Outline of quantum mechanics

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Abstract

This is a brief outline of the mathematics of quantum mechanics. It begins with examples of unitary time evolution given by the Schrödinger equation. It is then shown how the spectral theorem for self-adjoint operators gives a general framework for studying solutions of the Schrödinger equation. There is a discussion of the role of Planck's constant and uncertainty principles. This is followed by a section on spin and statistics. The exposition concludes with remarks about the various roles played by self-adjoint operators in the formulation of quantum mechanics. While the main purpose of this outline is to give a succinct and mathematically correct account of the basic notions of quantum mechanics, there is also an attempt to explain why giving a coherent interpretation of quantum mechanics is so difficult.

Contents

1 The setting for quantum mechanics

1.1 Introduction

Quantum mechanics is the framework for the current theory of matter, viewed as consisting of constituents on the molecular, atomic, and sub-atomic scale. The characteristic feature of quantum mechanics is the occurrence of Planck's constant

$$\hbar = 1.05443 \times 10^{-27} \text{erg s} \tag{1}$$

This has the dimensions of energy times time, or momentum times distance. In other words, it has the dimensions of angular momentum. This number is unbelievably small, but it affects many features of our world. The mass of an electron is

$$m = 9.1083 \times 10^{-28} \text{g}. \tag{2}$$

The ratio

$$\sigma^2 = \frac{\hbar}{m} = 1.157 \text{cm}^2/\text{s} \tag{3}$$

has the dimensions of a diffusion constant. This is the parameter that determines the propagation of a free electron. It is perhaps too optimistic to think of quantum mechanics as a theory that can be derived from classical mechanics by some process called quantization. It may even be misleading to think of classical mechanics as a limit of quantum mechanics, in view of the fact that $\hbar$ is a fixed number.

The mathematical structure of quantum mechanics is based on three fundamental ideas. These are:

- State
- Time evolution
- Observable

As we shall see, the first two may be defined as mathematical objects: vectors in Hilbert space and unitary operators acting on these vectors. The notion of observable will turn out to be remarkably obscure. In some accounts it is identified with the notion of self-adjoint operator, but we shall see that this leads to problems.

The mathematical description of a quantum state is as a unit vector in a Hilbert space. Often this is represented in a concrete form as a normalized wave function, that is, a complex valued function depending on a space variable. The normalization condition says that the absolute value squared of this function is a probability density, that is, has integral equal to one. In this case it is regarded as giving the probability density describing the random position of a particle at a single fixed time.

Time evolution in quantum mechanics is given by unitary linear operators from the Hilbert space to itself. Each such operator is simply an automorphism of the Hilbert space. Typically, these unitary operators fit together to form a

one-parameter group of unitary operators, where the parameter is the time displacement. In practice this time evolution is obtained by solving a conservative evolution equation, the famous Schrödinger equation. It is an odd situation: the dynamics takes place on the level of the wave function, but the observed quantity is interpreted as a particle.

An observable is sometimes identified as a self-adjoint operator acting in the Hilbert space. It behaves something like a random variable in probability theory, but there is a crucial difference. Given a quantum state, a self-adjoint operator gives rise to a random variable. More generally, a family of commuting self-adjoint operators gives rise to a family of random variables on the same probability space. There is a problem, however, with interpreting the values of these random variables as describing intrinsic properties of the system. The problem comes when one considers non-commuting families of self-adjoint operators. As we shall see, there is a serious consistency problem that prevents such an interpretation.

A possible resolution of this issue is to maintain that different observables correspond to different experimental contexts. There is no absolute notion of the value of an observable, apart from such a context. In particular, a measurement of one observable may preclude the measurement of another observable. However, if the notion of measurement is needed to complete the concept of observable, then there is the problem of describing exactly what constitutes a measurement. It is thus doubtful that every self-adjoint operator represents an observable in the sense described here. In fact, it may be that the question of which self-adjoint operators are associated with experimental measurements and thus represent observables depends on the details of the time evolution.

It is generally regarded that many of the most fundamental self-adjoint operators correspond to observables. These include operators corresponding to position, momentum, energy, and spin component. Some physicists have maintained that these all reduce to macroscopic position measurements (for example pointer readings) via some sort of measurement process. For example, when a particle with spin is passed through a region where there is a suitable magnetic field, then it is deflected in one way or the other, and this deflection is amplified into a macroscopic difference in position. Thus the apparatus with the magnetic field produces a measurement of the spin component along the field direction. This does not mean that the value of the spin component exists before the measurement; it emerges from the interaction with a particular apparatus, and it is this apparatus that defines the particular component being measured. The measurement is ultimately a determination of the position of the particle after the deflection.

Even position is problematical in quantum mechanics. The theory provides no mechanism for defining particle trajectories. The wave function determines the probability density for particle position at a fixed time. It does not determine the joint probability density for the positions of the particle at two or more different times. Thus quantum mechanics involves waves and particles, but their roles are very different. The waves propagate according to a well-defined linear partial differential equation. There is no description of particle motion,

but it is the particles that are ultimately observed.

1.2 Plan of the exposition

The following account begins with an account of states as vectors in Hilbert space and of time evolutions for particular systems. In other words, the story is about the Schrödinger equation.

The development then proceeds to the spectral theorem for self-adjoint operators. This theorem has remarkable consequences. It emerges that that the self-adjoint operators on a Hilbert space are in one-to-one correspondence with the one-parameter groups of unitary operators. In particular, there is a self-adjoint operator that determines the dynamics given by the Schrödinger equation.

The next parts are about special topics. Planck's constant and the uncertainty principle have important physical consequences. In many circumstances when the potential energy has negative singularities, the total energy is bounded below, with a bound that depends on the value of Planck's constant. This is at least part of the explanation for the stability of atoms. Other topics include spin and statistics. The fact that electrons obey Fermi-Dirac statistics leads to the Pauli exclusion principle, another ingredient in explaining the stability of matter.

Finally, there is a discussion of other roles for self-adjoint operators. Another consequence of the spectral theorem is that, given a particular quantum state, every self-adjoint operator may be realized as a random variable. This tempts some to say that every self-adjoint operator is an observable, and certainly there is nothing to forbid this choice of terminology. However if the notion of observable is restricted to something that can be measured in an experiment, then it most likely the case that relatively few self-adjoint operators correspond to observables. For the ones that do correspond to observables it is necessary to give an account of how this is accomplished by measurement. A complete account is not known to the author, but the final section will give some hints suggested by the conventional wisdom of quantum mechanics. The perceptive reader will notice the occurrence of the word "macroscopic," which is a hint that nothing is understood.

It should be emphasized that there is very little that is controversial about quantum dynamics. The part that is obscure is how the objects described by the dynamics are reflected in reality.

Before proceeding to the topics outlined in this subsection, there is one more point that should be mentioned. The usual expositions of quantum theory, including this one, emphasize the vector space description of quantum states. However, while in quantum mechanics each non-zero vector determines a state, it turns out that two vectors that are multiples of each other determine the same state. As a consequence, that space of states in quantum mechanics is actually a projective space. Furthermore, while the automorphisms of this space are typically determined by unitary operators, in some circumstances anti-unitary operators are appropriate. While these are important foundational issues, they

will not play a major role in what follows. See the appendix to David Wick's book [10] for further information about the projective space interpretation.

Here are warnings about terminology and notation. In the following, when there is talk of real or complex functions on some set, it is taken that the set has the structure of a standard measurable space and that the functions are Borel measurable functions. In general, the goal is to bypass technical issues that are not relevant to the discussion of the main subject. For instances, Hilbert spaces are always taken to be separable. For simplicity almost all of what follows will be about quantum mechanics in one space dimension. Nevertheless, space derivatives are written in the partial derivative notation $\frac{\partial}{\partial x}$. Such space derivatives are interpreted in a non-classical sense: $\frac{\partial}{\partial x}\psi = \chi$ holds whenever ψ is an indefinite integral of the locally integrable function χ. (That is, ψ is required to be an absolutely continuous function.) In particular, ψ can have a slope discontinuity. The term operator is a synonym for linear transformation defined on a vector space. For instance, in the following $\frac{\partial}{\partial x}$ is typically interpreted as an operator defined on the vector space of all square-integrable ψ such that $\frac{\partial}{\partial x}\psi = \chi$ is also square-integrable. Since every square-integrable function χ on the line is also locally integrable, the derivative makes sense.

1.3 Hilbert space

A *Hilbert space* $\mathcal{H}$ (or complex Hilbert space) is a complex vector space with an inner product that is a complete metric space with respect to the norm associated with the inner product. In general, we shall write a vector in $\mathcal{H}$ as ψ and its norm as $\|\psi\|$.

The definition of inner product that we use is the following. For each ordered pair of vectors ϕ and ψ in $\mathcal{H}$, the inner product is a complex number $\langle \phi, \psi \rangle$. The inner product must have the following properties.

1. Linear in the second variable: $\langle \phi, a\psi + b\chi \rangle = a\langle \phi, \psi \rangle + b\langle \phi, \chi \rangle$.
2. Conjugate linear in the first variable: $\langle a\psi + b\chi, \phi \rangle = \bar{a}\langle \psi, \phi \rangle + \bar{b}\langle \chi, \phi \rangle$.
3. Hermitian symmetric: $\langle \phi, \psi \rangle = \overline{\langle \psi, \phi \rangle}$.
4. Positive on all vectors: $\langle \psi, \psi \rangle \geq 0$.
5. Strictly positive on non-zero vectors: If $\psi \neq 0$, then $\langle \psi, \psi \rangle > 0$.

The convention that the inner product is linear in the second variable is somewhat unusual in the mathematics literature, but it is quite standard in physics. One advantage is that it gives a particularly convenient notation for the dual space, that is, the space of continuous linear functions from the Hilbert space to the complex scalars. Thus, if ϕ is a vector in $\mathcal{H}$, then ϕ^* is the element of the dual space such that the value of ϕ^* on ψ is $\langle \phi, \psi \rangle$. A fundamental result of Hilbert space theory states that every element of the dual space may be represented in this way. This notation is consistent with the usual notation in matrix theory, in which ψ is given by a column vector, and ϕ^* is a row vector.

The inner product $\phi^*\psi$ is a scalar, while the outer product $\psi\phi^*$ is a linear transformation from the Hilbert space to itself (a projection). In particular, the inner product $\psi^*\psi = \|\psi\|^2$, while $\psi\psi^*$ is an orthogonal projection.

The norm associated with the inner product is $\|\psi\| = \sqrt{\langle\psi, \psi\rangle}$. The positivity axiom says that $\|\psi\| \geq 0$; the strict positivity says that for ψ not equal to the zero vector we even have $\|\psi\| > 0$. It is assumed that the reader is familiar with the properties of inner products and their associated norms. As usual, we say that ϕ and ψ are orthogonal if $\langle\phi, \psi\rangle = 0$. In this case we write $\phi\perp\psi$, and we have $\|\phi\|^2 + \|\psi\|^2 = \|\phi + \psi\|^2$. This is the theorem of Pythagoras.

A norm defines a metric that makes the space into a metric space. To say that the Hilbert space is a complete metric space is to say that every Cauchy sequence of vectors in the Hilbert space converges to a vector in the Hilbert space.

Here is one of the most useful examples of a Hilbert space. Consider the space $\mathcal{H}$ of complex functions ψ defined on the real line such that

$$\|\psi\|^2 = \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx < \infty. \tag{4}$$

Define the inner product by

$$\langle\phi, \psi\rangle = \int_{-\infty}^{\infty} \overline{\phi(x)}\psi(x) \, dx < \infty. \tag{5}$$

This satisfies all the axioms, except for the strict positivity. However if we regard each pair of functions that differ on a set of measure zero as defining the same element of the Hilbert space, then after this identification all the axioms are satisfied. The resulting Hilbert space is denoted $\mathcal{H} = L^2(\mathbf{R}, dx)$. This notation indicates that the functions are complex functions on the real line $\mathbf{R}$ that are square integrable in the sense of Lebesgue. In the quantum mechanical context, such a function is called a *wave function*.

Another important example of a Hilbert space is an ℓ^2 space of complex sequences that are square-summable with respect to a given weight function. The weights $w_j > 0$ are strictly positive. A sequence c in this space satisfies

$$\|c\|^2 = \sum_j w_j |c_j|^2 < \infty. \tag{6}$$

In quantum mechanics there is always an underlying Hilbert space $\mathcal{H}$. A *state* is determined by a unit vector ψ in $\mathcal{H}$. Two unit vectors define the same state if one is a complex multiple of the other. Since the two vectors have the same length, this complex multiple must be a phase $e^{i\theta}$.

1.4 Unitary operators

A *Hilbert space isomorphism* from a complex Hilbert space $\mathcal{H}$ to another complex Hilbert space $\mathcal{H}'$ is a linear transformation $U : \mathcal{H} \to \mathcal{H}'$ that is a bijection and

also preserves the norm, so that $\|U\psi\| = \|\psi\|$. It may be shown that a Hilbert space isomorphism automatically preserves the inner product.

Here is a fundamental example, the Fourier transform. The Fourier transform of the complex function $\psi(x)$ in $\mathcal{H} = L^2(\mathbf{R}, dx)$ is another complex function $\hat{\psi}(k)$. The mapping F that takes ψ to $\hat{\psi}$ is the Fourier transform mapping. It is a unitary operator from the Hilbert space $\mathcal{H}$ to the Hilbert space $\hat{\mathcal{H}} = L^2(\mathbf{R}, \frac{dk}{2\pi})$ with norm

$$\|\hat{\psi}\|^2 = \int_{-\infty}^{\infty} |\hat{\psi}(k)|^2 \frac{dk}{2\pi}. \tag{7}$$

It is determined by the relation

$$\hat{\psi}(k) = \int_{-\infty}^{\infty} e^{-ikx} \psi(x)\, dx. \tag{8}$$

The identity that expresses the fact that F is unitary from $\mathcal{H}$ to $\hat{\mathcal{H}}$ is

$$\int_{-\infty}^{\infty} |\hat{\psi}(k)|^2 \frac{dk}{2\pi} = \int_{-\infty}^{\infty} |\psi(x)|^2\, dx. \tag{9}$$

We can write this as

$$\hat{\psi} = F\psi, \tag{10}$$

with

$$\|\hat{\psi}\|^2 = \|\psi\|^2. \tag{11}$$

Notice that the integral over k that defines the left hand side has an extra factor of $1/(2\pi)$. The inverse F^{-1} of the Fourier transform is a unitary operator from $\hat{\mathcal{H}}$ to $\mathcal{H}$ determined by

$$\psi(x) = \int_{-\infty}^{\infty} e^{ikx} \hat{\psi}(k) \frac{dk}{2\pi}. \tag{12}$$

The Fourier transform variable k is called the *wave number*, and its dimension is that of inverse length. Thus to the extent that we can compute these integrals, we get a way of translating statements about position x to statements about wave number k. Sometimes a Hilbert space isomorphism is called a unitary operator. In the following we shall mainly refer to a *unitary operator* as a linear transformation $U : \mathcal{H} \to \mathcal{H}$ of a complex Hilbert space to itself that is a Hilbert space isomorphism.

We shall often use the fact that the Fourier transform of $-i\frac{\partial}{\partial x}\psi(x)$ is $k\hat{\psi}(k)$ and that the Fourier transform of $x\psi(x)$ is $i\frac{\partial}{\partial k}\hat{\psi}(k)$. In fact, for many purposes we could think of these as defining the derivatives.

Here is a fundamental example of a unitary operator. Consider the space $\hat{\mathcal{H}} = L^2(\mathbf{R}, \frac{dk}{2\pi})$. Let $\alpha(k)$ be a real function on the real line. Then the operator V defined by

$$(V\psi)(k) = e^{-i\alpha(k)}\psi(k) \tag{13}$$

is a unitary operator. A composition of unitary operators is again a unitary operator. For example, the composition $U = F^{-1}VF$ is a quite non-trivial example of a unitary operator.

Often unitary operators combine to form a *one-parameter unitary group*. This refers to a homomorphism of the additive group of the line to the group of unitary operators on the Hilbert space $\mathcal{H}$. In other words, for each real t there is a unitary operator $U_t : \mathcal{H} \to \mathcal{H}$. The group homomorphism property says that $U_0 = I$ and that

$$U_{t+t'} = U_t U_{t'}. \tag{14}$$

Finally, it is require that for each ψ in $\mathcal{H}$ the map $t \mapsto U_t\psi$ is continuous from the real line to $\mathcal{H}$.

Here is an example of such a unitary group. Consider the space $\hat{\mathcal{H}} = L^2(\mathbf{R}, \frac{dk}{2\pi})$. Let $\alpha(k)$ be a real function on the real line. Then for each t the operator V_t defined by

$$(V_t\psi)(k) = e^{-it\alpha(k)}\psi(k) \tag{15}$$

is a unitary operator, and this defines a unitary group. The composition $U_t = F^{-1}V_tF$ provides a non-trivial example of a unitary group.

There are analogous constructions for isomorphisms with ℓ^2 spaces. Say that ϕ_j is an orthogonal basis for the Hilbert space $\mathcal{H}$. Define the ℓ^2 space with the weight function $w_j = 1/\langle\phi_j, \phi_j\rangle$. Then the map $Z : \mathcal{H} \to \ell^2$ given by $(Z\psi)_j = \langle\phi_j, \psi\rangle$ is an isomorphism from $\mathcal{H}$ to ℓ^2. The inverse isomorphism is given by $Z^{-1}c = \sum_j w_j c_j \phi_j$. Suppose that λ_j are real numbers. Then the composition given by Z followed by multiplication by $e^{-it\lambda_j}$ followed by Z^{-1} defines a unitary group U_t. Explicitly

$$U_t\psi = \sum_j w_j \phi_j e^{-it\lambda_j} \langle\phi_j, \psi\rangle. \tag{16}$$

2 The Schrödinger equation

2.1 Diffusion and the free motion Schrödinger equation

The diffusion equation (or heat equation) describes diffusing particles. The equation is

$$\frac{\partial}{\partial t}u = \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}u \tag{17}$$

We look for a solution $u(x,t) = (Q_t\psi)(x)$ satisfying $u(x,0) = \psi(x)$. In order to apply the Fourier transform, we take ψ in $L^2(\mathbf{R})$. The Fourier transform satisfies

$$\frac{d}{dt}\hat{u} = -\frac{\sigma^2}{2}k^2\hat{u} \tag{18}$$

with initial condition $\hat{u}(k,0) = \hat{\psi}(k)$. This has solution

$$\hat{u}(k,t) = e^{-\frac{\sigma^2}{2}k^2 t}\hat{\psi}(k). \tag{19}$$

Recall that the Gaussian density with variance parameter ϵ^2 is defined by

$$g_{\epsilon^2}(x) = \frac{1}{\sqrt{2\pi\epsilon^2}} e^{-\frac{x^2}{2\epsilon^2}}. \tag{20}$$

Its Fourier transform is

$$\hat{g}_{\epsilon^2}(k) = \int_{-\infty}^{\infty} e^{ikx} g_{\epsilon^2}(x)\, dx = e^{-\frac{\epsilon^2 k^2}{2}} \tag{21}$$

The expression for $\hat{u}(k,t)$ is the product of the Fourier transform of the Gaussian density of variance $\sigma^2 t$ with $\hat{\psi}(k)$. To evaluate the inverse Fourier transform $u(x,t)$ use the fact that the inverse Fourier transform of a product is a convolution. This proves the following result.

