An Introduction to Mathematical Quantum Mechanics

and eventually The Feschbach-Schur map

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June 4 2020

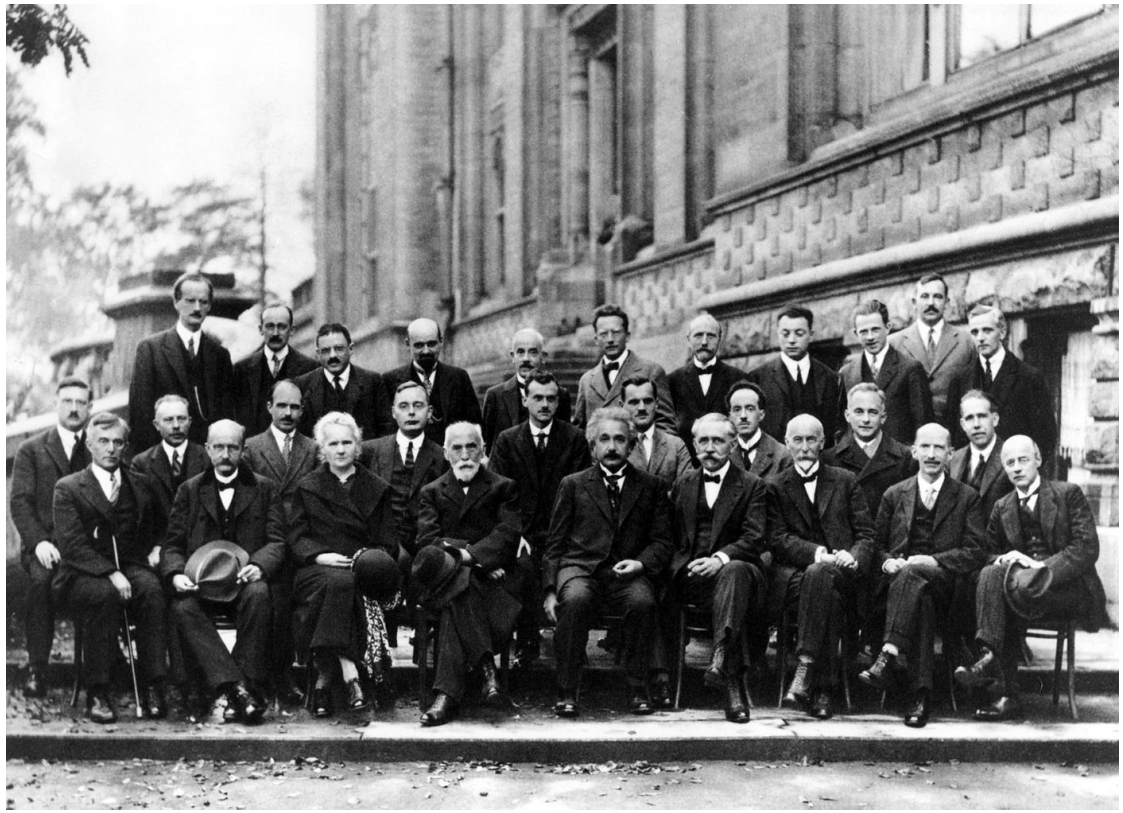
Path of Least Action

I propose the following sequence of topics for today:

1) An introduction to the mysteries of Quantum Phenomena
2) The mathematical formalism of the theory of quantum mechanics and its **axioms**
3) A basic example: The energy spectra of Hydrogen!
4) Perturbation Theory
5) The Feshbach-Schur Map

Invented by...

Quantum Mechanics was discovered and worked on at from the turn of the 20th century throughout the 1930s. Some important names include: Plank, Einstein, Bohr, Dirac, Pauli, Heisenberg, Schrödinger, ...



Formalised by...

The mathematical formalism was first established by Von Neumann in his 1932 work "Mathematical Foundations of Quantum Mechanics."

A question of scale

Our daily experience consists of dealing with *macroscopic objects*. This allows us to assign a reality for any statement in classical physics ie. *a measure of the magnetic field*. We regard the result of the measurement as independent in principle from the apparatus used and from the observer.

QM deals with phenomena at the atomic scales: where the concept of measurement itself becomes problematic because any measurement apparatus will exchange information with the quantum system and affect it.

We don't experience quantum phenomena at our scale as the effects are extremely subtle and hard to measure.

Some Physical Phacts

A few things have been observed experimentally that have formed the basis of the theory:

1) Wave/Particle duality: matter exhibits both particle-like (point-mass) and wavelike properties.
2) Discrete Energy states: the energy of a quantum field comes in integer multiples of a fundamental energy.
3) QM is probabilistic: the outcome of a physical experiment has a number of different possible outcomes each with a certain probability
4) QM is non-local: entanglement allows measurements to depend on properties of distant objects in ways that cannot be explained by signals moving at the speed of light

