides a nice introduction to random operators, and the interested reader can find much more information in the specialized books by Carmona and Lacroix [4], Pastur and Figotin [19], and Stollmann [27].

The second main application in Chapter 5 focuses on the use of scattering theory to describe the continuous spectrum of various families of Schrödinger operators and operators that arise in the scattering of waves by obstacles. In the first part, the authors discuss the problem of determining the continuous spectrum for random operators with decaying randomness using wave operators. In the second part, the methods of stochastic analysis, presented in Chapter 4, play a role. Stochastic methods are well suited to analysis involving semigroups and, via the Laplace transform, resolvents. Scattering problems with boundary conditions on the boundary of obstacles fit nicely into the theory of singular perturbations presented in Chapter 4. The semigroup is naturally expressed as an expectation with respect to various stochastic processes. For example, for closed regions $\Gamma \in \mathbb{R}^d$ with finite capacity, the authors prove that the absolutely continuous spectrum of the Laplacian on $\mathbb{R}^d \backslash \Gamma$, with Dirichlet boundary conditions, is the positive half-line.

There are now several books on various aspects of functional analysis and probability theory, spectral and scattering theory, and mathematical quantum mechanics. In addition to the four volume work of Reed and Simon [20], the interested reader may also consult books such as Blank, Exner, and Havlíček [3], Cycon, Froese, Kirsch, and Simon [5], E. B. Davies [6], Dereziński and Gérard [8], Gustafson and Sigal [11], Hislop and Sigal [13], Simon [25], and Yafaev [30]. Although there are overlaps in these texts, each has a different perspective and focuses on a different aspect of the field. The text of Demuth and Krishna complements these texts in focusing on what spectral information can be obtained from various transforms of spectral measures. I found the book very enjoyable to read. It is a clearly written and accessible reference for many techniques of spectral analysis that are commonly used in contemporary research in Schrödinger operators. Anyone with a background in basic real analysis, including the fundamentals of measure theory, and basic functional analysis, including Banach and Hilbert space theory, should be able to read and profit from the book.

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