Proposition 2.1 *The solution of the diffusion equation is given in terms of the Fourier transform F for $t \geq 0$ by*

$$u(t) = Q_t \psi = F^{-1} \hat{Q}_t F \psi, \tag{22}$$

where $\hat{Q}_t$ is multiplication by $e^{-\frac{\sigma^2 t k^2}{2}}$. Its explicit form for $t > 0$ is given by the convolution

$$u(x,t) = (Q_t\psi)(x) = (g_{\sigma^2 t} * \psi)(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-\frac{(x-y)^2}{2\sigma^2 t}} \psi(y)\, dy. \tag{23}$$

Notice that Q_t is not unitary, but it does satisfy the stability condition $\|Q_t\psi\| \leq \|\psi\|$ for $t > 0$. Typically the initial condition $\psi(x)$ is taken to be a positive function, and then it follows that the solution $u(x,t) \geq 0$ is also positive. Furthermore, in this case the total integral is constant. This explains why the solution is interpreted as a density.

The interpretation of the Schrödinger equation is quite different. The function ψ represents the quantum state. In this case the position observable is the x coordinate. If ψ is normalized so that the L^2 norm $\|\psi\| = 1$, then $|\psi(x)|^2$ is a probability density for x. The state makes the observable a random variable: the expectation of a function $f(x)$ is given by

$$E_\psi[f(x)] = \int_{-\infty}^{\infty} f(x) |\psi(x)|^2\, dx. \tag{24}$$

The Schrödinger equation for free motion is

$$\frac{\partial}{\partial t} u = i \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} u. \tag{25}$$

The same manipulations as for the diffusion equation give the solution

$$\hat{u}(k,t) = e^{-i\frac{\sigma^2}{2}k^2 t} \hat{\psi}(k). \tag{26}$$

Proposition 2.2 *The solution of the free Schrödinger equation is given in terms of the Fourier transform F for real t by*

$$u(t) = U_t\psi = F^{-1}\hat{U}_t F\psi, \tag{27}$$

where $\hat{U}_t$ is multiplication by $e^{-i\frac{\sigma^2 tk^2}{2}}$. The solution operator U_t is unitary. Its explicit form for $t \neq 0$ is given by the convolution

$$u(x,t) = (U_t\psi)(x) = (g_{i\sigma^2 t} * \psi)(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi i\sigma^2 t}} e^{\frac{i(x-y)^2}{2\sigma^2 t}} \psi(y)\, dy. \tag{28}$$

The only modification that must be made to pass from the diffusion equation to quantum mechanics is to replace t by it. The same kinds of formula continue to hold true, even though the convergence of the integrals is more delicate.

2.2 The free particle

The free particle solution describes motion at constant velocity, but with a spread of initial velocities. Here is a more detailed description of how this works.

Both the spatial shift and the time dynamics have nice expressions in terms of wave number. The spatial shift is a unitary operator from $\mathcal{H}$ to $\mathcal{H}$ with the obvious expression

$$(V_a\psi)(x) = \psi(x-a). \tag{29}$$

This may be written

$$V_a = F^{-1}\hat{V}_a F, \tag{30}$$

where the unitary operator $\hat{V}_a$ from $\hat{\mathcal{H}}$ to $\hat{\mathcal{H}}$ is given by

$$(\hat{V}_a\hat{\psi})(k) = e^{-iak}\hat{\psi}(k). \tag{31}$$

Notice that a has the dimensions of length, while k has the dimensions of inverse length, so ak is dimensionless, as it must be.

The free particle unitary time dynamics U_t on $\mathcal{H}$ is given by a similar expression. Now we have t with the dimension of time, and k with the dimension of inverse length. In quantum mechanics we have the diffusion constant $\frac{1}{2}\sigma^2$ with dimensions of length squared over time. So a suitable dimensionless combination is $t\frac{1}{2}\sigma^2 k^2$. The corresponding unitary operator on $\hat{\mathcal{H}}$ is

$$(\hat{U}_t\hat{\psi})(k) = e^{-it\frac{1}{2}\sigma^2 k^2}\hat{\psi}(k). \tag{32}$$

In the position representation we have

$$U_t = F^{-1}\hat{U}_t F. \tag{33}$$

We have already computed this explicitly as a convolution by a Gaussian with a complex variance parameter. The result of this explicit computation has an interesting physical interpretation.

Proposition 2.3 *Define the unitary operator from $\mathcal{H}$ to $\mathcal{H}$ by*

$$(M_t\psi)(y) = e^{\frac{iy^2}{2\sigma^2 t}}\psi(y). \tag{34}$$

Define another unitary operator from $\hat{\mathcal{H}}$ to $\mathcal{H}$ by

$$(Z_t\chi)(x) = \frac{1}{\sqrt{2\pi i\sigma^2 t}}\chi(\frac{x}{\sigma^2 t}). \tag{35}$$

Then the free particle solution operator is given by

$$U_t = M_t Z_t F M_t. \tag{36}$$

This last identity determines the long time asymptotics of the solution. Consider the difference $U_t\psi - M_t Z_t F\psi$. This has norm

$$\|U_t\psi - M_t Z_t F\psi\| = \|M_t Z_t F M_t\psi - M_t Z_t F\psi\|. \tag{37}$$

This is equal to

$$\|M_t Z_t F(M_t\psi - \psi)\| = \|M_t\psi - \psi\|. \tag{38}$$

However the right hand side goes to zero as $t \to \pm\infty$. This proves the following result.

Proposition 2.4 *In the limit $t \to \pm\infty$ the solution of the free particle Schrödinger equation has the asymptotic form*

$$U_t\psi \sim M_t Z_t\hat{\psi}. \tag{39}$$

Explicitly,

$$(U_t\psi)(x) \sim e^{\frac{ix^2}{2\sigma^2 t}}\frac{1}{\sqrt{2\pi i\sigma^2 t}}\hat{\psi}(\frac{x}{\sigma^2 t}). \tag{40}$$

From this we see that the velocity of propagation at wave number k is asymptotically $\sigma^2 k$. When t is large and x is large with $x/t \sim \sigma^2 k$, the amplitude $(U_t\psi)(x)$ is proportional to the value $\hat{\psi}(k)$. So the solution spreads out in space according to wave number. This proposition gives a particularly simple form for the asymptotic position probability density.

Proposition 2.5 *The position probability density for the free particle is given asymptotically by*

$$|(U_t\psi)(x)|^2 \sim \frac{1}{2\pi\sigma^2 t}|\hat{\psi}(\frac{x}{\sigma^2 t})|^2. \tag{41}$$

This leads to the notion of taking the wave number k or the corresponding velocity $\sigma^2 k$ as an observable . Its probability density would then be $|\hat{\psi}(k)|^2$. The expectation of a function of k is given by

$$E_{\hat{\psi}}[f(k)] = \int_{-\infty}^{\infty} f(k)|\hat{\psi}(k)|^2\,\frac{dk}{2\pi} = \int_{-\infty}^{\infty} f(\frac{x}{\sigma^2 t})\frac{1}{2\pi\sigma^2 t}|\hat{\psi}(\frac{x}{\sigma^2 t})|^2\,dx. \tag{42}$$

Compare this to

$$E_{U_t\psi}[f(\frac{x^2}{\sigma^2 t})] = \int_{-\infty}^{\infty} f(\frac{x}{\sigma^2 t})|U_t\psi(x)|^2\,dx \tag{43}$$

The asymptotic relation expressed in the previous proposition leads to the following important result.

Proposition 2.6 *An expectation involving wave number may be expressed in terms of asymptotic position by*

$$E_{\hat{\psi}}[f(k)] \sim E_{U_t\psi}[f(\frac{x^2}{\sigma^2 t})]. \tag{44}$$

In quantum mechanics it is customary to take the observable as the momentum $p = \hbar k = m\sigma^2 k$ instead of the velocity $\sigma^2 k$. So the notion is that position and momentum are both observables, but a measurement of one is incompatible with the measurement of the other. This is because for position one uses the position density $|\psi(x)|^2$ now, while for momentum one uses the position density $|(U_t\psi)(x)|^2$ much later, that is, for large t.

If the probability for x is initially very localized near a point, then there will be many wave numbers represented in the Fourier transform, and so the probability for k will be spread out. In particular, there will be many different propagation velocities, and with time the dynamics will filter the various wave numbers to make them occupy different regions in space.

2.3 Shift operators

In quantum mechanics there is a remarkable duality between position and wave number (or momentum). The position shift operator V_a is the unitary operator given by

$$(V_a\psi)(x) = \psi(x - a). \tag{45}$$

We have already seen its form in the wave number representation. The wave number shift operator $\hat{W}_b$ is the unitary operator given by

$$(\hat{W}_b\hat{\psi})(k) = \hat{\psi}(k - b). \tag{46}$$

Since the momentum is $p = \hbar k$, this is closely related to the corresponding momentum shift operator. In the position representation this shift operator becomes

$$(W_b\psi)(x) = e^{ibx}\psi(x). \tag{47}$$

These unitary operators operators satisfy the algebraic relation

$$W_bV_a = e^{iab}V_aW_b. \tag{48}$$

That is, if the order of the shifts are reversed, then the result is the same, up to a phase factor. Of course this phase factor makes no difference when determining the quantum state.

There is a remarkable uniqueness theorem that says that there is only one irreducible solution of this operator equation, up to isomorphism. This theorem gives an abstract characterization of the framework involving position and wave number and the Fourier transform. This shows that the basic structure of quantum mechanics may be derived from a purely algebraic relation for unitary operators.

2.4 The Schrödinger equation with a potential energy function

Schrödinger discovered the fundamental dynamical equation of quantum mechanics. The most common way of writing the *Schrödinger equation* is

$$i\hbar \frac{\partial}{\partial t} u = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} u + v(x)u. \tag{49}$$

Both sides of the equation have the units of energy. Here $v(x)$ is the potential energy function. The problem is to find the solution $u(x,t)$ of this equation with some initial condition $u(x,0) = \phi(0)$.

For some purposes it is convenient to write the equation in a slightly different but equivalent form. The only changes are the sign change and division by $\hbar$. This other form is

$$-i \frac{\partial}{\partial t} u = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} u - \frac{1}{\hbar} v(x)u. \tag{50}$$

Both sides of this equation have the units of inverse time. The potential energy term is divided by $\hbar$ in order to convert energy units into inverse time units. For each form of the potential energy function $v(x)$ one has a separate problem, and such problems are difficult to solve in general. We shall look at a few simple cases where it is possible to make progress.

There is a closely related equation *diffusion with removal equation*

$$\frac{\partial}{\partial t} u = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} u - \frac{1}{\hbar} v(x)u. \tag{51}$$

Suppose that $v(x) \geq 0$. Then this equation has an interpretation in terms of diffusion. The σ^2 is the usual diffusion constant. The $v(x)/\hbar$ indicates a spatially dependent rate at which the diffusing particles are being removed from the system. So the particles diffuse and occasionally vanish.

2.5 Motion with constant force

The next natural topic is the problem of Galileo: find the motion of a particle under the influence of a constant force ϵ. The solution would not have surprised Galileo: constant acceleration implies linear increase in velocity and quadratic increase in position.

Proposition 2.7 *The solution of the Schrödinger equation with constant force ϵ is*

$$u(t) = G_t\psi = c(t)W_{\frac{\epsilon t}{\hbar}}V_{\frac{1}{2}\frac{\epsilon}{m}t^2}U_t\psi. \tag{52}$$

Here $c(t)$ is a phase factor. The unitary operator U_t describes the free particle evolution. The unitary operator $W_{\frac{\epsilon t}{\hbar}}$ represents a shift in momentum $p = \hbar k$ by ϵt. The unitary operator $V_{\frac{1}{2}\frac{\epsilon}{m}t^2}$ represents a shift in position by $\frac{1}{2}\frac{\epsilon}{m}t^2$.

One can write the solution in a more explicit form as

$$(G_t\psi)(x) = c(t)e^{i\frac{\epsilon t}{\hbar}x}(U_t\psi)(x - \frac{1}{2}\frac{\epsilon}{m}t^2). \tag{53}$$

The value of the phase $c(t)$ is not important for the physics, but if we take $c(t) = e^{-i\frac{1}{6}\frac{\epsilon^2 t^3}{m\hbar}}$, then we get the group homomorphism property $G_{t+t'} = G_tG_{t'}$. In any case, it will emerge with the systematic derivation of the result.

Here is the derivation. Take $v(x) = -\epsilon x$ in the Schrodinger equation. The Fourier transformed equation is then

$$\frac{\partial}{\partial t}\hat{u} + \frac{\epsilon}{\hbar}\frac{\partial}{\partial k}\hat{u} = -i\frac{1}{2}\sigma^2k^2\hat{u}. \tag{54}$$

This is the equation for translation in wave number space, but with a source term.

This equation is not difficult to solve directly, but it is illuminating to put it in the form of a conservation law by the change of change of variable $\hat{u} = a(k)w$. If we choose $a(k)$ so that $\frac{\epsilon}{\hbar}a'(k)/a(k) = -i\frac{1}{2}\sigma^2k^2$, then the new equation no longer has a source term; it is simply the translation equation in wave number space

$$\frac{\partial}{\partial t}w + \frac{\epsilon}{\hbar}\frac{\partial}{\partial k}w = 0. \tag{55}$$

.

This equation is easy to solve by integrating along the lines that are solutions of $dk/dt = \frac{\epsilon}{\hbar}$. These are the lines $k = k_0 + \frac{\epsilon}{\hbar}t$. Along such a line the solution is constant, and so we have $w(k,t) = f(k_0) = f(k - \frac{\epsilon}{\hbar}t)$. The solution is translation at constant velocity in wave number space.

We have $\hat{u} = a(k)w$, where

$$a(k) = \exp(-i\frac{1}{6}\frac{\hbar}{\epsilon}\sigma^2k^3). \tag{56}$$

The initial conditions are related by $\hat{\psi}(k_0) = a(k_0)f(k_0)$. So the solution for $\hat{u}$ is

$$\hat{u}(k,t) = a(k)w(k,t) = a(k)f(k_0) = a(k)a(k_0)^{-1}\hat{\psi}(k_0). \tag{57}$$

Insert $k = k_0 + \frac{\epsilon}{\hbar}t$ to get

$$\hat{u}(k,t) = \exp(-i\frac{1}{6}\frac{\sigma^2\epsilon^2}{\hbar^2}t^3 - i\frac{1}{2}\frac{\sigma^2\epsilon}{\hbar}t^2k_0 - i\frac{1}{2}\sigma^2k_0^2t)\hat{\psi}(k_0). \tag{58}$$

Alternatively,

$$\hat{u}(k,t) = \exp(-i\frac{1}{6}\frac{\epsilon^2}{m\hbar}t^3 - i\frac{1}{2}\frac{\epsilon}{m}t^2 k_0 - i\frac{1}{2}\sigma^2 k_0^2 t)\hat{\psi}(k_0), \tag{59}$$

where $k_0 = k - \frac{\epsilon}{\hbar}t$. The result stated in the proposition follows by taking the inverse Fourier transform.

2.6 Spectral and propagator solutions

The following subsections treat other simple examples where it is possible to find explicit solutions of the Schrödinger equation with a potential energy function (or of the corresponding diffusion with removal equation). These examples are the quantum description of a particle confined to a bounded interval, a particle confined to a half-line, and a particle with a linear force (the harmonic oscillator). The problem is to find the operator that maps the initial wave function at time zero to the wave function at time t. Typically, there are two ways of exhibiting the solution. A *spectral solution* is obtained by mapping the Hilbert space to a weighted L^2 space of functions via a unitary operator W, multiplying by a complex phase $e^{-i\lambda(k)t}$, and then mapping back to the original Hilbert space via W^{-1}. Typically, the unitary operator will be an integral operator of the form

$$(W\psi)(k) = \int \overline{\phi_k(y)}\psi(y)\,dy. \tag{60}$$

The inverse operator is of the form

$$(W^{-1}f)(x) = \int \phi_k(x)f(k)w(k)\,dk. \tag{61}$$

in the continuous case or

$$(W^{-1}f)(x) = \sum_k \phi_k(x)f(k)w(k) \tag{62}$$

in the discrete case. In either case the weights $w(k) \geq 0$.

A *propagator* is a family of integral operators given by a functions $p_t(x,y)$ indexed by t. The solution is then given by

$$(U_t\psi)(x) = \int p_t(x,y)\psi(y)\,dy. \tag{63}$$

The propagator may be expanded to give a spectral solution. Sometimes this expansion is continuous, as in

$$p_t(x,y) = \int \phi_k(x)e^{-i\lambda(k)t}\overline{\phi_k(y)}w(k)\,dk. \tag{64}$$

Other times it is discrete, as in

$$p_t(x,y) = \sum_k \phi_k(x)e^{-i\lambda(k)t}\overline{\phi_k(y)}w(k). \tag{65}$$

Unfortunately, in most cases it is impossible to find an explicit solution of either kind. This means that it is necessary to use various approximation methods, such as perturbation theory or variational calculations, in order to understand the dynamics. These approximation methods are at the heart of the mathematics of quantum mechanics. Unfortunately these topics are too extensive to include in an short introductory account.

2.7 Particle in a box

Consider a particle confined to a bounded interval (often called a particle in a box). The idea is that the potential energy $v(x) = 0$ for $0 < x < a$ and $v(x) = +\infty$ elsewhere. The effect of this is to restrict the problem to the interval $[0, a]$ and impose zero boundary conditions at the end points of the interval when solving the Schrödinger equation.