An Experiment with Bullets

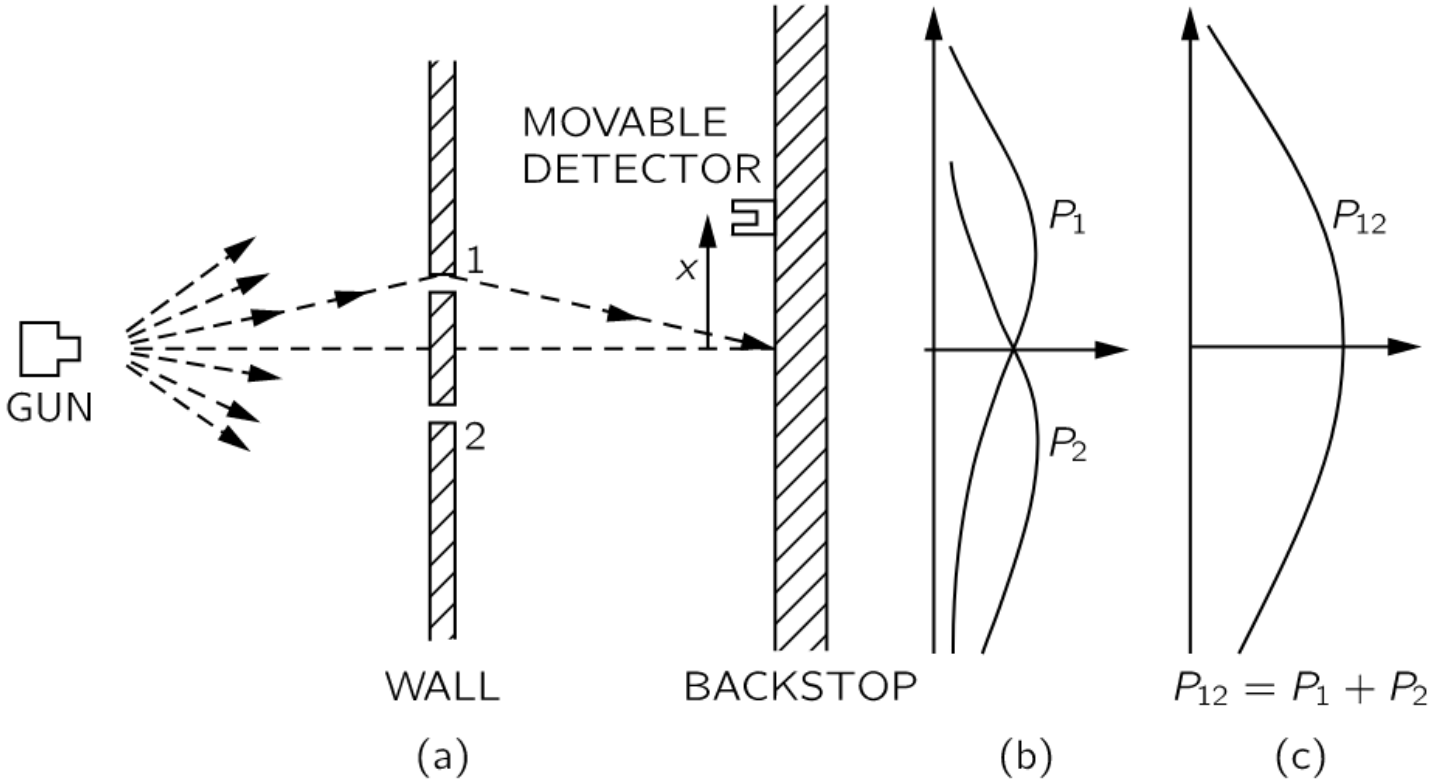


Fig. 1–1. Interference experiment with bullets.

An Experiment with Bullets

We assume the bullets are *indestructible*. We say that "bullets always arrive in identical lumps."
Note then the following fact:

$$P_{12} = P_1 + P_2$$

So we say this result is an observation of *no interference*.

An Experiment with Water Waves

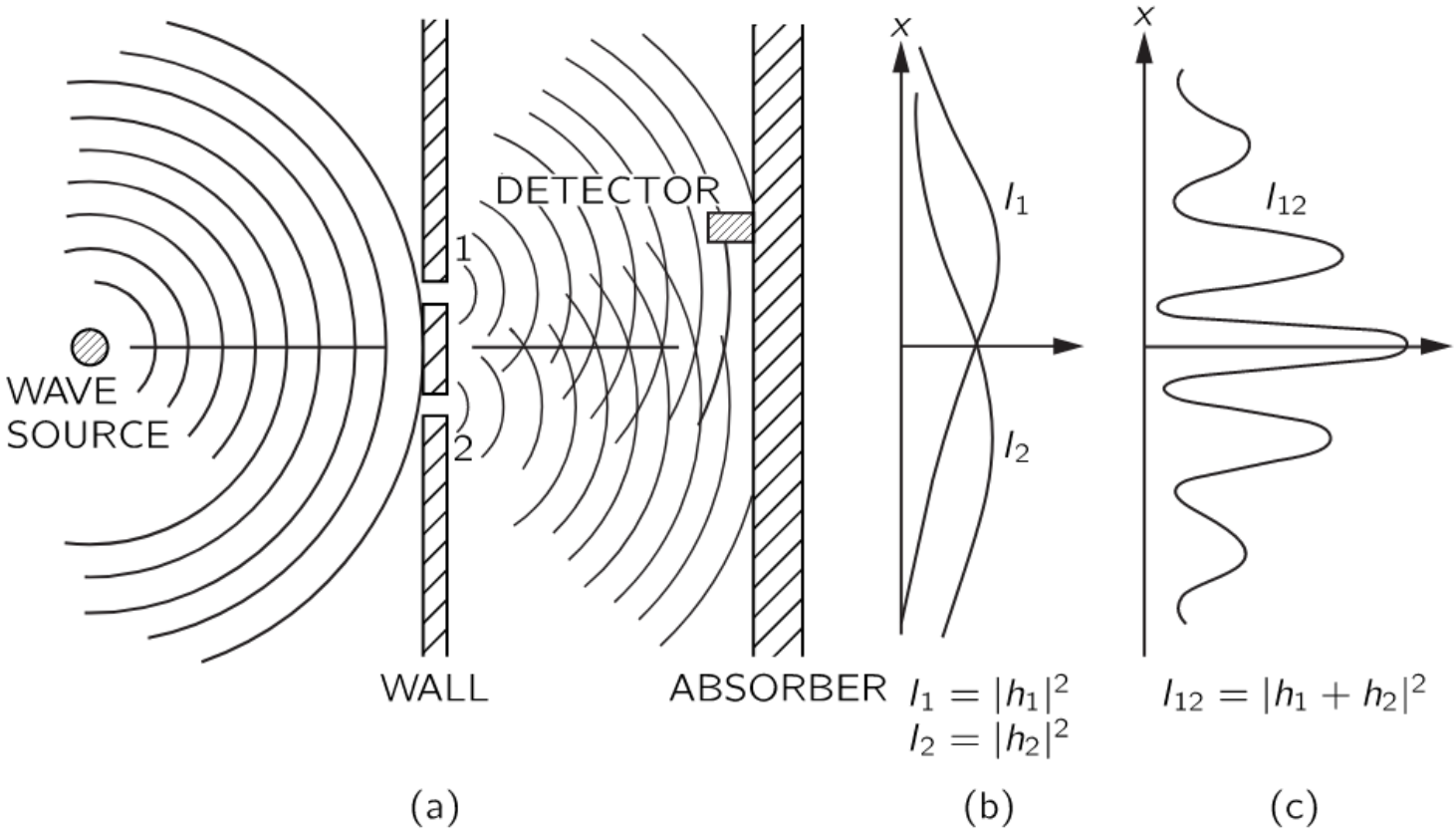


Fig. 1–2. Interference experiment with water waves.

An Experiment with Water Waves

First thing to notice: the wave intensity can have any size! We would not say there is any "lumpiness" in the wave intensity.

We then get the following *interference pattern* I_{12}. In the spots where I_{12} has maxima the wave peaks add together to give a large amplitude ("constructive interference.")

At the places where the waves arrive out of phase (a phase difference of π) they interfere "destructively", and the intensity is lower.

An Experiment with Water Waves

The instantaneous height of the water wave at the detector for the wave from hole 1 is $\mathcal{R}\{h_1 e^{i\omega t}\}$ where the amplitude $h_1 \in \mathbb{C}$, in general. Hence, $I_1 = |h_1|^2$.

The wave heights add up to give $(h_1 + h_2)e^{i\omega t}$. And hence we have

$$I_1 = |h_1|^2, \;\; I_2 = |h_2|^2, \;\; I_{12} = |h_1 + h_2|^2$$

An Experiment with Electrons

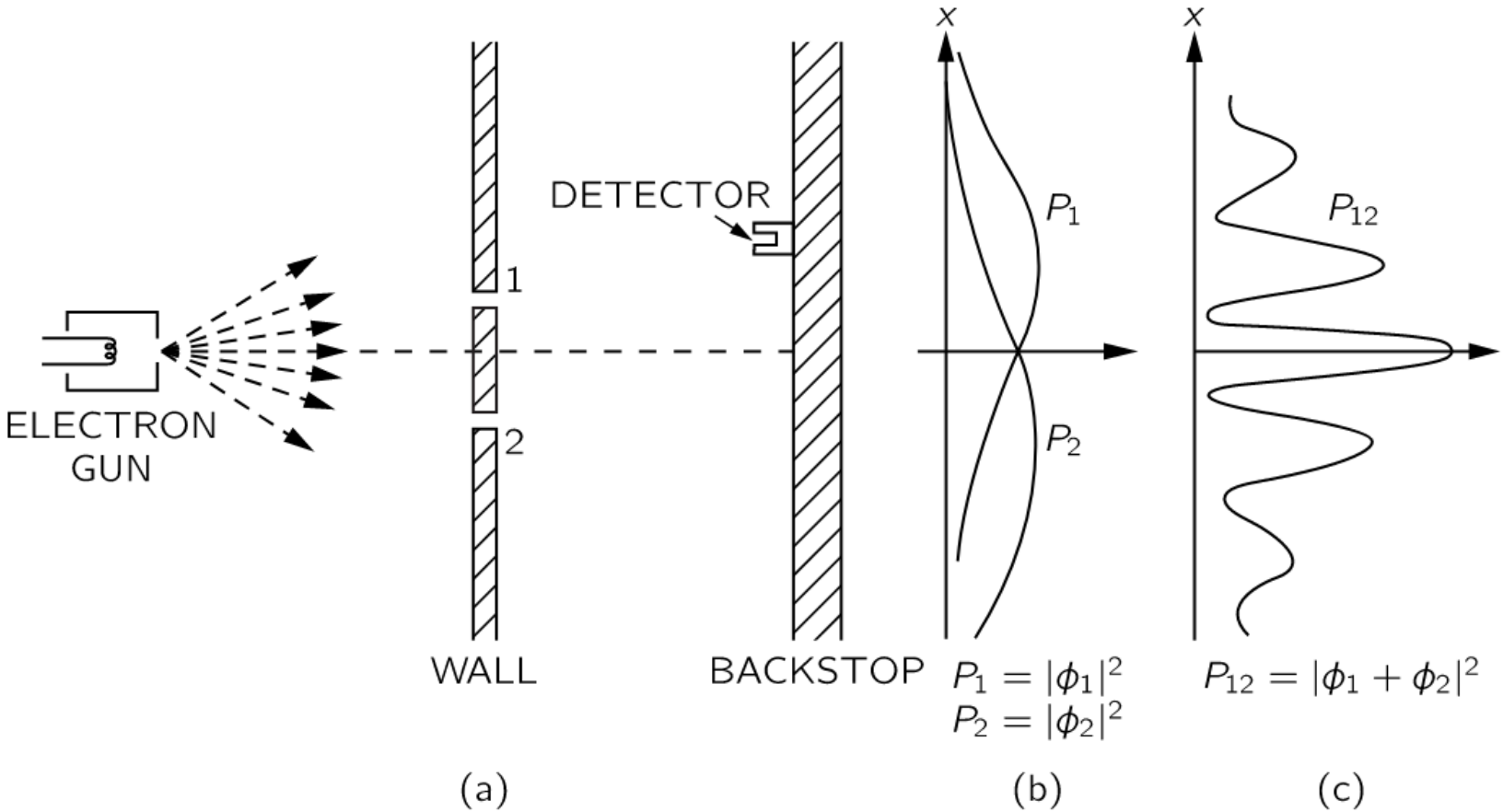


Fig. 1–3. Interference experiment with electrons.

The Double-slit Experiment

First thing we notice is that we hear sharp "clicks" from the detector. So "electrons always arrive in identical lumps."

Conclusion: You cannot explain the results of this experiment by assuming that electrons (like the bullets) either go through hole 1 or hole 2.
For electrons:

$$P_{12} \neq P_1 + P_2$$

But if we treat the electrons as water waves, describe outcomes from the holes 1 and 2 by complex functions ϕ_1 and ϕ_2, then like before:

$$P_1 = |\phi_1|^2, \;\; P_2 = |\phi_2|^2, \;\; P_{12} = |\phi_1 + \phi_2|^2$$

The Double-slit Experiment

We have to conclude that it is not true that the electrons go *either* through hole 1 or hole 2.