First look for a spectral solution. There is a new phenomenon: discrete frequencies. This comes from solving the eigenvalue problem

$$-\frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2}\phi_n(x) = \lambda_n \phi_n(x) \tag{66}$$

with the boundary condition $\phi(0) = \phi(a)$. The solution is

$$\phi_n(x) = \sin(\frac{n\pi x}{a}). \tag{67}$$

We conclude that

$$\lambda_n = \frac{1}{2}\sigma^2 \frac{n^2\pi^2}{a^2}. \tag{68}$$

Multiplying by $\hbar$, we see that the discrete energy levels are

$$E_n = \hbar\lambda_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{a^2}. \tag{69}$$

We can solve the evolution equation by writing an arbitrary initial condition as

$$\psi(x) = \frac{1}{a}\sum_{n=1}^{\infty} c_n \phi_n(x) \tag{70}$$

Here

$$c_n = 2\int_0^a \phi_n(y)\psi(y)\, dy. \tag{71}$$

Then for the diffusion equation the solution is

$$u(x,t) = \sum_n e^{-\lambda_n t} c_n \phi_n(x). \tag{72}$$

This describes diffusion where the particles are killed as soon as the encounter the boundary of the interval $[0, a]$.

For the Schrödinger equation the solution is

$$u(x,t) = \sum_n e^{-i\lambda_n t} c_n \phi_n(x). \tag{73}$$

These solutions are oscillatory waves that bounce off the boundary.

Proposition 2.8 *The spectral solution of the Schrödinger equation in a box is given by a composition of unitary operators. The original Hilbert space is $\mathcal{H} = L^2(0,a)$. It is mapped to a Hilbert space ℓ^2 of sequences with norm given by*

$$\|c\|^2 = \frac{1}{a}\sum_{n=1}^{\infty} |c_n|^2. \tag{74}$$

The unitary map S from $L^2(0,a)$ to ℓ^2 is given by

$$(S\phi)_n = 2\int_0^a \phi_n(y)\phi(y)\, dy. \tag{75}$$

The inverse map is

$$(S^{-1}c)(x) = \frac{1}{a}\sum_{n=1}^{\infty} c_n \phi_n(x). \tag{76}$$

The solution operator for the Schrödinger equation is given by S followed by multiplication by $e^{-it\lambda_n}$ followed by S^{-1}.

The propagator solution gives complementary information. It may be obtained from the above solution by using the Poisson summation formula. This formula says that if f is a rapidly decreasing function with Fourier transform $\hat{f}$, then

$$\sum_{m=-\infty}^{m=\infty} f(x-2ma) = \frac{1}{2a}\sum_{n=-\infty}^{n=\infty} \hat{f}(\frac{\pi n}{a}) e^{\frac{i\pi n x}{a}}. \tag{77}$$

This formula is derived by noticing that the left hand side is a periodic function with period $2a$ and hence may be expanded in a Fourier series.

The previous result says that the time evolution for the diffusion equation on the interval $[0,a]$ is given by a propagator

$$k_t(x,y) = \frac{2}{a}\sum_{n=1}^{\infty} e^{-\lambda_n t}\phi_n(x)\phi_n(y) = \frac{2}{a}\sum_{n=1}^{\infty} \hat{g}_{\sigma^2 t}(\frac{\pi n}{L}) \sin(\frac{n\pi}{a}x)\sin(\frac{n\pi}{a}y). \tag{78}$$

Write $2\sin(\frac{n\pi}{a}x)\sin(\frac{n\pi}{a}y) = \cos(\frac{n\pi}{a}(x-y)) - \cos(\frac{n\pi}{a}(x+y))$. Convert the cosine terms to complex exponentials and use the Poisson summation formula. The result is that

$$k_t(x,y) = \sum_{m=-\infty}^{\infty} [g_{\sigma^2 t}(x-y-2ma) - g_{\sigma^2 t}(x+y-2ma)]. \tag{79}$$

For the Schrödinger equation we should get the correct formula if we replace t by it. This gives the following result.

Proposition 2.9 *The propagator solution of the Schrödinger equation for a particle confined to the interval* $[0, a]$ *is given by the propagator*

$$p_t(x, y) = \sum_{m=-\infty}^{\infty} [g_{i\sigma^2 t}(x - y - 2ma) - g_{i\sigma^2 t}(x + y - 2ma)] \tag{80}$$

The interpretation of this result is the following. Consider x in the interval from 0 to a. Take free particle solutions starting at $y+2am$ and take negatives of free particle solutions starting at $-y+2am'$. The points $y+2am$ and $-y+2am'$ are mirror images, where the mirror is placed at the point $(m+m')a$. Thus there is a mirror at each integer multiple of a. The final effect is a cancellation at these mirror points that confines the wave to the interval. In fact, it is evident that the solution vanishes when either x or y is equal to 0 or to a. There are only standing waves that slosh back and forth in the interval.

2.8 Particle on the half-line

The particle on the half-line gives a simple illustration of scattering. The potential energy $v(x) = 0$ for $0 < x < +\infty$ and $v(x) = +\infty$ elsewhere. The effect of this is to restrict the problem to the interval $[0, +\infty)$ and impose zero boundary conditions at 0.

One way to get a spectral solution of the Schrödinger equation for this case is to start with the box solution and let $k_n = n\pi/a$. Then one can let $a \to +\infty$, and the variable k becomes a continuous variable. We get a unitary map S from $L^2(0, +\infty)$ to $L^2(0, +\infty)$ given by the sine transform

$$(S\psi)(k) = 2\int_0^{\infty} \phi_k(y)\psi(y)\, dy. \tag{81}$$

Here

$$\phi_k(x) = \sin(kx). \tag{82}$$

The inverse map is also a sine transform

$$(S^{-1}c)(x) = \int_0^{\infty} \phi_k(x)c(k)\, \frac{dk}{\pi}. \tag{83}$$

Proposition 2.10 *Consider the quantum particle on the half-line with Hilbert space* $\mathcal{H}_+ = L^2(0, \infty)$*. Let* S *be the sine transform. Let*

$$\lambda(k) = \frac{1}{2}\sigma^2 k^2. \tag{84}$$

Define M_t *to be multiplication by* $e^{-it\lambda(k)}$*. Then the spectral solution for the Schrödinger equation is given by the operator composition* $S^{-1}M_t S$*.*

This spectral solution gives the a formula for the propagator in the spectral form

$$p_t(x, y) = \frac{2}{\pi}\int_0^{\infty} e^{-it\lambda(k)} \sin(kx)\sin(ky)\, dk. \tag{85}$$

This can also be written as

$$p_t(x,y) = \frac{1}{\pi}\int_0^\infty e^{-it\lambda(k)}[\cos(x-y)-\cos(x+y)]\,dk = \frac{1}{2\pi}\int_{-\infty}^\infty e^{-i\frac{1}{2}\sigma^2 tk^2}[e^{ik(x-y)}-e^{ik(x+y)}]\,dk. \tag{86}$$

The inverse Fourier transform may be expressed in terms of free particle solutions. This gives the following result.

Proposition 2.11 *The propagator solution of the Schrödinger equation for a particle confined to the interval* $[0,+\infty]$ *is given by*

$$p_t(x,y) = g_{i\sigma^2 t}(x-y) - g_{i\sigma^2 t}(x+y) \tag{87}$$

Thus for $x \geq 0$ *the solution is given by*

$$u(x,t) = \int_0^\infty p_t(x,y)\psi(y)\,dy = (U_t\psi^-)(x), \tag{88}$$

where U_t *is the evolution operator for free motion and* ψ^- *is the reflected initial condition* $\psi^-(y) = \text{sign}(y)\psi(|y|)$.

This solution says that the solution is obtained by placing a mirror at the origin and having the solution with initial condition at y matched by a solution with initial condition at the reflected point $-y$ that has the opposite sign. If a solution comes in traveling to the left, then it is eventually replaced by the reflected solution traveling right. The effect is that the solution coming in traveling to the right appears to be scattered at the origin, with a sign change, and it emerges traveling right.

2.9 The diffusion with drift representation

We have already seen that the Schrödinger equation is intimately related to a diffusion with removal equation. In this subsection we show that there is yet another representation as a *diffusion with drift equation*. This is an important topic in probability theory, and it is striking that it is so closely connected with quantum mechanics. See the introductory chapter in [4] or the book [9] for more information on this topic.

Let $v(x)$ represent a continuous real function that is bounded below. Let

$$-A = \frac{1}{2}\sigma^2\frac{\partial^2}{\partial x^2} - \frac{1}{\hbar}v(x). \tag{89}$$

As we have seen, the equation

$$\frac{\partial u}{\partial t} = -Au \tag{90}$$

represents diffusion with removal at rate $\frac{1}{\hbar}v(x)$ when the diffusing particle is at location x. It is shown in probability theory that this diffusion has an underlying stochastic process, a probability measure on paths that describes diffusing particles that move in irregular paths, and sometimes vanish.

In the following, we shall often use an exponential notation for the solution of such an equation, writing

$$u(t) = e^{-tA}\psi. \tag{91}$$

This notation will later be justified by the spectral theorem for self-adjoint operators.

Suppose that A has a smallest eigenvalue λ corresponding to an eigenvector ϕ in the Hilbert space. Furthermore, suppose that $\phi(x) > 0$ at each x. Then we can make the change of variable

$$L = \phi^{-1}(A - \lambda I)\phi. \tag{92}$$

Then

$$-L = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} + \sigma^2 \frac{\phi'(x)}{\phi(x)} \frac{\partial}{\partial x}. \tag{93}$$

Alternatively, we can make the change of variable

$$L^* = \phi(A - \lambda I)\phi^{-1}. \tag{94}$$

Then

$$-L^* = \frac{1}{2}\sigma^2 \frac{\partial^2}{\partial y^2} - \sigma^2 \frac{\partial}{\partial y}\left(\frac{\phi'(y)}{\phi(y)}\,\cdot\,\right). \tag{95}$$

These operators have an interpretation as diffusion with drift $\sigma^2\phi'(y)/\phi(y)$. In addition to the random diffusive motion there is a systematic drift depending on position. The drift has units of velocity. It is shown in probability theory that this diffusion has an underlying stochastic process, a probability measure on paths that describes diffusing particles that move in paths that are irregular but have a tendency to drift in a direction given by the drift coefficient.

Why are there two such operators? Think of starting the diffusion at x and letting it evolve for time $t > 0$. The resulting probability density after the diffusion has taken place is a function of y. The forward equation (Fokker-Planck equation) is

$$\frac{\partial}{\partial t} w(y,t) = -L^* w(y,t). \tag{96}$$

It has solution

$$w(y,t) = (e^{-tL^*}h)(y) \tag{97}$$

which describes the density as a function of the final y when the diffusion is started at the random position $h(x)$. The diffusion and drift combine to produce an equilibrium with probability density $\rho(y) = \phi(y)^2$. In fact, it is easy to check that $L^*\rho = 0$ and $e^{-tL^*}\rho = \rho$.

The backward equation is

$$\frac{\partial}{\partial t} u(x,t) = -Lu(x,t). \tag{98}$$

It has solution

$$u(x,t) = (e^{-tL}f)(x) \tag{99}$$

which describes the describes the expectation of a function f of the final position as a function of the initial point x. One can even combine the forward and backward solutions to get the expectation of a function f of the final position when the initial point is random with density h. This is

$$\langle h, e^{-tL} f \rangle = \langle e^{-tL^*} h, f \rangle. \tag{100}$$

As an example, consider the particle in the box $[0, a]$. The smallest eigenvalue of the generator A is $\lambda_1 = \frac{1}{2}\sigma^2\pi^2/a^2$ with eigenfunction $\phi_1(x) = \sin(\pi x/a)$. So the drift term is $\sigma^2 \frac{\pi}{a} \cot(\pi x/a)$. It is very positive near 0 and very negative near a. So the particle diffuses, but it is repelled from the end points, leading to diffusive equilibrium with the largest part of the probability near the center of the interval.

In conclusion, there is a deep mathematical connection between quantum mechanics and diffusion. The solution of the Schrödinger equation is e^{-itA}. The solution of the diffusion with removal equation is given by e^{-tA}. The solutions of the forward and and backward equations for diffusion with drift are e^{-tL^*} and e^{-tL}. Moreover, since $A - \lambda I$ and L and L^* are similar, they have the same spectral properties.

2.10 The harmonic oscillator

One of the most famous quantum mechanical systems is the harmonic oscillator. This has many special properties that do not generalized to more complicated systems. However it is a landmark in the subject. The potential energy for the harmonic oscillator is the quadratic expression

$$v(x) = \frac{1}{2} m\omega^2 x^2. \tag{101}$$

The operator that occurs in the Schrödinger equation is then

$$A = -\frac{1}{2}\sigma^2 \frac{\partial^2}{\partial x^2} + \frac{1}{2}\frac{\omega^2}{\sigma^2} x^2. \tag{102}$$

This subsection will be devoted to establishing formulas for the solution operator e^{-itA}. As usual, we may express the solution operator in terms of a propagator $p_t(x, y)$. In this case the expression for the propagator is complicated, but a brief inspection of the formula shows that it is indeed a function that is periodic in t with angular frequency ω.

Proposition 2.12 *The propagator solution to the quantum harmonic oscillator equation is given by the Mehler formula*

$$p_t(x, y) = \sqrt{\frac{\omega}{2\pi i \sigma^2 \sin(\omega t)}} \exp(i \frac{\omega}{2\sigma^2 \sin(\omega t)} [\cos(\omega t)(x^2 + y^2) - 2xy]). \tag{103}$$

The spectral formula is also somewhat complicated, but again it exhibits the fact that solutions are periodic in t with angular frequency ω.

Proposition 2.13 *Let $g(x)$ denote the Gaussian function $g_{\frac{\sigma^2}{2\omega}}(x)$. Let $\phi(x) > 0$ be such that $\phi(x)^2 = g(x)$. Let $\chi_n(x) = \phi(x)^{-1}(-\frac{\partial}{\partial x})^n \phi(x)^2$. Then the spectral solution to the harmonic oscillator equation is given by*

$$p_t(x, y) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\sigma^2}{2\omega}\right)^n \chi_n(x) e^{-i(n+\frac{1}{2})\omega t} \chi_n(y). \tag{104}$$

The function $\phi(x)$ is the ground state wave function, and $g(x) = \phi(x)^2$ is the corresponding ground state position probability density. The eigenfunctions $\chi_n(x)$ are expressed in terms of the ground state wave function $\phi(x)$. These eigenfunctions define an isomorphism from $L^2(\mathbf{R})$ to a weighed ℓ^2 space. The solution operator e^{-itA} is given by the isomorphism followed by multiplication by $e^{-i(n+\frac{1}{2}\omega)t}$ followed by the inverse isomorphism. It follows that the eigenvalues of A are $\lambda_n = (n + \frac{1}{2})\omega$, and the corresponding energy values are $E_n = \hbar\lambda_n = (n + \frac{1}{2})\hbar\omega$.

The remainder of this subsection contains the derivation of these formulas. They result from a single general formula for the solution. This formula says that after several changes of variables the solution of the quantum harmonic oscillator is given by a rotation in the plane. Thus the dynamics of the quantum harmonic oscillator reduces to the dynamics of a classical harmonic oscillator. Indeed, the solution for a classical harmonic oscillator has a very simple representation in phase space (position and momentum together); it is just a rotation. If the classical phase space for a single particle is represented by the complex z plane, then a rotation with angular frequency ω is a map that sends z into $e^{-i\omega t}z$. This kind of rotation is precisely what underlies the dynamics of the quantum harmonic oscillator.

Even though the dynamics is essentially classical, there is still something essentially quantum mechanical about this system. For example, in the stationary state the position is random, in fact Gaussian distributed with variance $\sigma^2/(2\omega)$.

The change of variables operator W is given by a multiplication operator followed by the Fourier transform followed by another multiplication operator. Let $g(x)$ denote the Gaussian function $g_{\frac{\sigma^2}{2\omega}}(x)$. Let the ground state wave function $\phi(x) > 0$ be such that $\phi(x)^2 = g(x)$. Then the image of $L^2(\mathbf{R}, dx)$ under multiplication by $\phi(x)$ is a space of rapidly decreasing functions. The Fourier transforms of these functions are entire analytic functions of a Fourier transform variable z. The operator W is defined by

$$W\psi = \hat{g}^{-1} F \, \phi\psi. \tag{105}$$

For each complex number w define a corresponding rescaling operator by

$$(R_w f)(z) = f(wz). \tag{106}$$

This rescaling operator sends entire analytic functions to entire analytic functions. If $w = e^{-i\omega t}$, then the corresponding rescalings rotate the entire functions about the origin at angular frequency ω.

Proposition 2.14 *The operator e^{-itA} that gives the solution of the quantum harmonic oscillator equation is given in terms of rotation operators $R_{e^{-i\omega t}}$ by*

$$We^{-itA}\psi = e^{-i\frac{1}{2}\omega t}R_{e^{-i\omega t}}W\psi. \tag{107}$$

There is of course a corresponding result for the operators e^{-tA} that give the solution of the diffusion with removal equation. In this case the scalings are real scalings of the form $R_{e^{-\omega t}}$. The proof goes through for this case; at the end we can just replace t by it.

There are three change of variable operators that go into W. The first is multiplication by ϕ. First note that $\phi > 0$ is an eigenfunction of A with eigenvalue $\lambda = \frac{1}{2}\omega$. From this we can compute the corresponding forward diffusion with linear drift operator L^*. It is given by

$$-L^* = \frac{1}{2}\sigma^2\frac{\partial^2}{\partial x^2} + \omega\frac{\partial}{\partial x}x. \tag{108}$$

It describes the diffusion of a probability density when the drift toward the origin is $-\omega x$. It satisfies $\phi(A - \lambda I)\psi = L^*\phi\psi$ and hence $\phi e^{-tA}\psi = e^{-\lambda t}e^{-tL^*}\phi\psi$.

The next change of variable is from x to the Fourier transform variable z. Write $h = \phi\psi$. Say that $u(t) = e^{-tL^*}h$ is the solution of

$$\frac{\partial u}{\partial t} = -L^*u. \tag{109}$$

Take the Fourier transform

$$\hat{u}(z,t) = \int_{-\infty}^{\infty} e^{-izx}u(x,t)\,dy. \tag{110}$$

The equation becomes

$$\frac{\partial \hat{u}}{\partial t} + \omega z\frac{\partial \hat{u}}{\partial z} = -\frac{1}{2}\sigma^2 z^2\hat{u}. \tag{111}$$

It is convenient to make a third change of variable $w = \hat{g}(z)^{-1}\hat{u}$. The equation then becomes a conservation law

$$\frac{\partial w}{\partial t} + \omega z\frac{\partial w}{\partial z} = 0. \tag{112}$$

The solution of this equation may be found by integrating along the curves $dz/dt = \omega z$. These are the curves $z = e^{\omega t}z_0$. The solution is constant along such curves and hence is given by

$$w(z,t) = f(z_0) = f(e^{-\omega t}z). \tag{113}$$

This proves the result that the solution is given by scaling.