To truely test this, let's perform another experiment.

Watching the Electrons

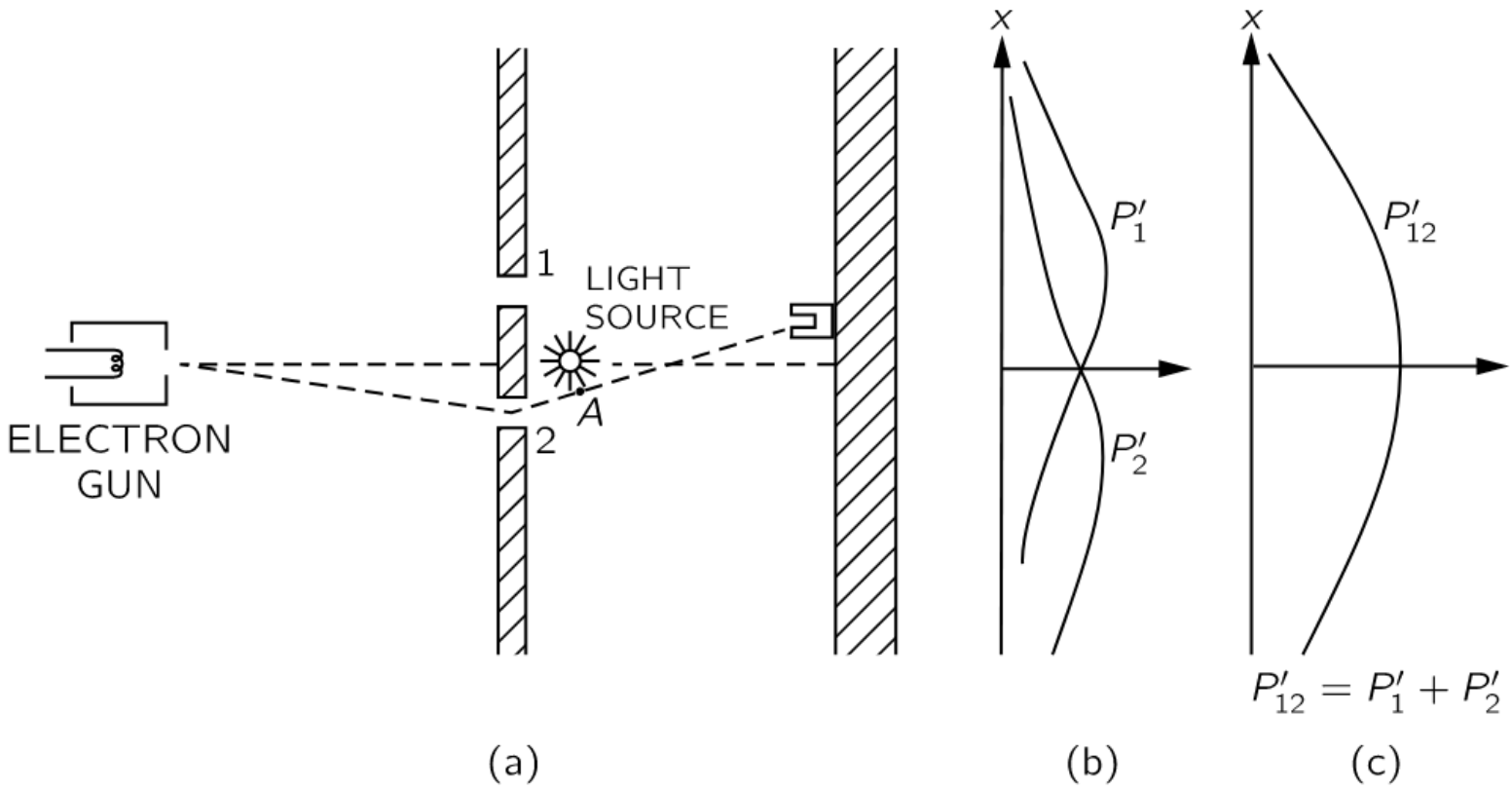


Fig. 1–4. A different electron experiment.

Watching the Electrons

What we see: every time we hear a "click" from the detector, we also see a flash of light either near hole 1 or hole 2. (so the electrons remain in lumps.) So we can index the electrons as going through either hole.

Notice that $P_1' = P_1$ and $P_2' = P_2$. BUT $P_{12}' \neq P_{12}$!!!

Conclusion: when we look at the electrons the distribution is different than when we don't look.

By trying to watch the electrons, we have changed their motions.

Watching the Electrons

This is all due to the interference of light. Lets try the same experiment again but dim the light. What we notice: the flashes do not get any weaker. Instead, sometimes we hear a click from the detector but see no flash! So light also acts like electrons: we knew it was wavy but it is also "lumpy." (See: the photoelectric effect)

The electrons that are seen by hole 1 look like P_1', those seen by hole 2 like P_2', but those that aren't seen look like P_{12}!

If the electrons are not seen, we have interference.

For this experiment: "It is impossible to design an apparatus to determine which hole the electron passes through, that will not at the same time disturb the electrons enough to destroy the interference pattern."

Enough Physics: Let's do Math

Axiom 1: With every quantum system there is associated an infinite-dimensional separable complex Hilbert space $\mathcal{H}$, (the *space of states*.) The Hilbert space of a composite quantum system is a tensor product of Hilbert spaces of component systems.

Axiom 2: The set of observables $\mathcal{A}$ of a quantum system with the Hilbert space $\mathcal{H}$ consists of all self-adjoint operators on $\mathcal{H}$.

Recall an operator A is self-adjoint (S-A) if $A = A^*$, or equivalently A is symmetric and $D(A) = D(A^*)$ or $\mathrm{Ran}(A \pm i\mathbf{1}) = \mathcal{H}$.