Next we work backward to compute the propagator. We have

$$\hat{u}(z,t) = \hat{g}(z)\hat{g}(e^{-t\omega}z)^{-1}\hat{h}(e^{-\omega t}z) = \hat{g}_{\sigma_t^2}(z)\hat{h}(e^{-\omega t}z), \tag{114}$$

where the variance parameter is

$$\sigma_t^2 = \frac{\sigma^2}{2\omega}(1 - e^{-2\omega t}). \tag{115}$$

Scaling and multiplication in the Fourier transform representation correspond to scaling and convolution in the x representation. So

$$(e^{-tL^*}h)(x) = \int_{-\infty}^{\infty} g_{\sigma_t^2}(x - y')h(e^{\omega t}y')e^{\omega t}\, dy' = \int_{-\infty}^{\infty} g_{\sigma_t^2}(x - e^{-\omega t}y)h(y)\, dy. \tag{116}$$

From this we can compute e^{-tA}. The result is the Mehler formula in the form $(e^{-tA}\psi)(x) = \int k_t(x, y)\psi(y)\, dy$, where

$$k_t(x, y) = \sqrt{\frac{\omega}{2\pi\sigma^2 \sinh(\omega t)}} \exp(-\frac{\omega}{2\sigma^2 \sinh(\omega t)}[\cosh(\omega t)(x^2+y^2)-2xy]). \tag{117}$$

As an immediate consequence we also have the corresponding Mehler formula for the propagator for the quantum harmonic oscillator.

We can also begin to see the spectral properties. If we compute the action of $R_{e^{-\omega t}}$ on z^n we get $e^{-n\omega t}z^n$. From this we see that the eigenvalues are are $e^{-n\omega t}$. Higher powers decay more rapidly. For the quantum mechanical problem the action of $R_{e^{-i\omega t}}$ on z^n gives $e^{-in\omega t}z^n$. In this case higher powers oscillate more rapidly.

Now we want to undo all these transformations. Back in the original Fourier transform representation we write the eigenfunctions as $(-iz)^n\hat{g}(z)$. (The $(-i)^n$ factor is put in to make the final formulas take on a somewhat more familiar form.) Back in x space this is $\left(-\frac{\partial}{\partial x}\right)^n \phi(x)^2$. This eigenfunction of e^{-tL^*} is a polynomial times a Gaussian. These polynomials are closely related to Hermite polynomials. Finally, we can go back to the original Hilbert space and the original e^{-tA}. The eigenvalues are $e^{-(n+\frac{1}{2})\omega t}$ and the eigenfunctions are $\chi_n(x) = \phi(x)^{-1}\left(-\frac{\partial}{\partial x}\right)^n \phi(x)^2$.

Finally, in order to get the spectral representation of the propagator, it is convenient to look at the operator $e^{-tL^*}\phi^2$, the composition of the e^{-tL^*} with multiplication by $\phi^2 = g$. The advantage of this operator is that it is self-adjoint. In the Fourier transform representation multiplication by $\phi^2 = g$ corresponds to convolution by $\hat{g}(z)$. An easy computation shows that in the Fourier transform representation $e^{-tL^*}\phi^2$ is an integral operator with kernel

$$\hat{r}(z, w) = \hat{g}(z)\hat{g}(e^{-\omega t}z)^{-1}\hat{g}(e^{-\omega t}z - w) = \hat{g}(z)e^{\frac{\sigma^2}{2\omega}e^{-\omega t}zw}\hat{g}(w). \tag{118}$$

Expand the exponential to get

$$\hat{r}(z, w) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\sigma^2}{2\omega}\right)^n (-iz)^n\hat{g}(z)e^{-n\omega t}(iw)^n\hat{g}(w). \tag{119}$$

Take the inverse Fourier transform. This leads to the conclusion that $e^{-tL^*}\phi^2$ is an integral operator with kernel

$$r(x, y) = \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{\sigma^2}{2\omega}\right)^n (-\frac{\partial}{\partial x})^n\phi(x)^2e^{-n\omega t}(-\frac{\partial}{\partial y})^n\phi(y)^2. \tag{120}$$

From this it is immediate that e^{-tA} is an integral operator with kernel

$$k_t(x,y) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{\sigma^2}{2\omega} \right)^n \chi_n(x) e^{-(n+\frac{1}{2})\omega t} \chi_n(y). \tag{121}$$

This leads immediately to the spectral formula for the propagator for the quantum harmonic oscillator.

3 Self-adjoint operators

3.1 Stone's theorem

This subsection features Stone's theorem, which gives a correspondence between one-parameter unitary groups satisfying a continuity condition and self-adjoint operators.

Consider a one-parameter group $t \mapsto U_t$ of unitary operators acting in the Hilbert space $\mathcal{H}$. Suppose also that it satisfies the continuity condition: for each vector ψ in the Hilbert space, the map $t \mapsto U_t\psi$ is continuous from the real line to the Hilbert space $\mathcal{H}$. Consider the linear subspace D of $\mathcal{H}$ of all ψ such that $t \mapsto U_t\psi$ is differentiable as a function from the real line to $\mathcal{H}$. Then it may be shown that D is dense in $\mathcal{H}$ and that U_t sends D to itself. Furthermore, there is a unique linear operator A defined on the domain D with values $\mathcal{H}$ satisfying the abstract Schrödinger equation

$$i\frac{dU_t\psi}{dt} = AU_t\psi. \tag{122}$$

Stone's theorem says that the operators A that arise in this way are precisely the self-adjoint operators, and that furthermore the self-adjoint operator A uniquely determines the unitary group U_t. In view of this result, it is natural to denote the unitary group determined by the self-adjoint operator A by $U_t = e^{-itA}$. It will turn out that this notion of exponential is compatible with the notion given by the spectral theorem.

An operator A is self-adjoint if it is equal to its adjoint A^*. The following is a description of the general notion of adjoint operator. Let $\mathcal{H}$ be a Hilbert space. Let $D(A)$ be a dense linear subspace of $\mathcal{H}$. Let $\mathcal{H}'$ be another Hilbert space, and let $A : D(A) \to \mathcal{H}'$ be a linear operator. Then A is said to have *adjoint* operator $A^* : D(A^*) \to \mathcal{H}$ with domain $D(A^*) \subseteq \mathcal{H}'$ if the following conditions are satisfied.

1. For every ϕ in $D(A^*)$ and ψ in $D(A)$ we have $\langle A^*\phi, \psi\rangle = \langle \phi, A\psi\rangle$.

2. If there are ϕ and χ such that for all ψ in $D(A)$ we have $\langle \chi, \psi\rangle = \langle \phi, A\psi\rangle$, then ϕ is in $D(A^*)$ and $A^*\phi = \chi$.

The notion of adjoint operator is fundamental in Hilbert space theory. Here are some examples. In the first two examples we must have $\mathcal{H}' = \mathcal{H}$. In the last two examples the domain is the entire Hilbert space.

- A is self-adjoint if $A^* = A$.
- E is an orthogonal projection if $E^* = E$ and $E^2 = E$.
- U is unitary if $U^* = U^{-1}$.

For another interesting example consider a vector χ in $\mathcal{H}$. It defines a linear transformation $z \mapsto z\chi$ from $\mathbf{C}$ to $\mathcal{H}$. It is natural to denote the adjoint transformation by χ^*. By the definition of adjoint $\langle \chi^* \phi, z \rangle = \langle \phi, z\chi \rangle = z\langle \phi, \chi \rangle = \overline{\langle \chi, \phi \rangle} z$. This proves that $\chi^* \phi = \langle \chi, \phi \rangle$. So χ^* is a linear transformation from $\mathcal{H}$ to $\mathbf{C}$.

The considerations are relevant to Stone's theorem. Suppose that A is self-adjoint, so the adjoint of A is A. Then the adjoint of $-iA$ is iA. This makes it plausible that the adjoint of e^{-itA} is e^{itA}, that is, the adjoint of U_t is $U_{-t} = U_t^{-1}$. In other word, each U_t is unitary. In fact, all of this is true, and the situation is summarized in the following theorem.

Theorem 3.1 (Stone's theorem) *Suppose there is a one-parameter unitary group $t \mapsto U_t$ that satisfies the continuity condition. Then there exists a unique self-adjoint operator A that generates this group via $U_t = e^{-itA}$. Conversely, each self-adjoint operator A determines a unique unitary group $U_t = e^{-itA}$ satisfying the continuity condition.*

This remarkable result is ample justification for the study of self-adjoint operators. In particular, it shows that any reasonable time dynamics for a quantum system must be given by a self-adjoint operator. See [7] for a proof.

3.2 Multiplication operators

Multiplication operators are simple and concrete, but they play a crucial role in operator theory. Suppose there is a space $L^2(K, \mu)$ consisting of functions that are square-integrable with respect to some measure. The measure might be continuous or discrete. In the continuous case we would write the square of the norm as

$$\|f\|^2 = \int |f(k)|^2 \, \mu(dk). \tag{123}$$

In the discrete case we would have

$$\|f\|^2 = \sum |f(k)|^2 \, \mu(\{k\}). \tag{124}$$

There is also the possibility of mixed situations involving part integral and part sum. The notion of integral encompasses all such cases.

Let α be a complex function on K. Then there is a corresponding operator mult_α that sends the function f in $L^2(K, \mu)$ to the pointwise product $\alpha \cdot f$. If α is a bounded function, then mult_α is defined on all functions in L^2. In general, mult_α is defined on the domain consisting of all f in L^2 such that $\alpha \cdot f$ is also in L^2.

Consider the complex conjugate function $\bar{\alpha}$. This also defines a multiplication operator $\text{mult}_{\bar{\alpha}}$ with the same domain. These two operators are adjoint; in particular $\langle \bar{\alpha} \cdot f, g \rangle = \langle f, \alpha \cdot g \rangle$. If α is a real function, then mult_α is self-adjoint. If α only takes on the values 0 and 1, then it is an orthogonal projection. If $|\alpha| = 1$, then mult_α is unitary.

We say that an operator A is isomorphic to another operator B if there is a Hilbert space isomorphism U such that $A = U^{-1}BU$. Note that in particular, U must be a bijection between the domain of A and the domain of B.

Proposition 3.1 *Every real multiplication operator is self-adjoint. As a consequence, every operator that is isomorphic to a real multiplication operator is self-adjoint.*

Here are some examples in the case when the Hilbert space is $L^2(\mathbf{R}, dx)$.

- The first order differential operator $-i\frac{\partial}{\partial x} = F^{-1}\text{mult}_k F$ is self-adjoint. Its role in quantum mechanics is that the operator $-i\hbar\frac{\partial}{\partial x}$ is isomorphic via the Fourier transform to multiplication by $p = \hbar k$. This is the momentum operator.

- The second order differential operator $-\frac{\partial^2}{\partial x^2} = F^{-1}\text{mult}_{k^2} F$ is self-adjoint. This is the square of the operator in the first example. Its role in quantum mechanics is that the operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is isomorphic via the Fourier transform to multiplication by $\frac{p^2}{2m}$. This is the kinetic energy operator.

- Let $v(x)$ be a real function on the line. Then $\text{mult}_{v(x)}$ is a self-adjoint operator. This may be thought of as a potential energy operator. Often it is denoted more briefly as $v(x)$.

- The operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$ is an operator for the total energy of the quantum harmonic oscillator. We have seen that it isomorphic to multiplication by $(n + \frac{1}{2})\hbar\omega$ on a weighted ℓ^2 space of sequences.

The last example is a special case of the Schrödinger operator

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v(x). \tag{125}$$

This is the total energy operator in quantum mechanics. In general it is a difficult problem to know whether or not this operator is self-adjoint. One way to prove that such an operator is self-adjoint would be to find an explicit isomorphism with a multiplication operator. However is usually impossible to accomplish. For instance, if $v(x) = \lambda x^4$ with $\lambda > 0$, then the operator is self-adjoint, but it requires heroic effort to get even partial information about an isomorphism with a multiplication operator. In the case $\lambda < 0$, there is no unambiguous definition as self-adjoint operator, because such a definition would require a choice of boundary conditions at $x = \pm\infty$.

3.3 The spectral theorem

The spectral theorem says that every self-adjoint operator is A is isomorphic to an operator that is multiplication by a real function. Here we state and explain this result. See [7] for a succinct proof.

Theorem 3.2 (Spectral theorem) *Suppose A is a self-adjoint operator acting in a Hilbert space $\mathcal{H}$. Then there is a space $L^2(K,\mu)$, an isomorphism $U : \mathcal{H} \to L^2(K,\mu)$, and a real measurable function α such that*

$$A = U^{-1}\mathrm{mult}_\alpha U. \tag{126}$$

More specifically, if ψ is in $\mathcal{H}$, then ψ is in the domain $D(A)$ of A if and only if $\alpha \cdot U\psi$ is in $L^2(K,\mu)$, and in this case

$$(UA\psi)(k) = \alpha(k)(U\psi)(k). \tag{127}$$

An isomorphism that makes A into a multiplication operator is called a *spectral representation*. A spectral representation is not unique. One way to get a new one is to make a change of labeling. For example, suppose that $g : K' \to K$ is a measure space isomorphism that carries the measure μ' to the measure μ. Define an isomorphism $W : L^2(K,\mu) \to L^2(K',\mu')$ by $(Wf)(k') = f(g(k'))$. Similarly, define a new multiplication operator by $\alpha'(k') = \alpha(g(k'))$. Then $WU : \mathcal{H} \to L^2(K',\mu')$ defines a new spectral representation that makes A isomorphic to multiplication by α'.

Another way to get a new spectral representation is to change the measure via a density. Say that ρ is a measurable function such that $\rho(k) > 0$ for all k. Define a new measure $\tilde{\mu}$ by

$$\int h(k)\,\tilde{\mu}(dk) = \int h(k)\rho(k)\,\mu(dk). \tag{128}$$

Define a Hilbert space isomorphism $R : L^2(K,\mu) \to L^2(K,\tilde{\mu})$ by $(Rf)(k) = \rho(k)^{-\frac{1}{2}} f(k)$. Then $RU : \mathcal{H} \to L^2(K,\tilde{\mu})$ defines a new spectral representation that makes A isomorphic to multiplication by α.

The power of the spectral theorem is that it permits taking functions of a self-adjoint operator. Let f be a complex function on the line. Then $f(A)$ is defined as the operator that has spectral representation given by multiplication by $f(\alpha)$. It may be proved that this definition of a function of A is independent of the spectral representation. Here is an important special case. It is the part of Stone's theorem that says that a self-adjoint operator determines a unitary group.

Proposition 3.2 *Let A be a self-adjoint operator. Then $U_t = e^{-itA}$ as defined by the spectral theorem is a one-parameter unitary group.*

The proof is to note that $U_t = e^{-itA}$ is isomorphic to multiplication by $e^{-it\alpha}$, which is unitary for each real t. Furthermore, the continuity condition is

satisfied: for each vector ψ the map $t \mapsto U_t\psi$ is continuous. This continuity condition is not difficult to prove from the spectral representation by an application of the dominated convergence theorem.

Let A be a self-adjoint operator. Suppose that S is a subset of the line, and 1_S is the indicator function of this set. Then $1_S(A)$ is a well-defined self-adjoint operator, called the *spectral projection* of A corresponding to the subset S. We say that λ is in the *spectrum* of A if for every $\epsilon > 0$ the projection $1_{(\lambda-\epsilon,\lambda+\epsilon)}(A)$ is a non-zero projection. We say that λ is in the *point spectrum* of A if $1_{\{\lambda\}}(A)$ is a non-zero projection. If λ is in the point spectrum of A, then λ is an eigenvalue of A, and $1_{\{\lambda\}}(A)$ projects onto the corresponding eigenspace. Finally, we say that λ is in the *continuous spectrum* of A if λ is in the spectrum but not in the point spectrum. Here are examples.

- The first order differential operator $-i\frac{\partial}{\partial x} = F^{-1}\mathrm{mult}_k F$ has the same spectrum as mult_k. This is continuous spectrum including all of $\mathbf{R}$. The same is true for the momentum operator $-i\hbar\frac{\partial}{\partial x}$ isomorphic to multiplication by $p = \hbar k$.

- The second order differential operator $-\frac{\partial^2}{\partial x^2} = F^{-1}\mathrm{mult}_{k^2} F$ has the same spectrum as mult_k^2. This is continuous spectrum constituting the semi-infinite interval $[0, +\infty)$. The same is true for the kinetic energy operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ isomorphic to multiplication by $\frac{p^2}{2m}$.

- Let $v(x)$ be a real function on the line. Then $\mathrm{mult}_{v(x)}$ is a self-adjoint operator. Its spectrum is the essential range of the function v. The spectrum may be a combination of continuous and point spectrum. The point spectrum would corresponding to portions of the graph of $v(x)$ that are flat. The values at such points are eigenvalues of infinite multiplicity.

- The harmonic oscillator total energy operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2$ has the same spectrum as multiplication by the diagonal operator with entries $(n + \frac{1}{2})\hbar\omega$ on a weighted ℓ^2 space of sequences. This is point spectrum, eigenvalues of multiplicity one.

3.4 Spectral measures

Consider a self-adjoint operator A and a state vector ψ (a unit vector in the Hilbert space). The spectral theorem provides a unitary operator $U : \mathcal{H} \to L^2(K, \mu)$ and a real function α defined on a space K equipped with a measure μ. Furthermore, the measure $|(U\psi)(k)|^2\mu(dk)$ is a probability measure on K. Thus α is a *random variable* in the standard sense of mathematical probability theory, that is, a real function defined on a probability space.

As usual, the random variable has a *distribution* ν, a measure on the real line. This is defined by requiring that for each bounded real function h on the line the corresponding expectation is

$$\int h(\alpha(k))|(U\psi)(k)|^2\,\mu(dk) = \int_{-\infty}^{\infty} h(x)\,\nu(dx). \tag{129}$$

In other words, it is the image of the probability measure $|(U\psi)(k)|^2\,\mu(dk)$ under α.