Axioms of Quantum Mechanics

Axiom 3: The set of states $\mathcal{P}$ of a quantum system with space $\mathcal{H}$ consists of all positive (and hence S-A) trace-class operators M with $\mathrm{Tr}M = 1$.
Pure states are projection operators onto 1-dim subspaces of $\mathcal{H}$. The projection onto the subspace spanned by $\psi \in \mathcal{H}$ with $\|\psi\| = 1$ is denoted by P_ψ. All other states are called *mixed states*, ie.

$$\sigma = \sum_n c_n P_{\psi_n}, \quad c_n > 0, \quad \sum_n c_n = 1$$

In the Schrödinger picture states are elements $\psi \in \mathcal{H}$.

A positive operator is said to be of trace-class if

Recalling some definitions

Recall that the trace of an operator is defined by

$$\mathrm{Tr}A = \sum_{n=1}^{\infty}(Ae_n, e_n)$$

and is independent of choice of orthonormal basis $\{e_n\}$. A positive operator is of trace class if

$$\sum_{n=1}^{\infty}(Ae_n, e_n) < \infty$$

for some orthonormal basis. The space of trace class operators is a Banach algebra with norm $\|A\|_1 = \mathrm{Tr}\sqrt{A^*A}$.

Axioms of Quantum Mechanics

Axiom 4: The mean value of the measurements of the observable represented by A in the state represented by P_ψ is given by:

$$\langle A \rangle_\psi := \mathrm{Tr}(AP_\psi) = (\psi, A\psi)$$

In the case of a mixed state,

$$\langle A \rangle_\sigma := \mathrm{Tr}(\sigma A) = \sum_n c_n \mathrm{Tr}(P_{\psi_n} A)$$

Axioms of Quantum Mechanics

Axiom 5: Consider the observable A. The possible values of the observable A must belong to the spectrum of A. In the case where A only have a discrete simple spectrum, the possible outcomes of measurement are its eigenvalues. Denote in this case the eigenvalues a_k with corresponding eigenvectors ψ_k. Then the probability of the outcome a_k is given by

$$p_k^A = |(\psi_k^A, \phi)|^2$$

Axiom 6: If the measurement of A gives a_k as a result (assuming it is non-degenerate) then immediately after the measurement the state of the system is described by the vector ψ_k^A (or $P_{\psi_k^A}$.)

Recalling some more definitions

Recall the spectrum of an operator A on the Hilbert space $\mathcal{H}$ is:

$$\sigma(A) := \{\lambda \in \mathbb{C} : (A - \lambda) \text{ is not invertible (has no bounded inverse)}\}$$

The discrete spectrum $\sigma_d(A)$ of the operator consists of its isolated eigenvalues of finite multiplicity. The rest of the spectrum is called the essential spectrum of the operator A:

$$\sigma_{\text{ess}}(A) = \sigma(A) \setminus \sigma_d(A)$$

Two basic results: 1) The spectrum $\sigma(A) \subset \mathbb{C}$ is a closed set.
2) The spectrum of a S-A operator is real ie. $\sigma(A) \subset \mathbb{R}$.

Dynamics

Given a quantum system that currently lies in a state, how does it evolve in time? The analogue of Hamilton's eq in classical mechanics is the Heisenberg picture of quantum mechanics. We postulate that like in classical mechanics the time-evolution is completely determined by a special observable $H \in \mathcal{A}$, called the Hamiltonian.

The interpretation of H is that it is the energy operator. Its spectra determine the allowed energy states of the system. Generally H has the form

$$H = -\frac{\hbar^2}{2m}\Delta + V$$

Dynamics: Heisenberg Representation

We treat the states as independent of time and evolve the observables:

$$\frac{dM}{dt} = 0, \quad M \in \mathcal{P}$$

$$\frac{dA}{dt} = \frac{i}{\hbar}[H, A]$$

To solve this we can define the family of unitary operators

$$U(t) = e^{-\frac{i}{\hbar}tH}$$

for $t \in \mathbb{R}$. This is well defined when H is both bounded or unbounded (requires a bit of work) and S-A.

Dynamics: Heisenberg Representation

For an observable A define

$$A(t) = U(t)^{-1} A U(t)$$

The dynamics is implied by this formula, we define the *time evolution operator* $U_t : \mathcal{A} \to \mathcal{A}$ by $U_t(A) = A(t)$.

In this sense all quantum observables obey the Heisenberg equation of motion.

Dynamics: Schrödinger Picture

In the Schrödinger picture we time-evolve the states and the observables A remain fixed. So the time evolution operator acts like $U_t : \mathcal{P} \to \mathcal{P}$ so that $U_t(M) = M(t) := U(t)MU(t)^{-1}$.

Infinitesimally the evolution of quantum states is described by the Schrödinger equation:

$$\frac{dM}{dt} = -\frac{i}{\hbar}[H, M]$$

For a pure state $M = P_\psi$ we recover the usual *time-dependent Schrödinger equation:*

$$i\hbar\frac{d\psi}{dt} = H\psi$$

Dynamics

If we prescribe initial conditions $\psi(0) = \psi_0$ then we together with the SE we form a Cauchy problem.

Fundamental result: H is S-A iff dynamics exist, ie. the Cauchy problem for the SE has a unique solution that conserves probability. (this can be done for H bounded or unbounded.)

Take-away for the rest of this presentation: The spectral analysis of the operator H is fundamental to understanding the dynamics and allowed energy states of a quantum system.

Example: The Hydrogen Atom

A hydrogen consists of a proton and an electron, interacting via a Coulomb force law. The appropriate Schrödinger operator is:

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{e^2}{|x|}$$

on the Hilbert space $L^2(\mathbb{R}^3)$.

What is the spectra of H? An important bound:

$$\|V\psi\| \leqslant a\|H_0\psi\| + b\|\psi\|$$

for all $\psi \in \mathcal{D}(H_0)$ and some a, b with $a < 1$.

The Hydrogen Atom

Theorem

Assume H_0 is a S-A operator and V is a symmetric operator satisfying the earlier bound with $a < 1$. Then the operator $H := H_0 + V$ with $\mathcal{D}(H) = \mathcal{D}(H_0)$ is S-A.

This is an extension of a more simple result for V real and bounded.

Idea: show $\|V(H_0 - i\lambda)^{-1}\| < 1$, and use this to show that the equation

$$(H + i\lambda)\psi = f$$

has a unique solution for every $f \in \mathcal{H}$ and some $\lambda \in \mathbb{R}, \pm\lambda > 0$.

Trying to Characterize the Essential Spectrum

Is there some sort of characterization of the essential spectrum like the eigenvalue problem for the discrete spectrum? Define a *spreading sequence*.

Let A be an operator on $L^2(\mathbb{R}^d)$. A sequence $\{\psi_n\} \subset L^2(\mathbb{R}^d)$ is called a spreading sequence for A and λ if:

1) $\|\psi_n\| = 1$ for all n
2) for any bounded set $B \subset \mathbb{R}^d$, $\operatorname{supp}\ (\psi_n) \cap B = \emptyset$ for n sufficiently large
3) $\|(A - \lambda)\psi_n\| \to 0$ as $n \to \infty$

Note that the second condition eliminates the possibility of a repeated eigenfunction.

The Essential Spectrum

Easy calculation: $\sigma_{ess}(-\frac{\hbar^2}{2m}\Delta) = [0, \infty)$. (use the FT)

Theorem

If $H = -\frac{\hbar^2}{2m}\Delta + V$ is a Schrödinger operator with real potential $V(x)$ continuous and bounded from below, then

$$\sigma_{ess}(H) = \{\lambda : \ \textit{there is a spreading sequence for } H \textit{ and } \lambda\}$$

Theorem

Let $V : \mathbb{R}^d \to \mathbb{R}$ be continuous, with $V(x) \to 0$ as $|x| \to \infty$. Then $\sigma_{ess}(H) = [0, \infty)$. So H can only have negative isolated eigenvalues, possibly accumulating at 0.

Idea of proof: use the bound:

$$\|(H-\lambda)\psi_n\| - \|V\psi_n\| \leqslant \|(-\frac{\hbar^2}{2m}\Delta - \lambda)\psi_n\| \leqslant \|(H-\lambda)\psi_n\| + \|V\psi_n\|$$

Back to the Hydrogen Atom

Hence we know that H is S-A and $\sigma_{ess}(H) = [0, \infty)$. Let's find the bound-states (eigenfunctions) and bound-state energies (eigenvalues).

Exploit the radial symmetry of the Coulomb Potential and change to spherical coordinates. The solve the eigenvalue problem for H by separation of variables!

$$\psi(r, \theta, \phi) = R(r) Y_l^k(\theta, \phi)$$

$$(\frac{\hbar^2}{2m}[-\Delta_r + \frac{l(l+1)}{r^2}] - \frac{e^2}{r})R = ER$$

and Y_l^k is a spherical harmonic.

The Hydrogen Atom

We can thus calculate that we have solutions in the following regime:

$$l = 0, 1, 2, \ldots; \quad k \in \{-l, -l+1, \ldots, l\}; \quad n \in \{l+1, l+2, \ldots\}$$

with solutions $R_{nl}(r) = \rho^l e^{-\rho/2} F_{nl}(\rho)$ where $\rho = \frac{2me^2}{n\hbar^2} r$ and F_{nl} is a polynomial.

The eigenvalues (allowed energy states) are

$$E_n = -(\frac{me^4}{2\hbar^2})\frac{1}{n^2}$$

General Coulomb Operators

In general people have studied so-called Coulomb operators, of the form

$$H = H_0 + V(x), \quad H_0 = -\frac{1}{2m}\Delta + \frac{\alpha}{|x|}$$

for $m > 0$ and $x \in \mathbb{R}^3$. We are in the case $V = 0$.

Theorem

If $\alpha \geqslant 0$ the discrete spectrum is empty. If $\alpha < 0$ the spectrum is bounded below, the eigenvalues are all negative, they are infinite in number and have 0 as a limit point.

Perturbation Theory

Theme: break down the operator in question into pieces we understand. If the operator is "close" to an operator we already know, then we can estimate its spectrum to be "close" to the one we already know.

$$H_\kappa = H_0 + \kappa W$$

κ is a real parameter called the *coupling constant* and as an operator W is referred to as the *perturbation*.

As we have seen, if W is H_0-bounded,

$$\|W\psi\| \leqslant a\|H_0\psi\| + b\|\psi\|$$

then "standard" perturbation theory applies.

Comparison Theorems

Theorem

Let $A \geqslant 0$ and B be S-A operators on $\mathcal{H}$. Without getting into quadratic forms, assume (roughly speaking) that $\mathcal{D}(A) \cap \mathcal{D}(B)$ is dense in $\mathcal{H}$ and that the negative part of B is "infinitesimal" with respect to A. Suppose that for any $\kappa \geqslant 0$,

$$\sigma_{ess}(A + \kappa B) = [0, \infty)$$

Then every negative eigenvalue $\mu_n(\kappa)$ of the operator $A + \beta B$ is a non decreasing monotone function of κ.

Example: Let $V \in L^2 + L^\infty$, then $\sigma_{ess}(-\Delta + \beta V) = [0, \infty)$. So if V has a "negative part" the eigenvalues (if they exist) are not decreasing functions of κ.

"Projecting-out" Procedure

Theorem (Raileigh-Ritz)

Let H be a S-A operator bounded below on $\mathcal{H}$. Denote by μ_n, for $n = 1, \ldots, N$ its eigenvalues that lie below the essential spectrum, in increasing order. Let $M_n, n \leqslant N$ be an n-dimensional subspace of $\mathcal{H}$ contained in $\mathcal{D}(H)$. Let P_n be the orthogonal projection onto M_n.
Let the operator P_nHP_n be defined in the sense of quadratic forms (moral: its defined) and let $\hat{\mu}_n$ be its corresponding eigenvalues. Then for $m = 1, \ldots, n$ we have $\hat{\mu}_n \geqslant \mu_n$.