The distribution may also be called a spectral measure, since it is non-zero only on the essential range of α, which is the spectrum of A. Since $h(A)$ is a well-defined self-adjoint operator, the expectation with respect to this distribution may be written in Hilbert space language as

$$E_\psi[h(A)] = \langle \psi, h(A)\psi\rangle = \int \overline{(U\psi)(k)} h(\alpha(k))(U\psi)(k)\,\mu(dk) = \int_{-\infty}^{\infty} h(x)\,\nu(dx). \tag{130}$$

Say that ψ is in the operator domain $D(A)$ of A. Then we can define the expectation (mean) and second moment of A. Thus

$$E_\psi[A] = \langle \psi, A\psi\rangle = \int \alpha(k)|(U\psi)(k)|^2\,\mu(dk) = \int_{-\infty}^{\infty} x\,\nu(dx). \tag{131}$$

and

$$E_\psi(A^2) = \|A\psi\|^2 = \int \alpha(k)^2|(U\psi)(k)|^2\,\mu(dk) = \int_{-\infty}^{\infty} x^2\,\nu(dx).. \tag{132}$$

Then as usual the variance is given by

$$(\Delta A)_\psi^2 = E_\psi[(A - E_\psi[A])^2] = E_\psi[A^2] - E_\psi[A]^2. \tag{133}$$

The second moment is an upper bound for the variance. The standard deviation is defined as the square root of the variance.

Define the form domain $Q(A) = D(|A|^{\frac{1}{2}})$. We have $D(A) \subseteq Q(A)$, but in general the form domain is larger. Then for ψ in the form domain of A we can at least define the expectation (mean) by

$$E_\psi[A] = \langle \psi, A\psi\rangle = \int \alpha(k)|U\psi(k)|^2\,\mu(dk) = \int x\,\nu(dx). \tag{134}$$

Strictly speaking, the notation $\langle \psi, A\psi\rangle$ should be interpreted as $\langle |A|^{\frac{1}{2}}\psi, \mathrm{sign}(A)|A|^{\frac{1}{2}}\psi\rangle$. In a similar way we can define the form $\langle \chi, A\psi\rangle$ for χ and ψ each in $Q(A)$. Again $\langle \chi, A\psi\rangle$ means $\langle |A|^{\frac{1}{2}}\chi, \mathrm{sign}(A)|A|^{\frac{1}{2}}\psi\rangle$.

3.5 Generalized vectors

Generalized vectors give another perspective on the unitary operators that occur in spectral representations. Here is a brief account. Consider an isomorphism $U : \mathcal{H} \to L^2(K, \mu)$. Choose a vector ψ in $\mathcal{H}$. For each point k in the set K there is an evaluation $(U\psi)(k)$ that is defined for almost every k in K. With some optimism one may hope that the exceptional set may be taken independent of ψ, so that the map $\psi \mapsto (U\psi)(k)$ is defined for almost every k and is linear in ψ. In general this map will not be continuous in ψ. In this circumstance, it is convenient to write the linear functional in the form

$$(U\psi)(k) = \langle \phi_k, \psi\rangle. \tag{135}$$

In the case when the map is not continuous the ϕ_k will not be given by vectors in the Hilbert space $\mathcal{H}$, and the inner product is not the usual inner product in this space.

Here is a framework that makes sense of this notation. The vectors ψ belongs to some smaller Hilbert space $\mathcal{H}_+ \subseteq \mathcal{H}$ that is dense in $\mathcal{H}$, and the ϕ_k belong to some larger Hilbert space $\mathcal{H}_-$ with $\mathcal{H} \subseteq \mathcal{H}_-$ and in which $\mathcal{H}$ is dense. The pairing between $\mathcal{H}_-$ and $\mathcal{H}_+$ given by the brackets is conjugate linear in the first variable and linear in the second variable, and it coincides with the usual inner product on pairs taken from $\mathcal{H}$.

Here is an example that is common when dealing with Schrödinger operators. Let $\rho > 0$ be a bounded real function with finite integral over the line. The smaller Hilbert space is $\mathcal{H}_+ = L^2(\mathbf{R}, \rho(x)^{-1}\, dx)$, the original Hilbert space is $\mathcal{H} = L^2(\mathbf{R}, dx)$, while the bigger Hilbert space is $\mathcal{H}_- = L^2(\mathbf{R}, \rho(x)\, dx)$. If ϕ is in $\mathcal{H}_-$ and ψ is in $\mathcal{H}_+$, then the pairing that agrees with the usual inner product on $\mathcal{H}$ is $\langle \phi, \psi \rangle$. Since this may also be written in terms of an $\mathcal{H}$ inner product as $\langle \rho^{\frac{1}{2}} \phi, \rho^{-\frac{1}{2}} \psi \rangle$, it follows from the Schwarz inequality that it is finite.

A classic example where this choice of Hilbert spaces works is for the Schrödinger operator for free motion. Then the spectral representation is given by the Fourier transform. The ϕ_k in this case is the function $\phi_k(x) = e^{ikx}$. This is not in $\mathcal{H}$, but it is in $\mathcal{H}_-$. Furthermore, the Fourier transform is determined by the condition that

$$(F\psi)(k) = \langle \phi_k, \psi \rangle = \int_{-\infty}^{\infty} e^{-ikx} \psi(x)\, dx \tag{136}$$

for all ψ in $\mathcal{H}_+$.

One common use of this notation is to express quantities like

$$\langle \chi, \psi \rangle = \int \overline{(U\chi)(k)} (U\psi)(k)\, \mu(dk). \tag{137}$$

or

$$\langle \chi, A\psi \rangle = \int \overline{(U\chi)(k)} \alpha(k) (U\psi)(k)\, \mu(dk) \tag{138}$$

or

$$\langle \chi, e^{-itA} \psi \rangle = \int \overline{(U\chi)(k)} e^{-it\alpha(k)} (U\psi)(k)\, \mu(dk) \tag{139}$$

It is reasonable to write $\langle \chi, \phi_k \rangle$ for the complex conjugate of $\langle \phi_k, \chi \rangle$. Then the equations become

$$\langle \chi, \psi \rangle = \int \langle \chi, \phi_k \rangle \langle \phi_k, \psi \rangle\, \mu(dk). \tag{140}$$

or

$$\langle \chi, A\psi \rangle = \int \langle \chi, \phi_k \rangle \alpha_k \langle \phi_k, \psi \rangle\, \mu(dk) \tag{141}$$

or

$$\langle \chi, e^{itA} \psi \rangle = \int \langle \chi, \phi_k \rangle e^{-it\alpha_k} \langle \phi_k, \psi \rangle\, \mu(dk) \tag{142}$$

It is also reasonable to introduce that notation ϕ_k^* for the possibly discontinuous linear map $\psi \mapsto \langle \phi_k, \psi \rangle$. One can then identify ϕ_k with the complex conjugate of this map, so $\chi \mapsto \langle \chi, \phi_k \rangle = \overline{\langle \phi_k, \chi \rangle}$ is conjugate linear. The identity

$$\langle \chi, U^{-1} f \rangle = \int \langle \chi, \phi_k \rangle f(k) \, \mu(dk) \tag{143}$$

suggests writing

$$U^{-1} f = \int \phi_k f(k) \, \mu(dk). \tag{144}$$

If one is willing to interpret the expressions in a suitable weak form, then one can write the spectral theorem is the particularly succinct form

$$A = \int \phi_k \alpha_k \phi_k^* \, \mu(dk). \tag{145}$$

The propagator also has a expression

$$e^{-itA} = \int \phi_k e^{-it\alpha_k} \phi_k^* \, \mu(dk). \tag{146}$$

With the appropriate interpretation, this last formula is true in complete generality, and furthermore it is simple enough to be memorable. However, it should be remembered that it is just a summary of a statement about composition of unitary maps.

The generalized vectors ϕ_k are mathematical objects that one can study in their own right. They belong to a larger Hilbert space $\mathcal{H}_-$ that includes $\mathcal{H}$? How small can this space be and still be large enough to include these generalized vectors? See [2] for a possible answer. (It is sufficent that the injections from $\mathcal{H}_+$ to $\mathcal{H}$ and from $\mathcal{H}$ to $\mathcal{H}_-$ be Hilbert-Schmidt operators, but in specific cases it is often possible to make do with a weaker condition.)

In theoretical work it may not be necessary to make explicit use of generalized vectors, and it may even be clumsy to do so. All that is needed for quantum theory is the isomorphism U from $\mathcal{H}$ to the Hilbert space to L^2 and its inverse U^{-1}. The generalized vectors are hidden within the definition of each particular U, and they often need not be isolated as individual objects.

3.6 Dirac notation

The Dirac notation is a clever way of denoting vectors and generalized vectors. Consider an isomorphism $U : \mathcal{H} \to L^2(K, \mu)$. One can think of the set K as a set of labels. Implicitly, one assumes that different spectral representations involve different label sets. In the Dirac notation one writes

$$(U\psi)(k) = \langle k \mid \psi \rangle. \tag{147}$$

It is natural to define $\langle \chi \mid k \rangle = \overline{\langle k \mid \chi \rangle}$. Then in the Dirac notation

$$\langle \chi, \psi \rangle = \int \langle \chi \mid k \rangle \langle k \mid \psi \rangle \, \mu(dk). \tag{148}$$

and

$$\langle \chi, A\psi \rangle = \int \langle \chi \mid k \rangle \alpha_k \langle k \mid \psi \rangle \, \mu(dk). \tag{149}$$

Sometimes one encounters expressions like $\langle k \mid$ in isolation. It is clear what this means: it is a possibly discontinuous linear mapping from vectors ψ to scalars given by $\langle k \mid \psi \rangle = (U\psi)(k)$. Similarly, $\mid k \rangle$ is the corresponding conjugate linear map given by complex conjugation of the linear map. In this spirit, sometimes one sees expressions like

$$I = \int \mid k \rangle \langle k \mid \, \mu(dk). \tag{150}$$

and

$$A = \int \mid k \rangle \alpha_k \langle k \mid \, \mu(dk). \tag{151}$$

One can also write

$$U^{-1} f = \int \mid k \rangle f(k) \, \mu(dk). \tag{152}$$

Consider another spectral representation given by $(V\psi)(\ell) = \langle \ell \mid \psi \rangle$. The composition VU^{-1} is given by

$$(VU^{-1} f)(\ell) = \int \langle \ell \mid k \rangle f(k) \, \mu(dk). \tag{153}$$

The expression $\langle \ell \mid k \rangle$ is called a *bracket*. In general it is not a function, but some kind of generalized function. The standard terminology in physics is that $\langle \ell \mid$ is called a *bra*, and $\mid k \rangle$ is called a *ket*. Sometimes a ket is thought of as a generalized vector, as suggested by the expression for $U^{-1} f$ above, which writes a vector as a superposition of kets.

Here are some examples. In the Dirac notation the inverse Fourier transform might be written

$$\langle x \mid \psi \rangle = \int_{-\infty}^{\infty} \langle x \mid k \rangle \langle k \mid \psi \rangle \frac{dk}{2\pi}. \tag{154}$$

Here ψ is a vector in some abstract Hilbert space, $\langle x \mid \psi \rangle$ is its representation as a function of position x, and $\langle k \mid \psi \rangle$ is its representation as a function of wave number k. The bracket $\langle x \mid k \rangle$ is just another notation for the e^{ikx} factor that gives the transformation between wave number and position representations. It is possible to distinguish x values from k values because they have different units.

Another common situation is when a vector ψ is representented by coefficients in terms of an orthonormal basis ϕ_n, where n runs over some index set. The coefficients are $\langle n \mid \psi \rangle = \langle \phi_n, \psi \rangle$. Since $\langle \psi \mid n \rangle = \langle \psi, \phi_n \rangle$, it is natural to identify the ket $\mid n \rangle$ with the unit vector ϕ_n. So the expansion of the vector is

$$\psi = \sum_n \mid n \rangle \langle n \mid \psi \rangle. \tag{155}$$

If we wanted this in the position representation, it would become

$$\langle x \mid \psi \rangle = \sum_n \langle x \mid n \rangle \langle n \mid \psi \rangle. \tag{156}$$

While in an example like the last one the ket $\mid n\rangle$ is a normalized basis vector, this is not the only possible situation. In fact, the wave number ket $\mid k\rangle$ is given in the position representation by the function $x \mapsto e^{ikx}$, which is not even in the Hilbert space L^2. This corresponds to the fact that the map $\psi \mapsto \langle k \mid \psi \rangle$ given by the corresponding bra is not continuous as a function on the Hilbert space $\mathcal{H}$. Ultimately, this is because the value of the Fourier transform of a function at a point is not continous as a function on L^2.

The clever feature of the Dirac notation is the use of the label set for the representation to denote various kinds of vectors and generalized vectors. However, the only place in science where the Dirac notation is in common use is in quantum theory, and it is not necessary even there.

3.7 Spectral representation for multiplicity one

The spectral theorem as stated above is somewhat mysterious, since there are many possible spectral representations. It would be nice to find a standard form for a spectral representation. This would also shed light on how one could prove the spectral theorem: construct the standard representation explicitly.

Let A be a self-adjoint operator and let $U_t = e^{-itA}$ be the corresponding unitary group. We say that the unit vector ψ is a *cyclic vector* if the smallest closed subspace that contains all $U_t\psi$ is the whole Hilbert space $\mathcal{H}$.

Not every self-adjoint operator has a cyclic vector. However, there is the following decomposition into cyclic subspaces.

Proposition 3.3 *Let A be a self-adjoint operator acting in $\mathcal{H}$. Then $\mathcal{H}$ is an orthogonal direct sum of closed subspaces $\mathcal{H}_j$ that are each invariant under the unitary operators e^{-itA}. Furthermore, the subspaces may be chosen so that there are vectors ψ_j in $\mathcal{H}_j$ that are cyclic for these restrictions.*

The proof of this proposition is easy. Choose an arbitrary unit vector ψ_1 and consider the smallest closed subspace $\mathcal{H}_1$ with ψ_1 in it and invariant under the e^{-itA}. The orthogonal complement of $\mathcal{H}_1$ is also invariant under the e^{-itA}. If this orthogonal complement is not the zero subspace, choose ψ_2 in the orthogonal complement. Let $\mathcal{H}_2$ be the smallest closed subspace of the orthogonal complement with ψ_2 in it and invariant under the e^{-itA}. Continue in this way until the result is a maximal family of non-zero cyclic subspaces. These will automatically span the entire Hilbert space.

From now on we focus on finding a standard form associated with the self-adjoint operator A and the cyclic vector ψ. Actually, we shall describe two standard forms. Here is the first.

Proposition 3.4 *Consider a self-adjoint operator with a unit cyclic vector ψ. Then there is a spectral representation $W : \mathcal{H} \to L^2(\mathbf{R}, \nu)$. Here ν is the*

probability measure that is the distribution associated with ψ and A. The spectral representation is determined by the requirement that $(We^{-itA}\psi)(x) = e^{-itx}$. The operator that represents A is multiplication by x.

There is a characterization of measures associated with the real line. Here is a brief review. As always, we consider subsets and functions to be measurable (Borel measurable) by default. We consider measures defined on subsets of the line that are finite on bounded intervals. Thus each subset $B \subseteq \mathbf{R}$ has a measure $\nu(B) \geq 0$. The assignment of measures satisfies the usual requirements from measure theory.

Every such measure is given by a function F that is increasing and right continuous. To say that F is increasing is to say that $x \leq y$ implies $F(x) \leq F(y)$. (In some accounts this is called non-decreasing.) To say that F is right-continuous is to say that the right hand limit $\lim_{x \downarrow a} F(x) = F(a)$. We can write this more succinctly as $F(x+) = F(x)$. The measure of a subset $(a, b] \subseteq \mathbf{R}$ is given by the difference $\nu((a, b]) = F(b) - F(a)$. The function F associated with ν is determined up to an arbitrary constant. Once one has specified the measure on such special subsets, then it is determined for all subsets. In particular, for a single point $\nu(\{b\}) = F(b) - F(b-)$. Once the measure is available, there is also a corresponding integral defined for bounded functions g by

$$\int_{-\infty}^{\infty} g(x)\, \nu(dx) = \int_{-\infty}^{\infty} g(x)\, dF(x). \tag{157}$$

In the special case when the measure of the whole real line $\nu(\mathbf{R}) = 1$, the measure is a probability measure, the corresponding integral is the expectation, and there is a choice of the arbitrary constant so that the function F takes values in the unit interval. For the moment continue to consider the general case.

The function F may have both flat places and jumps, but nevertheless it has a kind of inverse. Let I be the open interval from $\inf F$ to $\sup F$. For y in I define

$$G(y) = \sup\{x \mid F(x) < y\}. \tag{158}$$

Then G is increasing and left continuous. Furthermore, $a < G(y) \leq b$ is equivalent to $F(a) < y \leq F(b)$.

This allows a remarkable representation of the measure ν in terms of Lebesgue measure λ on the interval I. We have

$$\nu((a, b]) = F(b) - F(a) = \lambda(\{y \mid F(a) < y \leq F(b)\}) = \lambda(\{y \mid a < G(y) \leq b\}). \tag{159}$$

It then follows that

$$\nu(B) = \lambda(\{y \mid G(y) \in B\}). \tag{160}$$

In addition, it may be shown that

$$\int_{-\infty}^{\infty} h(x)\, \nu(dx) = \int_I h(G(y))\, dy. \tag{161}$$

In other words, every Lebesgue-Stieltjes measure on the real line is the image of Lebesgue measure on an interval by some increasing function G.

This representation is not a perfect correspondence between measures, since a point measure at a discontinuity of F corresponds to Lebesgue measure on a subinterval of I. However consider the case when F is continuous. Then this is not an issue. There is also no problem with places where F is flat, since these are places where the measure is zero, and these correspond to single points in I, which have Lebesgue measure zero. So in this case the two measure spaces (the real line $\mathbf{R}$ with ν and the interval I with Lebesgue measure ν) are in quite natural correspondence.

Proposition 3.5 *Consider a self-adjoint operator A with a unit cyclic vector ψ. Suppose A only has continuous spectrum. Then there is a spectral representation $U : \mathcal{H} \to L^2(I, \lambda)$. Here I is the unit interval, and λ is Lebesgue measure. Let F be the increasing right-continuous function associated with the spectral measure. Let G be the inverse function (taken in the above sense) of F. The spectral representation is determined by the requirement that $(Ue^{-itA}\psi)(y) = e^{-itG(y)}$. The operator that represents A is multiplication by $G(y)$.*

The meaning of this result is the following. If we consider self-adjoint operators with a cyclic vector (which implies spectral multiplicity one), then we have only two kinds of spectral representation. We have point spectrum with distinct eigenvalues; the spectral representation is given by eigenvectors in the Hilbert space. Or we have continuous spectrum; the spectral representation is given by Lebesgue measure on an interval (which may be taken to be the unit interval). In the continuous spectrum case, the operator itself is represented by multiplication by an increasing real function γ. The spectrum of the operator is the essential range of γ. The distribution in a state is a probability measure on the spectrum. It is a continuous measure that may be rather complicated, depending on how complicated the function γ is.

3.8 Form sums and Schrödinger operators

Stone's theorem implies that a self-adjoint Schrödinger operator generates a quantum dynamics, but how does one show that a Schrödinger operator is self-adjoint? One method might be to write the Schrödinger total energy operator as the sum of a kinetic energy operator and a potential energy operator. Each of these has an explicit spectral representation that exhibits it as a self-adjoint operator. So all that is required is a mechanism of showing that the sum of two self-adjoint operators is self-adjoint. This is not true in general for unbounded self-adjoint operators, but when the operators are both positive there is no problem. This observation gives a very general way of determining a quantum dynamics.

There is another way to think of this issue. How could the sum of kinetic and potential energies fail to determine the dynamics? The kinetic energy (which is positive) could rush to plus infinity while the potential energy could rush to

minus infinity, and after a finite time there could be some kind of catastrophe. However, if the potential energy is positive, or even bounded below, then this cannot happen. The following discussion presents the details of this argument.

Suppose that A is a self-adjoint operator. Then it is a linear transformation from the dense linear subspace $D(A) \subseteq \mathcal{H}$ to $\mathcal{H}$. Consider $D(A)$ with a new Hilbert space inner product given by

$$\langle \phi, \chi \rangle_{(2)} = \langle A\phi, A\chi \rangle + \langle \phi, \chi \rangle. \tag{162}$$

The norm is given by

$$\|\phi\|^2_{(2)} = \|A\psi\|^2 + \|\psi\|^2. \tag{163}$$

This Hilbert space has a very different character from the original Hilbert space. From the point of view of the spectral theorem, the norm in this Hilbert space is related to the second moment of the random variable.

As an example, consider the Hilbert space $L^2(\mathbf{R}, dx)$ with the usual inner product. Let $A = -\frac{\partial^2}{\partial x^2}$. In the Fourier transform representation this becomes multiplication by k^2. So the (2)-norm in this case is given by

$$\|\psi\|^2_{(2)} = \|\frac{\partial^2 \psi(x)}{\partial x^2}\|^2 + \|\psi\|^2 = \|k^2 \hat{\psi}(k)\|^2 + \|\psi(k)\|^2. \tag{164}$$

Suppose that A is a positive self-adjoint operator. Then it defines a positive quadratic form on the form domain $Q(A) = D(A^{\frac{1}{2}})$. This includes the operator domain $D(A)$, but for an unbounded operator it is strictly larger. Consider the corresponding bilinear form $\langle A^{\frac{1}{2}}\chi, A^{\frac{1}{2}}\psi \rangle$, defined for χ and ψ in $Q(A)$. Henceforth this will be written in the more attractive form $\langle \chi, A\psi \rangle$. In the same spirit, the corresponding quadratic form satisfies $0 \leq \langle \psi, A\psi \rangle < \infty$ for ψ in $Q(A)$.

Consider $Q(A)$ with the new Hilbert space inner product

$$\langle \phi, \chi \rangle_{(1)} = \langle \phi, A\chi \rangle + \langle \phi, \chi \rangle. \tag{165}$$

The norm is given by

$$\|\phi\|^2_{(1)} = \|A^{\frac{1}{2}}\psi\|^2 + \|\psi\|^2. \tag{166}$$

From the point of view of the spectral theorem, the norm in this Hilbert space is related to the first moment of the corresponding random variable.

As an example, consider the Hilbert space $L^2(\mathbf{R}, dx)$ with the usual inner product. Let $A = -\frac{\partial^2}{\partial x^2}$. In the Fourier transform representation this becomes multiplication by k^2. So the (1)-norm in this case is given by

$$\|\psi\|^2_{(1)} = \|\frac{\partial \psi(x)}{\partial x}\|^2 + \|\psi\|^2 = \|k \hat{\psi}(k)\|^2 + \|\psi(k)\|^2. \tag{167}$$

Theorem 3.3 (Form representation theorem) *Let $\mathcal{H}$ be a Hilbert space. Let $a(\phi, \chi)$ be a positive form defined on a dense linear subspace $\mathcal{H}_{(1)} \subseteq \mathcal{H}$. Suppose that with the inner product*

$$\langle \phi, \chi \rangle_{(1)} = a(\phi, \chi) + \langle \phi, \chi \rangle \tag{168}$$

the space $\mathcal{H}_{(1)}$ is a Hilbert space. Then there is a unique positive self-adjoint operator A such that $\mathcal{H}_{(1)} = Q(A)$ and $a(\phi, \chi) = \langle \phi, A\chi \rangle$.

The form representation theorem gives a particularly simple way of constructing self-adjoint operators. Say that A and B are self-adjoint operators. In general it is not clear that the sum $A + B$ makes sense. However, if A and B are both positive, then in very general circumstances one can use the form representation theorem to define $A + B$ as a self-adjoint operator.

Theorem 3.4 (Positive form sum theorem) *Suppose that A and B are positive self-adjoint operators. Suppose that $Q(A) \cap Q(B)$ is dense in $\mathcal{H}$. Then there is a unique positive self-adjoint operator $A + B$ whose form is the sum of the forms of A and B.*

This form sum result has a simple generalization to self-adjoint operators that are bounded below. One simply has to add appropriate constants to reduce this case to the case of positive self-adjoint operators.

Here is an application to quantum mechanics. Consider the Hilbert space $\mathcal{H} = L^2(\mathbf{R}, dx)$ with the usual Lebesgue measure. Let P be the *momentum operator*. This is isomorphic via the Fourier transform to multiplication by $p = \hbar k$. So P has the simple explicit form

$$P = -i\hbar \frac{\partial}{\partial x}. \tag{169}$$

The *kinetic energy operator* is

$$H_0 = \frac{1}{2m} P^2. \tag{170}$$

Then H_0 is isomorphic in the Fourier transform representation to multiplication by $\frac{1}{2m} p^2 = \frac{\hbar^2}{2m} k^2$. It has the explicit form

$$H_0 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}. \tag{171}$$

The form of H_0 for ψ in $Q(H_0) = D(P)$ is

$$\langle \chi, H_0 \psi \rangle = \frac{1}{2m} \langle P\chi, P\psi \rangle = \frac{\hbar^2}{2m} \int \overline{\frac{\partial}{\partial x} \chi(x)} \frac{\partial}{\partial x} \psi(x)\, dx. \tag{172}$$

The derivative may be defined by the Fourier transform. This implies that $\psi(x)$ is an absolutely continuous function, that is, an indefinite integral of another function, and that both ψ and $\partial\psi/\partial x$ are in $L^2(\mathbf{R})$.

Let the *position operator* Q be multiplication by x. If v is a real function on the line, define the *potential energy operator* V to be the operator $v(Q)$. This is multiplication by $v(x)$, and so it is also a self-adjoint operator. The form of V is defined for ψ in $Q(V)$ by

$$\langle \chi, V\psi \rangle = \int \overline{\chi(x)} v(x) \psi(x)\, dx. \tag{173}$$

Suppose that v is positive (or more generally, bounded below). The total energy is

$$H = H_0 + V = \frac{P^2}{2m} + v(Q) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + v(x). \tag{174}$$

To use the method of form sums find a condition that guarantees that $Q(H_0) \cap Q(V)$ is dense in $L^2(\mathbf{R})$. For instance, take the dense set to be smooth functions with compact support. These are clearly in $Q(H_0)$. If v is locally integrable, then they are also in $Q(V)$. This proves the following result.

Proposition 3.6 *Suppose that $v(x)$ is bounded below and locally integrable. Then the Schrödinger operator $H = \frac{P^2}{2m} + v(Q)$, defined as a form sum, is a well-defined self-adjoint operator.*

One consequence of this result is that the unitary operator $e^{\frac{-itH}{\hbar}}$ is a well-defined unitary evolution that gives a solution of the Schrödinger equation. For more on form sums see the treatise [6]. The book [8] give many applications to quantum mechanics. For a brief account see [3].

4 The role of Planck's constant

4.1 The uncertainty principle

The Heisenberg uncertainty principle is perhaps the most famous assertion of quantum mechanics. In this subsection we shall see that this principle, interpreted suitably, has important physical interpretations. In particular, it shows that in some circumstances negative singularities of the potential energy are completely harmless.

There is particularly simple and symmetric mathematical formulation of the uncertainty principle that makes it an elementary result of Fourier analysis. This is not a strong enough version of the principle to give the desired physical result, but it is a place to start.

Proposition 4.1 (Heisenberg uncertainty principle) *For every unit vector ψ the standard deviations of position and wave number satisfy the inequality*

$$(\Delta x)_\psi (\Delta k)_\psi \geq \frac{1}{2}. \tag{175}$$

Since in quantum mechancs the position Q is multiplication by x and the momentum P is given in the Fourier transform representation by multiplication by $p = \hbar k$, the principle also takes the form

$$(\Delta Q)_\psi (\Delta P)_\psi \geq \frac{\hbar}{2}. \tag{176}$$

The Heisenberg uncertain principle is a standard result. It is a consequence of a simple identity together with the Cauchy-Schwarz inequality. However there is another, closely related, uncertainty principle that is just as simple but much more powerful in its physical applications.

Proposition 4.2 (Local uncertainty principle) *For every unit vector ψ the corresponding position probability density satisfies*

$$\sup_x |\psi(x)|^2 \leq (\Delta k)_{\hat{\psi}}. \tag{177}$$

In quantum mechanics this implies that the expectation of a function $v(Q)$ of position satisfies

$$\pm E_\psi[v(Q)] \leq \left(\int_{-\infty}^{\infty} |v(x)|\, dx \right) \frac{1}{\hbar} (\Delta P)_\psi. \tag{178}$$

The idea of this result is that concentration in momentum implies spread in position. The spread in position is in a very strong sense: the position probability density near every given point is small. It is proved at the end of this subsection.

For every $a > 0$ there is an estimate

$$(\Delta P)_\psi \leq E_\psi[P^2]^{\frac{1}{2}} \leq \frac{1}{2a} E_\psi[P^] + \frac{a}{2}. \tag{179}$$

This shows that in every state the expected potential energy is bounded by

$$\pm \langle \psi, v(Q)\psi \rangle \leq \left(\int_{-\infty}^{\infty} |v(x)|\, dx \right) \frac{1}{\hbar} \left[\frac{1}{2a} \langle \psi, P^2 \psi \rangle + \frac{a}{2} \right]. \tag{180}$$

An appropriate choice of a leads to the following lower bound.

Proposition 4.3 *Let*

$$E = \frac{1}{2} \frac{m}{\hbar^2} \left(\int_{-\infty}^{\infty} |v(x)|\, dx \right)^2. \tag{181}$$

In every state ψ the total energy in quantum mechanics satisfies the lower bound

$$\langle \psi, \frac{P^2}{2m} \psi \rangle + \langle \psi, v(Q)\psi \rangle \geq -E. \tag{182}$$

The physical meaning of this application of the uncertainty principle is striking. Suppose that the potential energy has a negative singularity, that is, it has arbitrarily large negative values near some point. Then it may still be true that the total energy is bounded below. The reason is that the probability of being near the point cannot be too large, unless this is compensated by a large kinetic energy.

The same kind of reasoning gives a rigorous proof of self-adjointness for certain Schrödinger operators for which the potential energy is not bounded below. The following theorem is the key.

Theorem 4.1 (Relatively small form sum theorem) *Suppose that A is a positive self-adjoint operator. Suppose that B is a self-adjoint operator with*

$Q(A) \subseteq Q(B)$. *Suppose that there exist positive constants* $\epsilon < 1$ *and* b *such that for all* ψ *in* $Q(A)$ *we have*

$$\pm\langle\psi, B\psi\rangle \leq \epsilon\langle\psi, (A+b)\psi\rangle. \tag{183}$$

Then there is a unique self-adjoint operator $A + B$ *whose form sum is the sum of the forms of* A *and* B.

This theorem is an easy consequence of the form representation theorem. It has an important consequence for Schrödinger operators. The hypothesis on the potential energy function is that it is the sum of an integrable function and a bounded function. In this case, one can take the integrable part arbitrarily small and apply the uncertainty principle bound. The result is the following assertion.

Proposition 4.4 *Suppose that* $v(x)$ *is the sum of an integrable function and a bounded function. Then the Schrödinger operator* $H = \frac{P^2}{2m} + v(Q)$*, defined as a form sum, is a well-defined self-adjoint operator.*

This subsection concludes with a proof of the local uncertainty principle. It is clear that

$$|\psi(x)|^2 \leq \left(\int_{-\infty}^{\infty} |\hat{\psi}(k)| \, \frac{dk}{2\pi}\right)^2. \tag{184}$$

By the Cauchy-Schwarz inequality

$$\left(\int_{-\infty}^{\infty} |\hat{\psi}(k)| \, \frac{dk}{2\pi}\right)^2 \leq \int_{-\infty}^{\infty} \frac{1}{k^2+a^2} \, \frac{dk}{2\pi} \int_{-\infty}^{\infty} (k^2+a^2)|\hat{\psi}(k)|^2 \, \frac{dk}{2\pi}. \tag{185}$$

These give

$$|\psi(x)|^2 \leq \frac{1}{2a}(\|k\psi\|^2 + a^2) = \frac{1}{2a}\|k\psi\|^2 + \frac{a}{2}. \tag{186}$$

The case $a = \|k\psi\|$ gives a bound of the left hand side in terms of the square root of the second moment. The bound in terms of the standard deviation follows from a shift in wave number, since such a shift does not change the absolute value of the position wave function.

4.2 Classical mechanics

This subsection treats the case when Planck's constant may be neglected. This is often called the classical limit, but this terminology gives a misleading impression of the physical situation. Since Planck's constant $\hbar = 1.05443 \times 10^{-27}$erg s is a constant, the success of classical mechanics cannot be due to the fact that $\hbar$ approaches zero.

One way to think of the role of Planck's constant is in terms of the original form of the uncertainty principle due to Heisenberg. This is the statement that in any state, the product of standard deviations $\Delta p \; \Delta q \geq \frac{\hbar}{2}$. A state with localized momentum must have a large position standard deviation.

However there is nothing in general to prevent a state from having a reasonably small position standard deviation. The idea is that a small position standard deviation should be compatible with classical behavior. The question arises: small compared to what? To understand this issue, we begin with Ehrenfest's theorem, which makes no reference at all to Planck's constant.

Proposition 4.5 (Ehrenfest's theorem) *Let $u(t)$ be a solution of the Schrödinger equation. Then*

$$m\frac{d^2\langle u(t), qu(t)\rangle}{dt^2} = -\langle u(t), v'(q)u(t)\rangle. \tag{187}$$

This theorem is true under appropriate hypotheses on the regularity of the solution of the Schrödinger equation. It proved by elementary computation. The problem with the result is that it does not give a closed form equation for the expected position $\langle u(t), qu(t)\rangle$.

Let $q_t = \langle u(t), qu(t)\rangle$ be the expected position. Expand $v'(q) \approx v'(q_t) + v''(q_t)(q - q_t) + \frac{1}{2}v'''(q_t)(q - q_t)^2$. Inserting this in the equation, we get

$$m\frac{d^2q_t}{dt^2} \approx -v'(q_t) - \frac{1}{2}v'''(q_t)(\Delta q)_t^2. \tag{188}$$

From this we see that a condition for neglecting the last term is that

$$(\Delta q)_t \ll \sup_x \sqrt{\frac{|v'(x)|}{|v'''(x)|}}. \tag{189}$$

In other words, the condition is that the position standard deviation should be small compared to a certain scale of variation of the potential energy function. The conclusion is that the classical equation

$$m\frac{d^2q_t}{dt^2} = -v'(q_t) \tag{190}$$

applies, at least in some loose approximation. This argument is not rigorous, but it is illuminating, in that it hints at why classical behavior can be relevant, even for a fixed value of Planck's constant.

Still, there is something odd about the situation. This argument shows at best that the expected position might come close to satisfying the classical law of motion. The expected position is only a statistical quantity. In orthodox quantum mechanics there is no attempt to characterize actual particle trajectories, even statistically. That is, there is no stochastic process underlying the motion of a quantum particle. So the quantum path cannot have a classical limit, because there is no quantum path.

5 Spin and statistics

5.1 Spin $\frac{1}{2}$

In quantum mechanics angular momentum is a discrete variable. Recall that Planck's constant $\hbar$ has the dimensions of angular momentum. It turns out that

the values of angular momentum that can occur have magnitudes $0, \frac{1}{2}\hbar, \hbar, \frac{3}{2}\hbar, 2\hbar, \frac{5}{2}\hbar, \ldots$. Either sign can occur. Particles such as electrons, protons, and neutrons have an intrinsic angular momentum of magnitude $\frac{1}{2}\hbar$. This is called *spin*. The possible spin values in a given direction are $\pm\frac{1}{2}\hbar$. So spin in a given direction is like a variable representing a coin toss. In the following we will mostly take the spin in units of $\frac{1}{2}\hbar$. Thus the values will be simply ± 1.

The Hilbert space that describes the states of a spin $\frac{1}{2}\hbar$ particle is two-dimensional. Write

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{191}$$

for a vector in the Hilbert space $\mathbf{C}^2$. Then $\|\psi\|^2 = |\psi_1|^2 + |\psi_2|^2$. It is a unit vector in $\mathbf{C}^2$ if this length is one. In this case it describes the quantum state. Such a vector is called a *spinor*, since it has a geometrical significance. The space of all spinors forms a three-sphere in four-dimensional space. This three-sphere maps to the two-sphere in three-dimensional space. In geometry this is called the *Hopf map*. A spinor ψ in $\mathbf{C}^2$ that maps to a unit vector (x, y, z) in $\mathbf{R}^3$ determines a quantum state that makes the spin in the direction (x, y, z) sure to have the value $+1$.

An easy way to define this map is to use spherical polar coordinates for three-dimensional space. We have $z = r\cos(\theta)$, $x = r\sin(\theta)\cos(\phi)$, and $y = r\sin(\theta)\sin(\phi)$. Here θ is the colatitude and ϕ is the longitude. To get a unit vector in the two-sphere set $r = 1$. The spinor ψ describes a unit vector as follows. Write ψ in the form

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \cos(\theta/2)e^{i\chi_1} \\ \sin(\theta/2)e^{i\chi_2} \end{pmatrix}. \tag{192}$$

Then θ is the colatitude, and the relative phase $\phi = \chi_2 - \chi_1$ is the longitude.