More on "Projecting-out"

Theorem

Let $\{e_n\} \in \mathcal{D}(H)$ be a complete orthonormal basis for $\mathcal{H}$. Let $H \geqslant E_0 I$ and let E_0 be an eigenvalue of H. Suppose

$$\liminf_{\psi \in \mathcal{H}, \|\psi\|=1; N \to \infty} (P_N \psi, H P_N \psi) = E_0$$

where P_N is the orthogonal projection on the subspace spanned by $\{e_1, \ldots, e_n\}$. Let $\hat{\mu}_0^N$ be the smallest eigenvalue of $P_N H P_N$. Then,

$$\lim_{N \to \infty} \hat{\mu}_0^N = E_0$$

One way operators can be "small" wrt one another

Let $\mathcal{R}$ denote the Rollnik class, potentials which are "small with respect to the laplacian": $V(x)$ with $x \in \mathbb{R}^3$ satisfies $V \in \mathcal{R}$ if

$$|V|_{\mathcal{R}}^2 := \int \frac{|V(x)||V(y)|}{|x-y|^2} d^3x d^3y < \infty$$

If $V(x) = \mathcal{R} + L^\infty$ one can say things like $V \prec\prec \Delta$, which means uniformly in $\phi \in \mathcal{H}$,

$$(\phi, |V|\phi) \leqslant a(\lambda)(\phi, (-\Delta + \lambda I)\phi), \quad \lim_{\lambda \to \infty} a(\lambda) = 0$$

In some spectral sense these potentials are "dominated" by the laplacian.

Estimating the number of eigenvalues in $d = 3$

Theorem

For $x \in \mathbb{R}^3$, suppose $\sigma_{ess}(-\Delta + V) = [0, \infty)$ and that there exist positive constants $R_0, \epsilon > 0$ such that for $x_0 > R_0$ one has $V(x) < -\frac{a}{|x|^{2-\epsilon}}$ for $a > 0$. Then $-\Delta + V$ has an infinite number of negative eigenvalues.

Theorem

Let $V(x) = \mathcal{R} + L^{\infty}_{\epsilon}, x \in \mathbb{R}^3$ and for $|x| > R$ let $V(x) \geqslant -\frac{1}{4}\frac{b}{|x|^2}$ for $b < 1$. Then $-\Delta + V$ has at most a finite number of negative eigenvalues.

Estimating the number of eigenvalues in $d < 3$

Theorem

Let $V \in L^d(\mathbb{R}^d) + (L^\infty(\mathbb{R}^d))_\epsilon, d = 1, 2$. Then for every $\kappa > 0$ the operator $-\Delta + \kappa V$ has at least one negative eigenvalue if at least one of the following is satisfied:

1) $V \leqslant 0$, $V \neq 0$
2) $\int |V(x)| dx < \infty$, $\int V(x) dx < 0$
3) $\int V_+(x) dx < \infty$, $\int V_- x dx = \infty$

Enlisting aid from my Stochastic manz

Difference between these cases is the following. The laplacian is the generator of brownian motion as a stochastic process.

In $d = 1, 2$ brownian motion is *recursive* (paths return with probability 1 to an arbitrarily small nbhd of the initial point) while in $d = 3$ brownian motion is *dispersive* (paths with probability 1 exit asymptotically from any compact set in $\mathbb{R}^d$.)

Bound states of the operator $-\Delta + V$ correspond to invariant measures of the resulting stochastic process.

Enlisting aid from my Stochastic manz

In this context the probabilistic analogue of the last theorem is the following: if brownian motion is recursive then the addition of an attractive vector field leads to a Stochastic process that has at least one invariant measure.

On the contrary if the brownian motion is dispersive in order to have an invariant measure one must add a sufficiently strong attractive vector field (this can be proved also within the theory of stochastic processes).

Ok finally: The Feschbach-Schur Map

Problem: determine (some of) the eigenvalues of the S-A operator

$$H_\kappa = H_0 + \kappa W$$

on a Hilbert space $\mathcal{H}$.

Idea: Reduce the problem to a (nonlinear) equation on some smaller space $\mathcal{K}$. In applications this space $\mathcal{K}$ is usually finite-dimensional and hence the solution can be found algebraically.

Introduced by Feschbach in his 1958 paper "Unified Theory of Nuclear Reactions". It was further refined in the 2003 paper by Bach, Chen, Frölich, and Sigal titled "Smooth Feschbach map and operator-theoretic renormalization group methods".

The Physical Problem

Consider a nucleus A of atomic number N (number of nuclei) of an incident problem. Denote by $x \in \mathbb{R}^3$ the coordinates of the particle and by $X = x_k, k = 1, \ldots, N$ the coordinates of the particles in the nucleus. The representation space is

$$L^2(\mathbb{R}^{3N+3}) = \mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2, \quad \mathcal{H}_1 = L^2(\mathbb{R}^3),\ \mathcal{H}_2 = L^2(\mathbb{R}^{3N})$$

We want to solve the eigenvalue problem:

$$H\Phi = E\Phi, \quad H = H_A - \frac{1}{2m}\Delta_x + V(x, X)$$

The solution will yield the bound states (discrete spectrum) of the composite system. The scattering states correspond to the essential spectrum.

The Abstract Problem

In math literature this abstract method is usually called the *Schur complement formula*. In applications to linear partial differential equations it is referred to as the *Grushin problem*.

Let $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ so that the entire S-A operator H can be written as

$$H = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

Let P_1 and P_2 be the orthogonal projections onto these subspaces, ie. they are S-A, $P_i^2 = P_i$ for $i = 1, 2$ and $P_1 + P_2 = 1$. We assume that $Ran(P) \subset \mathcal{D}(H)$. Define:

$$H_1 := P_1 H P_1, \quad H_2 := P_2 H P_2$$

We require that P be chosen such that H_2 is invertible (its inverse is bounded on $\mathcal{H}_2$.)