Proposition 5.1 *The map from the three-sphere of normalized spinors ψ in $\mathbf{C}^2$ to the two-sphere of unit vectors (x, y, z) in $\mathbf{R}^3$ is given by*

$$z = \cos(\theta) = \cos^2(\theta/2) - \sin^2(\theta/2) = |\psi_1|^2 - |\psi_2|^2 \tag{193}$$

and

$$x + iy = \sin(\theta)e^{i\phi} = 2\cos(\theta/2)\sin(\theta/2)e^{-i\chi_1}e^{i\chi_2} = 2\bar{\psi}_1\psi_2. \tag{194}$$

The inverse image of a unit vector in three-dimensional space is a circle. This corresponds to an arbitrary phase in the spinor. This inverse image also has an explicit representation.

Proposition 5.2 *The unit vector (x, y, z) determines the corresponding spinor up to a phase by the formula*

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = e^{i\chi_1}\frac{1}{\sqrt{\frac{1+z}{2}}}\begin{pmatrix} \frac{1+z}{2} \\ \frac{x+iy}{2} \end{pmatrix} = e^{i\chi_2}\frac{1}{\sqrt{\frac{1-z}{2}}}\begin{pmatrix} \frac{x-iy}{2} \\ \frac{1-z}{2} \end{pmatrix}. \tag{195}$$

The relation between a vector $\mathbf{R}^3$ and a spinor is complicated by the fact that the vector is quadratic in the spinor. The next proposition will show that there is a correspondence between the vector and the state defined by the spinor that is linear.

For this it is convenient to describe the spinors in terms of the *Pauli matrices* defined by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{196}$$

These combine to make a vector $\vec{\sigma}$ whose components are these three matrices.

Consider a vector $\vec{\mathbf{u}}$ with components (x, y, z). Then the corresponding Pauli matrix is

$$\vec{\sigma} \cdot \vec{\mathbf{u}} = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix}. \tag{197}$$

These matrices satisfy the algebraic relation

$$(\vec{\sigma} \cdot \vec{\mathbf{u}})(\vec{\sigma} \cdot \vec{\mathbf{v}}) = \vec{\mathbf{u}} \cdot \vec{\mathbf{v}}\, I + i\vec{\sigma} \cdot (\vec{\mathbf{u}} \times \vec{\mathbf{v}}). \tag{198}$$

In particular $(\vec{\sigma} \cdot \vec{\mathbf{u}})^2 = \vec{\mathbf{u}} \cdot \vec{\mathbf{u}}\, I$.

The formula for the product of Pauli matrices should seem familiar to most mathematicians. Recall that a *quaternion* is a sum $t + \vec{\mathbf{u}}$, where t is a scalar and $\vec{\mathbf{u}}$ is a vector in three dimensional space. It is obvious how to define the product of two quaternions, except for the term involving the product of two vectors. This quaternion product is given by combining the scalar dot product and the vector cross product to give a quaternion

$$\vec{\mathbf{u}}\, \vec{\mathbf{v}} = -\vec{\mathbf{u}} \cdot \vec{\mathbf{v}} + \vec{\mathbf{u}} \times \vec{\mathbf{v}} \tag{199}$$

If we represent the scalar t by t times the identity I, and if we represent the vector $\vec{\mathbf{u}}$ by $-i\vec{\sigma} \cdot \vec{\mathbf{u}}$, then the resulting matrices form an representation of the quaternion algebra.

Let $\vec{\mathbf{u}}$ be a unit vector, so that $(\vec{\sigma} \cdot \vec{\mathbf{u}})^2 = I$. Then $\vec{\sigma} \cdot \vec{\mathbf{u}}$ represents the spin along this axis. It has eigenvalues ± 1. Let

$$E(\vec{\mathbf{u}}) = \frac{1}{2}(I + \vec{\sigma} \cdot \vec{\mathbf{u}}) = \frac{1}{2} \begin{pmatrix} 1 + z & x - iy \\ x + iy & 1 - z \end{pmatrix}. \tag{200}$$

This $E(\vec{\mathbf{u}})$ projects onto the eigenspace of $\vec{\sigma} \cdot \vec{\mathbf{u}}$ with eigenvalue 1. The spinors in this eigenspace map to the unit vector $\mathbf{u}$. These represent states where the spin component in the $\mathbf{u}$ direction is 1. It is not hard to see that the spinors in the eigenspace with eigenvalue -1 map to the unit vector $-\mathbf{u}$. These represent states where the spin component in the $\mathbf{u}$ direction is -1.

Proposition 5.3 *Each state vector ψ of the spin $1/2$ system corresponding to the unit vector $\vec{\mathbf{u}}$ defines a corresponding projection operator $\psi\psi^*$. The correspondence between projection operators defining states and the unit vectors $\vec{\mathbf{u}}$ is given explicitly by*

$$\psi\psi^* = E(\vec{\mathbf{u}}). \tag{201}$$

5.2 Composite systems

This subsection contrasts two constructions of Hilbert spaces. A direct sum of Hilbert spaces corresponds to disjoint union of sets, while a tensor product of Hilbert spaces corresponds to cartesian product of sets. It is the tensor product construction that gives the quantum mechanical description of composite systems.

Suppose that $\mathcal{H}$ is a Hilbert space and that $\mathcal{H}_1$ is a closed linear subspace of $\mathcal{H}$. Let $\mathcal{H}_2$ be the orthogonal complement of $\mathcal{H}_1$ in $\mathcal{H}$. Then the *projection theorem* says that $\mathcal{H}$ is the orthogonal *direct sum* $\mathcal{H} = \mathcal{H}_1 \bigoplus \mathcal{H}_2$. Thus, for every vector ψ in $\mathcal{H}$ there is a vector ϕ in $\mathcal{H}_1$ and a vector χ in $\mathcal{H}_2$ with $\psi = \phi + \chi$, and this decomposition is unique. Finally, since ϕ is orthogonal to χ, we have the theorem of Pythagoras $\|\psi\|^2 = \|\phi\|^2 + \|\chi\|^2$. Sometimes this is called an internal direct sum.

If instead we are given two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, then we can form a new Hilbert space $\mathcal{H} = \mathcal{H}_1 \bigoplus \mathcal{H}_2$ that is an external direct sum. This consists of all ordered pairs $\phi \oplus \chi$ with ϕ in $\mathcal{H}_1$ and χ in $\mathcal{H}_2$. The norm of a pair is defined by taking the theorem of Pythagoras as a definition, so $\|\phi \oplus \chi\|^2 = \|\phi\|^2 + \|\chi\|^2$.

Say that the two Hilbert spaces are spaces of functions: $\mathcal{H}_1 = L^2(X_1)$ and $\mathcal{H}_2 = L^2(X_2)$. Then the direct sum $\mathcal{H} = L^2(X_1 \sqcup X_1)$, where $X_1 \sqcup X_2$ is the disjoint union. Thus if ϕ is a function on X_1, and χ is a function on X_2, then $\phi \oplus \chi$ is the function on $X_1 \sqcup X_2$ whose value on x is $\phi(x)$ if $x \in X_1$ and $\chi(x)$ if $x \in X_2$.

The tensor product construction is similar to the external direct sum. Given Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, there is a *tensor product* Hilbert space $\mathcal{H} = \mathcal{H}_1 \bigotimes \mathcal{H}_2$. Furthermore, given vectors ϕ in $\mathcal{H}_1$ and χ in $\mathcal{H}_2$, there is always a vector $\phi \otimes \chi$ in $\mathcal{H}_2$. However now the situation is more complicated; the vectors of this form need not constitute the entire tensor product space. For instance, linear combinations of such vectors also belong to the tensor product space.

One way to see what is going on is to represent the Hilbert spaces as $\mathcal{H}_1 = L^2(X_1)$ and $\mathcal{H}_2 = L^2(X_2)$. Then $\mathcal{H} = L^2(X_1 \times X_2)$, where $X_1 \times X_2$ is the cartesian product. So a function in $\mathcal{H}$ is a function $\psi(x_1, x_2)$ that is square-integrable with respect to the product measure. If ϕ and χ are vectors in $\mathcal{H}_1$ and $\mathcal{H}_2$, then their tensor product is

$$(\phi \otimes \chi)(x_1, x_2) = \phi(x_1)\chi(x_2). \tag{202}$$

There is certainly no reason to expect that the general function of two variables will have this product form. However, consider a vector ψ in the tensor product Hilbert space. If it factors as $\psi = \phi \otimes \chi$, then it is called *decomposable*. Obviously this is a very special case.

In addition to tensor product vectors, there are tensor product operators. For instance, if $A : \mathcal{H}_1 \to \mathcal{H}_1$ and $B : \mathcal{H}_2 \to \mathcal{H}_2$, then there is an operator $A \otimes B : \mathcal{H} \to \mathcal{H}$ determined by $(A \otimes B)(\phi \otimes \chi) = A\phi \otimes B\chi$. In the case when A and B are self-adjoint, it is also natural to consider the commuting operators $A \otimes I$ and $I \otimes B$ and their sum $A \otimes I + I \otimes B$. Then there is a corresponding

relation for unitary operators

$$\exp(-it(A \otimes I + I \otimes A_2)) = \exp(-itA) \otimes \exp(-itB). \tag{203}$$

In quantum mechanics, the tensor product describes composite systems. Thus, for instance, if $\mathcal{H}_1 = L^2(X_1)$ is the Hilbert space for particle 1, and $\mathcal{H}_2 = L^2(X_2)$ is the Hilbert space for particle 2, then $\mathcal{H} = L^2(X_1 \times X_2)$ is the Hilbert space for system consisting of the two particles. (Here the particles are assumed distinguishable.) This leads to the remarkable conclusion that the wave function $\psi(x_1, x_2)$ for the two particle system is a function of both particle position coordinates at once. In general, the wave function ψ will not be decomposable. In that case, the two particle system is said to be *entangled*. There is no longer a well-defined wave function for the individual particles. This is the typical case.

Consider the indecomposable case when $\psi = \phi \otimes \chi$, that is, $\psi(x_1, x_2) = \phi(x_1)\chi(x_2)$. Then it is possible to think of $\phi(x_1)$ and $\chi(x_2)$ as describing the states of the individual particles. However this case is very much the exception.

One famous case of the tensor product is the Hilbert space $\mathbf{C}^2 \bigotimes \mathbf{C}^2$ describing two spins. There is a maximally entangled state of the combined system called the *singlet state*. This is given by

$$\psi_0 = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right]. \tag{204}$$

The idea is that the spins are as opposite as they can get. We shall see in a later section that this state is invariant under rotations.

Physicists often use the Dirac notation in the context of spin systems. Thus they might use labels $\uparrow$ and $\downarrow$ for the vector indices. So the singlet state might be denoted

$$\psi_0 = \frac{1}{\sqrt{2}} \left[\, |\uparrow\rangle \otimes |\downarrow\rangle - |\downarrow\rangle \otimes |\uparrow\rangle \, \right]. \tag{205}$$

Or the indices for the tensor product states might be pairs of arrows, so the same state would be

$$\psi_0 = \frac{1}{\sqrt{2}} \left[\, |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \, \right]. \tag{206}$$

It is easy to compute the properties of spin in the singlet state. (See, for instance, the appendix to [10].) Consider unit vectors $\vec{\mathbf{u}}$ and $\vec{\mathbf{v}}$. There is an operators $\vec{\sigma} \cdot \vec{\mathbf{u}} \otimes I$ for the $\vec{\mathbf{u}}$ component of the first spin and and operator $I \otimes \vec{\sigma} \cdot \vec{\mathbf{v}}$ for the $\vec{\mathbf{v}}$ component of the second spin. In the singlet state these each have values ± 1 with equal probabilities. Since they commute, they have a joint distribution. If ρ is the angle between the unit vectors $\vec{\mathbf{u}}$ and $\vec{\mathbf{v}}$, then the probability that they have the same value is $\sin^2(\rho/2)$, and the probability that they have the opposite value is $\cos^2(\rho/2)$. In particular, when $\vec{\mathbf{u}} = \vec{\mathbf{v}}$ and $\rho = 0$ they are always opposite. This system is a building block for many remarkable quantum effects exhibiting some form of non-locality.

People sometimes argue about whether quantum mechanics is non-local. Of course, this depends on the meaning of the word "local." (See the appendix

to [10] for one analysis.) However there is already a rather evident sense in which quantum mechanics is non-local, namely, that the wave function for two particles is a single function of the two particle coordinates. This can have dramatic effects even when the particles are widely separated in space, provided this wave function is not decomposable. If the particles have spin, then their spin state can also be indecomposable, as in the example of the maximally entangled singlet state. Composite systems in quantum theory can behave very differently from what one would expect from their constituents.

5.3 Statistics

Another fact about quantum mechanics is the special treatment of composite systems of indistinguishable particles. There are two kinds of systems: Bose-Einstein (boson) and Fermi-Dirac (fermion). For Bose-Einstein systems the state vectors of a composite system are restricted to be symmetric under interchange, while for Fermi-Dirac systems they are restricted to be anti-symmetric under interchange. Fermi-Dirac statistics are particularly important in atomic systems, since they apply to electron systems. This leads to the famous *Pauli exclusion principle*, which says that two electrons cannot occupy the same quantum state.

Finally, there is a principle that connects spin and statistics. Identical particles of spin for $0, 1, 2, \ldots$ obey Bose-Einstein statitistics, while identical particles of spin $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ obey Fermi-Dirac statistics. In particular, since electrons have spin $\frac{1}{2}$, they obey Fermi-Dirac statistics. Hence the Pauli exclusion principle for electrons. Quantum mechanics is already an amazing subject; the extra features involving spin and statistics merely underline what a strange theory it is.

6 Fundamental structures of quantum mechanics

6.1 Self-adjoint operators as dynamics

The spectral theorem implies that for each self-adjoint operator A there is a corresponding one-parameter unitary group $t \mapsto U_t = e^{-itA}$. It satisfies the continuity condition: for each vector ψ in the Hilbert space, the map $t \mapsto U_t\psi$ is continuous from the real line to the Hilbert space. Stone's theorem also gives a converse statement: every one-parameter unitary group satisfying the continuity condition arises in this way. If one believes that quantum dynamics is given by unitary operators, then this result shows why self-adjoint operators play such a central role in quantum theory.

A densely defined operator $A : D(A) \to \mathcal{H}$ is said to be *Hermitian* if for each ϕ and ψ in $D(A)$ we have $\langle A\phi, \psi\rangle = \langle \phi, A\psi\rangle$. This is a purely algebraic property, but it is not enough to make the operator self-adjoint. For the operator to be self-adjoint there is an additional analytic condition. This says that if there are ϕ and χ such that for all ψ in $D(A)$ we have $\langle \chi, \psi\rangle = \langle \phi, A\psi\rangle$, then ϕ is in

$D(A)$ and $A\phi = \chi$. The significance of this condition is explained treatments of operator theory, such as [3].

The adjoint operator of a Hermitian operator may have a larger domain, and in general it will not be Hermitian. The usual interpretation of this situation is that the Hermitian operator A has too many boundary conditions, making its domain too small, while the adjoint A^* has too few boundary conditions, making its domain too big. A self-adjoint operator has just the right boundary conditions needed to allow it to define an unambiguous dynamics.

It is possible that A is Hermitian (but not self-adjoint) and A^* is also Hermitian. In that case A^* is self-adjoint, and A is said to be *essentially self-adjoint*. This corresponds to a case when the domain is restricted in some unimportant way, but still defines the correct boundary conditions. When an operator is essentially self-adjoint, it determines a unique self-adjoint operator, and this self-adjoint defines a quantum dynamics as before.

The self-adjointness problem is to define the quantum dynamics e^{-itA} for each real t. This is a problem of fixed time interval and large energy. Some of the main results were described in a previous section. Once this is accomplished, there is the task of finding the asymptotic behavior of the dynamics for $t \to \pm\infty$. This is the study of spectral theory and associated phenomena, such as scattering. This is a problem of fixed energy interval and large time. This subject is too extensive to cover in an outline of limited scope.

6.2 Self-adjoint operators as states

This subsection treats very special operators: positive self-adjoint operators with trace one. These give a particularly convenient way of describing quantum states. First we need some preliminary considerations.

An operator K is *Hilbert-Schmidt* if $\mathrm{tr}(K^*K) < \infty$. This trace is defined in the following way. Let ϕ_n be an orthonormal basis. Then

$$\mathrm{tr}K^*K = \sum_n \langle \phi_n, K^*K\phi_n \rangle = \sum_n \|K\phi_n\|^2. \tag{207}$$

It may be shown that this is independent of the choice of orthonormal basis. Also, the adjoint K^* is Hilbert-Schmidt, with $\mathrm{tr}KK^* = \mathrm{tr}K^*K$. If K acts in an L^2 space, then K is always given by an integral operator

$$(Kf)(x) = \int k(x,y)f(y)\,dy. \tag{208}$$

The product $W = K^*K$ is also an integral operator

$$(Wf)(x) = (K^*K)f(x) = \int\int \overline{k(z,x)}k(z,y)f(y)\,dz\,dy. \tag{209}$$

It may be shown that in this case

$$\mathrm{tr}(K^*K) = \int\int |k(z,y)|^2\,dz\,dy. \tag{210}$$

So Hilbert-Schmidt operators are easy to characterize: they are integral operators with square-integrable kernels.

If $W = M^*K$ is the product of two Hilbert-Schmidt operators M^* and K, then it itself is a Hilbert-Schmidt operator. However not every Hilbert-Schmidt operator arises in this way. An operator W is said to be *trace class* if it is the product $W = M^*K$ of two Hilbert-Schmidt operators. Its trace is defined by

$$\mathrm{tr}W = \mathrm{tr}M^*K = \sum_n \langle \phi_n, M^*K\phi_n\rangle = \sum_n \langle M\phi_n, K\phi_n\rangle. \tag{211}$$

If a trace class operator W acts on an L^2 space, it is an integral operator

$$W = \int w(x,y)f(y)\,dy \tag{212}$$

with square integrable kernel. One might hope that the trace would be defined by the integral

$$\mathrm{tr}(W) = \int w(x,x)\,dx. \tag{213}$$

On the other hand, it might seem too good to be true, since one is integrating over a set of measure zero in the product space. There is something delicate about checking that an operator is trace class. However, if W is represented as $W = M^*K$, and the kernel $w(x,y)$ is correspondingly represented as

$$w(x,y) = \int \overline{m(z,x)}k(z,y)\,dz, \tag{214}$$

then the integral expression for the trace is valid.