Motivation: Schur's Complement Method

Consider the matrix of operators:

$$\mathcal{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} : \mathcal{H}_1 \oplus \mathcal{H}_2 \to \tilde{\mathcal{H}}_1 \oplus \tilde{\mathcal{H}}_2$$

$$\mathcal{B} := \mathcal{A}^{-1} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} : \tilde{\mathcal{H}}_1 \oplus \tilde{\mathcal{H}}_2 \to \mathcal{H}_1 \oplus \mathcal{H}_2$$

Lemma

Suppose that A_{22} is invertible. Then B_{11} is invertible and

$$B_{11}^{-1} = A_{11} - A_{12}A_{22}^{-1}A_{21}$$

The Grushin Problem in Linear Programming

Solve the linear system of the following problem:

$$\begin{cases} Pu + R_- u_- = v \\ R_+ u = v_+ \end{cases}$$

where $P : \mathcal{H}_1 \to \mathcal{H}_2$, $R_- : \mathcal{H}_- \to \mathcal{H}_2$, $R_+ : \mathcal{H}_1 \to \mathcal{H}_+$. If it is invertible we call it well-posed and write the inverse as follows:

$$\begin{pmatrix} u \\ u_- \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix} \begin{pmatrix} v \\ v_+ \end{pmatrix}$$

Simple example of a Grushin Problem

Let $P : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ defined as convolution:

$$Pu = K \star u$$

where $\hat{K} \in L^\infty(\mathbb{R}^n)$. Take $H_\pm = L^2(\mathbb{R}^n)$ and let $R_+(u) = \hat{u}(\xi)$ and $R_-(u_-) = \check{u}_-$.

The Grushin problem is well-posed and $E_{-+} = \hat{K}$, the multiplication operator by $\hat{K}$.

The convolution operator is invertible on L^2 iff $\hat{K}^{-1} \in L^\infty$.

The Abstract Problem

Defining $R_{P_2} = P_2 H_2^{-1} P_2$, we further require that:

$$\|R_{P_2}\| < \infty, \quad \|P_1 H R_{P_2}\| < \infty, \quad \|R_{P_2} H P_1\| < \infty$$

So that we can define the *Feschbach-Schur Map/Operator*:

$$F_{P_1}(H) := H_1 - P_1 H R_{P_2} H P_1$$

Main Result for the Feschbach-Schur Map

Theorem

Assume that the previous relations hold. Then the operators H *and* $F_{P_1}(H)$ *are isospectral at* 0*, in the sense that:*

a) $0 \in \sigma(H)$ *if and only if* $0 \in \sigma(F_{P_1}(H))$

b) $H\psi = 0$ *if and only if* $F_{P_1}(H)\phi = 0$

where ψ *and* ϕ *are related by* $\phi = P_1\psi$ *and* $\psi = Q\phi$*, where* Q *is known as the resolvent and is defined by:*

$$Q = Q(H) = P_1 - R_{P_2} H P_1$$

Moreover, under the conditions above, if H is S-A then so is $F_P(H)$. (usually goes both ways.)

Back to Perturbation Theory

Recall: we are technically considering the operator family

$$H_\kappa = H_0 \otimes Id + Id \otimes \kappa W$$

Assume that the operator H_0 has an isolated eigenvalue λ_0 of finite multiplicity (this is usually true, like the ground state energy of the Hydrogen Atom).

Define P_1 to be the orthogonal projection onto the eigenspace corresponding to λ_0 and apply the Feschbach-Schur theorem to the family of operators $H = H_\kappa - \lambda$ for λ sufficiently close to λ_0 (conditions to be determined.)

Feschbach-Schur in Perturbation Theory

What we can use is the following:

1) $\lambda \in \sigma_d(H_k)$ if and only if $0 \in \sigma_d(H)$
2) If $F_{P_1}(H)$ is well-defined it is a family of *mxm* matrices (m is the multiplicity of λ_0)

Take-away: The perturbation problem reduces from finding an eigenvalue and eigenfunction of an infinite dimensional operator H to finding the values of λ (called the *singular values*) for which

$$0 \in \sigma_d(F_{P_1}(H_k - \lambda))$$

Feschbach-Schur in Perturbation Theory

What we need to check on a case by case basis is the following:

I. Is $F_{P_1}(H)$ well-defined?

II. Find the singular values of $F_{P_1}(H)$.

I. Is $F_{P_1}(H_\kappa - \lambda)$ well-defined?

Generally the conditions we seek are as follows:

1) WP_1 and P_1W are bounded operators
2) The operator $P_2H_\kappa P_2 - \lambda_0$ is invertible on its domain $Ran(P_2)$ for $0 < \kappa < \kappa_0$ for some κ_0.

These will guarantee that the conditions for the theorem are met and hence $F_{P_1}(H)$ is well-defined.

Condition 1) can follow from the S-A of H_0 and W and WP_1 bounded.

Generally condition 2) readily needs to be checked on a case-by-case basis. Uses the fact that the operator $P_2H_0P_2$ has no spectrum near λ_0 (projected-out) and hence neither does $P_2H_\kappa P_2$.

II. Computing $F_{P_1}(H_\kappa - \lambda)$

We can further help ourselves by writing

$$F_{P_1}(H_\kappa - \lambda) = \kappa P_1 W P_1 - \kappa^2 U(\lambda) + \lambda_0 - \lambda$$

which implies the relation:

$$\lambda \in \sigma_d(H_\kappa) \iff (\lambda - \lambda_0) \in \sigma_d(\kappa P_1 W P_1 - \kappa^2 U(\lambda))$$

where $U(\lambda) = P_1 W \hat{R}(\lambda) W P_1$ with $\overline{R_\kappa}(\lambda) = P_2(P_2 H_\kappa P_2 - \lambda)^{-1} P_2$.

More work needed....

A long story short

Theorem (Central Theorem of Perturbation Theory)

Assume condition 1) *holds, the operator* H_0 *has an isolated eigenvalue* λ_0 *of finite multiplicity* m*, and there is* $\kappa_0 > 0$ *such that condition* 2) *holds. Then for* $|\kappa|$ *sufficiently small, the operator* H_κ *has eigenvalues* $\lambda_k^{(i)}$ *near* λ_0 *of total multiplicity equal to* m*. Moreover if* H_κ *is S-A, then the eigenvalues have expansions of the form:*

$$\lambda_k = \lambda_0 + \kappa(\psi_0, W\psi_0) + \kappa^2(W\psi_0, \overline{R}_0 W\psi_0) + O(|\kappa|^3)$$

and we can further interpret the quadratic term.

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