The class of operators of present interest are positive self-adjoint trace class operators with trace equal to one. Thus W is such an operator if $W^* = W$ and $W \geq 0$ and $\mathrm{tr}W = 1$. By the spectral theorem these operators are of the form

$$W = \sum_n \lambda_n \chi_n \chi_n^*. \tag{215}$$

where the χ_n are unit vectors, and the $\lambda_n \geq 0$ satisfy $\mathrm{tr}(W) = \sum_n \lambda_n = 1$.

Two unit vectors define the same quantum state if they differ by a phase. So one can identify the state associated with the vector ψ with the orthogonal projection $E = \psi\psi^*$ onto the corresponding one-dimensional space. This orthogonal projection is a very special kind of positive self-adjoint operator with trace one. The expectation of the self-adjoint operator A in this state is

$$\langle \psi, A\psi\rangle = \mathrm{tr}(AE). \tag{216}$$

Consider a quantum mechanical system with a random state. This means that there is a given probability measure γ on the space of all states. The state space is identified as the space of all one-dimension orthogonal projections E. Form the operator average

$$W = \int E\gamma(dE). \tag{217}$$

It may be shown that W is a positive self-adjoint operator with trace one. he conventional term in quantum mechanics for such an operator is *density matrix*. The utility of this notion is due to the equation

$$\int \mathrm{tr}(AE)\gamma(dE) = \mathrm{tr}(AW). \tag{218}$$

The density matrix gives a convenient summary of the result of the averaging.

One cannot go backward from the density matrix W to recover the measure γ. It is true that the spectral representation of W produces a discrete measure with masses λ_j on a set of states corresponding to orthogonal vectors χ_j. However, there is no guarantee that this is the measure that actually gave rise to the density matrix. There is no obstacle, for instance, to obtaining a random quantum system by a random choice of state vectors that are not orthogonal.

Sometimes a density matrix is said to specify a *mixed state*. (In the case when it is a one-dimensional orthogonal projection it is a *pure state*. This is the notion of state that we have been using up to now.) When a mixed state arises by randomization, the actual randomization that is used is not determined by the state.

There is another way that a density matrix can occur. Consider a subsystem that is part of a larger system. The larger system may be in a pure state, but this does not mean that the subsystem has a description via a pure state. However observations on the subsystem may always be described by a density matrix. In this case, it is called a *reduced density matrix*. The use of the reduced density matrix represents a loss of information about the original larger system.

As an example, take the case when we have two particles with entangled wave function $\psi(x_1, x_2)$. Since this is a pure state, the density matrix is an integral operator given by the integral kernel $\psi(x_1, x_2)\overline{\psi(y_1, y_2)}$. Consider the first particle. This system has reduced density matrix given by the integral operator with kernel

$$w(x_1, y_1) = \int \psi(x_1, x_2)\overline{\psi(y_1, x_2)}\, dx_2. \tag{219}$$

This density matrix defines a quantum mixed state that suffices for predictions involving the first particle alone. It is not a pure state for the first particle, nor does it characterize a random quantum pure state for the first particle. In fact, the reduced density matrix for the first particle has lost much of the information about the original state of the two particle system.

There is an exception in the case when the original state of the two particle system is decomposable, so there is no entanglement. In that case the reduced density matrix is a pure quantum state for the first particle. The second particle has no influence on what is happening with the first particle, and so it may be ignored.

A particularly famous example is the composite system obtained by combining two spin 1/2 systems. In Dirac notion the density matrix for the singlet state is

$$\psi_0\psi_0^* = \frac{1}{2}\left[\, |{\uparrow\downarrow}\rangle\langle{\uparrow\downarrow}| + |{\downarrow\uparrow}\rangle\langle{\downarrow\uparrow}| - |{\uparrow\downarrow}\rangle\langle{\downarrow\uparrow}| - |{\downarrow\uparrow}\rangle\langle{\uparrow\downarrow}| \,\right]. \tag{220}$$

It is not difficult to rewrite this in matrix notation. For instance, the last term is

$$|{\downarrow}{\uparrow}\rangle\langle{\uparrow}{\downarrow}| = |{\downarrow}\rangle\langle{\uparrow}| \otimes |{\uparrow}\rangle\langle{\downarrow}| = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{221}$$

The resulting formula is

$$\begin{aligned} \psi_0\psi_0^* &= \frac{1}{2}\Big[\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ &\quad - \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \Big]. \end{aligned} \tag{222}$$

After some computation this becomes

$$\begin{aligned} \psi_0\psi_0^* &= \frac{1}{4}\Big[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\ &\quad - \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \Big]. \end{aligned} \tag{223}$$

The Pauli matrices make an appearance. In brief, this says that

$$\psi_0\psi_0^* = \frac{1}{4}\left(I \otimes I - \vec{\sigma} \otimes \vec{\sigma}\right). \tag{224}$$

The singlet state is a rotation invariant pure state.

Consider the combined system in the singlet state, and look at the reduced density matrix for one of the spins. This matrix is

$$W = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{225}$$

This mixed state gives incomplete information about the spin, since it neglects its intimate relation with the other spin. Another point of view would be to think of it as a randomized state. Choose an arbitrary spin direction. Then it is the randomization of the spin up and spin down states in this direction, when the spin up and spin down states are taken with equal probability. This representation as a random pure state is far from unique.

6.3 Self-adjoint operators as observables?

The dynamical role of self-adjoint operators as generators of one-parameter unitary groups is entirely clear. This is given by Stone's theorem. The role of self-adjoint operators as observables is comparatively mysterious.

It is not controversial that for every state and every self-adjoint operator A there is a realization of A as a random variable α defined on a probability space. It is even the case that for every state and every pair of commuting self-adjoint operators A, B there is a realization of A, B as a pair of random variables

α, β on a probability space. Suppose that A, D are another pair of commuting self-adjoint operators. Again there is a realization of A, D as a pair of random variables α', γ'. The problem comes when when B, D do not commute. The spectral theorem does not give a single probability space[1] that works for both pairs A, B and A, D.

The random variables α and α' both correspond to the self-adjoint operator A. One could imagine that in each concrete realization of the physical system the random variables α and α' have equal values. This could be explained if for each time the experiment is done there is a number Z_A associated with the self-adjoint operator A. This quantity would reflect an actual property of the system.

It turns out that there is no such quantity. Self-adjoint operators cannot correspond to intrinsic properties of the physical system. There are many impossibility results that show this. The most famous of these is based on Bell's inequality, a result of elementary probability theory. (See the appendix to [10] for an account.) It shows that if there were properties associated with self-adjoint operators, then this inequality would be violated. A nice feature of Bell's analysis is that the physical system is so simple; it is a system of two spin $1/2$ particles in the singlet state.

Hardy [5] derived an even more convincing result, in which the contradiction is exhibited on a certain fraction of the individual runs of the experiment, rather than statistically. We follow the account in [1]. Again the example involves a system of two spin $1/2$ particles and a certain state of the combined system. Curiously enough, the state in Hardy's example is not the singlet state.

Hardy defines certain spin component operators A, B, C, D. Each has a spectrum ± 1. Say that A, C are associated with the first particle, while B, D are associated with the second particle. Then the following pairs commute: $AB = BA$, $AD = DA$, $BC = CB$, and $CD = DC$.

Suppose that self-adjoint operators, considered in isolation, actually correspond to intrinsic properties. Suppose furthermore that calculations involving commuting self-adjoint operators proceed in the usual way. For the state considered by Hardy and the four self-adjoint operators A, B, C, D there would be corresponding physical quantities Z_A, Z_B, Z_C, Z_D with definite numerical values (depending on the realization). However Hardy shows that calculations involving only commuting self-adjoint operators give the following four results for the joint probabilities computed from the state:

1. $P[Z_A = 1, Z_B = 1] > 0$.
2. $P[Z_B = 1, Z_C = -1] = 0$.
3. $P[Z_D = -1, Z_A = 1] = 0$.

[1]Such a space exists. Let β and γ' be conditionally independent given α, and use the probability distribution for α and the conditional distributions for β given α and for γ' given α yielded by quantum mechanics. Since quantum mechanics is silent about the joint distribution of β and γ' one is free to do this. (The situation is different with the no-hidden-variables theorems, like Hardy's, for which the graph corresponding to the relevant quantum mechanical joint probabilities has cycles.) This example was communicated by Sheldon Goldstein.

4. $P[Z_C = 1, Z_D = 1] = 0$.

According to 1, in some substantial proportion of repetitions of the experiment the outcome is such that both Z_A and Z_B have the value 1. Consider only such outcomes. By 2 and 3 both Z_C and Z_D have the value 1. Then 4 says that this cannot happen. The supposition that there are such physical quantities has led to a contradiction. They do not exist.

Many physicists are aware of this situation, although perhaps not all realize that it is fatal for the concept of self-adjoint operator as observable. In fact, they often cheerfully acknowledge that for a particular experiment one self-adjoint operator may have an associated physical value, while another self-adjoint operator may not have such a value at all. Obviously, which is the case must depend on something more than the self-adjoint operator. The self-adjoint operator alone does not determine what is observed.

The result of this analysis is that a self-adjoint operators must be combined with some other ingredient in order to define an observable. This extra ingredient is the experimental context that defines the measurement. The random physical quantity, if it is defined at all, depends not only on the self-adjoint operator, but also on the experiment. So it is no surprise that the random variable α associated with A in a measurement of A, B may have different values from the random variable α' associated with A in measurement of A, D. A possible mechanism for this is presented in the next subsection.

Nothing in the above discussion proves that there cannot be intrinsic properties of the system, independent of the experimental context. All it shows is that such properties cannot be described exclusively by self-adjoint operators. There are variations of non-relativistic quantum mechanics in which a system does have intrinsic properties. See, for instance, [1] for Bohmian mechanics or the contribution by Carlen in [4] for stochastic mechanics. These formulations are often overlooked, but they have considerable conceptual value. In particular, they often provide instant counter-examples to a variety of careless assertions about quantum theory. It may also be that orthodox quantum mechanics describes at least some intrinsic properties of the system, if one can believe the account in the following subsection. If this were not the case, then it would be a puzzle that experiments can have outcomes.

6.4 Self-adjoint operators with measurement as observables

Here is a brief account of one possible interpretation of quantum mechanics. It is influenced by [1], a survey that considers a variety of approaches. The present description attempts to be close to quantum orthodoxy, and, given this constraint, reasonably precise and consistent. As in many such accounts, the exposition is marred by the introduction of undefined terms. In this case, the terms "measurement" and "experiment" are at least partially specified, but the term "macroscopic" is not subject to serious analysis.

The fundamental idea is that an observable consists of more than a self-adjoint operator; there is also an experimental context. The self-adjoint operator merely provides a convenient summary of certain aspects of the situation. There may be more than one experiment that gives rise to a particular self-adjoint operator. So the only kind of measurement involving the self-adjoint operator is when one is performing the experiment.

We only deal with the case of point spectrum. In this case a self-adjoint operator acting in the Hilbert space $\mathcal{H}$ may be written the form

$$A = \sum_j \lambda_j E_j \tag{226}$$

The eigenvalues λ_j are real numbers (not necessarily distinct). There is an orthogonal family $\mathcal{H}_j$ of closed subspaces of the Hilbert space $\mathcal{H}$ whose direct sum is $\mathcal{H}$. The operators E_j denote the orthogonal projections onto the subspaces $\mathcal{H}_j$.

The complete description involves the system together with an environment, forming what one might call the total system. The self-adjoint operator acts on the original system Hilbert space $\mathcal{H}$. The environment Hilbert space $\mathcal{H}'$ is intended to describe the apparatus used for the experiment. The total system Hilbert space is a tensor product $\mathcal{H} \bigotimes \mathcal{H}'$ of original system and environment Hilbert spaces. Thus the original system is a subsystem of the total system.

An original system vector of the form $E_j\psi$ is an eigenvector of the operator A with eigenvalue λ_j. Let Φ be the initial state of the environment. Suppose that it is possible to find a unitary time dynamics U for the total system that sends $E_j\psi \otimes \Phi$ to a state

$$U(E_j\psi \otimes \Phi) = R_j\psi \otimes \Phi_j. \tag{227}$$

The environment states Φ_j are taken to form an orthonormal family. The R_j are a family of linear operators on the original system Hilbert space $\mathcal{H}$ defined by the above equation. Since U is unitary, we see that $\|R_j\psi\|^2 = \|E_j\psi\|^2$ for each ψ. In other words, the operators R_j satisfy $R_j^* R_j = E_j^2 = E_j$. The effect of the unitary dynamics for the total system is to produce a correlation between original system and the environment in which the original system vector $R_j\psi$ goes with environment vector Φ_j.

Let ψ be a unit vector representing the initial state of the original system. Since $\psi = \sum_j E_j\psi$, the unitary dynamics for the total system gives a final state

$$U(\psi \otimes \Phi) = \sum_j R_j\psi \otimes \Phi_j. \tag{228}$$

The initial state of the original system was a pure state with state vector ψ. The final state of the original system is a mixed state with state vectors given by normalizing $R_j\psi$, taken with probability

$$p_j = \|(R_j\psi) \otimes \Phi_j\|^2 = \|R_j\psi\|^2 = \|E_j\psi\|^2 = \langle \psi, E_j\psi \rangle. \tag{229}$$

This kind of dynamical mapping of a pure state of the original system to a mixed state of the original system via a unitary map of the total system (of which the original system is a subsystem) is an example of *decoherence*. In the resulting description of the original system all information about the relative phases of the components $E_j\psi$ is lost.

It is impossible to map a pure state of the system to a mixed state of the system with a unitary dynamics of the system alone. In an example of this kind the mapping is accomplished with a unitary dynamics for the combined total system. There is no reason to believe that the original system should have a unitary dynamics obtained from the Schrödinger equation, since there is an interval of time for which it is not an isolated system.

If we associate the number λ_j with the random choice of j, then for each real function f we have the expectation

$$\sum_j f(\lambda_j)p_j = \sum_j f(\lambda_j)\langle\psi, E_j\psi\rangle = \langle\psi, f(A)\psi\rangle. \tag{230}$$

The system operator A together with the pure system state ψ gives the statistics of λ_j with the mixed state probabilities p_j.

Since the time of Bohr it has been customary to interpret the world on the atomic level in terms of experience on the macroscopic scale. In this spirit, consider the environment state vectors Φ_j as being wave functions with macroscopically disjoint supports. In this circumstance the correlation with the environment may be thought of as permanent, for all practical purposes. Therefore no contradiction arises from the supposition that the system state is realized with a particular value of j. It is then customary to regard λ_j as the actual experimental value and $R_j\psi$ (suitably normalized) as the actual state vector of the system after the measurement. This is called *reduction* or *collapse* of the state vector. It corresponds to the standard situation in applications of probability, where it is natural to think that experiments that are actually performed have outcomes.

The probabilities of these outcomes are given by the probabilities $p_j = \|E_j\psi\|^2$ associated with the self-adjoint operator and the state ψ. However, as we saw in the previous subsection, the actual outcomes that are obtained must depend on something else. It is the association with macroscopically distinct states and the associated collapse that provides the mechanism.

The Schrödinger equation is deterministic and thus cannot possibly provide a random outcome. So collapse is not obtained by solving the Schrödinger equation. It would seem that collapse is a problematic operation from the point of view of quantum dynamics. On the other hand, collapse does not contradict the Schrödinger equation, since no one expects that the system should obey this equation while it is in interaction with the environment. And the result is that the pure state given by ψ is mapped to another pure state given by $R_j\psi$, suitably normalized. The idea is that at the beginning and at the end of the experiment the original system may be regarded as a quantum mechanical system in its own right, rather than as a subsystem of a larger system. The mapping itself is

obtained by considering the original system as a subsystem of a larger system and invoking decoherence followed by collapse. From the point of the view of the original system it appears only as a rather mysterious random process. It is this process that allows quantum experiments to have physically realized outcomes. For a quantum mechanical system to have an intrinsic property it would seem that there must be an interaction with the macroscopic world.

Is this all there is to quantum reality? In other words, is it necessary to have this kind of amplification to the macroscopic level in order to make sense of the theory? Perhaps the answer is yes, but this leaves many questions unanswered.

We conclude this subsection with a technical comment. The above discussion showed that an experiment of a certain kind can provide a measurement for a self-adjoint operator. However there is a somewhat more general but still reasonable notion of experiment that need not provide a such a measurement. Suppose that there is a unitary time dynamics U such that for each system vector ψ we have

$$U(\psi \otimes \Phi) = \sum_j R_j \psi \otimes \Phi_j. \tag{231}$$

Here the R_j are bounded operators, without the restriction that $R_j^* R_j$ is an orthogonal projection. Each individual $O_j = R_j^* R_j$ is a bounded positive self-adjoint operator. The unitarity condition implies that for each initial ψ the sum $\sum_j \|R_j\psi\|^2 = \|\psi\|^2$. As a consequence, the operators O_j are normalized to satisfy $\sum_j O_j = I$. The same calculation as above shows that the probability of the support corresponding to index j is

$$p_j = \|(R_j\psi) \otimes \Phi_j\|^2 = \|R_j\psi\|^2 = \langle \psi, O_j \psi \rangle. \tag{232}$$

If we associate the number λ_j with this event, then there is no difficulty in computing

$$\sum_j f(\lambda_j) p_j = \sum_j f(\lambda_j) \|R_j\psi\|^2 = \sum_j f(\lambda_j) \langle \psi, O_j \psi \rangle. \tag{233}$$

So it would seem that the entire discussion of experiment carries over to this more general situation, where there is no reference to a self-adjoint operator at all. The system is in a mixed state in which $R_j\psi$ occurs with probability p_j. The collapse of the state to one of the $R_j\psi$ remains just as valid. This form of experiment seems just as reasonable as the more restrictive one presented above.

It is still possible to define a self-adjoint operator

$$A = \sum_j \lambda_j O_j, \tag{234}$$

but this representation is far from being a spectral representation. The self-adjoint operator A is useful for expressing the expectation (or mean)

$$\sum_j \lambda_j p_j = \sum_j \lambda_j \langle \psi, O_j \psi \rangle = \langle \psi, A\psi \rangle, \tag{235}$$

but it is not relevant to computing the distribution of the λ_j. In fact the distribution of A is concentrated on its eigenvalues, and the λ_j are not eigenvalues of A. Thus it is misleading to regard the experiment as providing a measurement for A.

This more general kind of experiment seems just as plausible as what we had before. The result is that certain numbers λ_j are observed, but they are not numbers associated with a self-adjoint operator. Perhaps the notion that observables must correspond to self-adjoint operators may be taken with some skepticism.

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