# Quantum Dynamics

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# Introduction

## 1.1 Quantum mechanics

The invention of quantum mechanics was the greatest revolution of modern science. It explained the properties of everyday matter, from density and heat capacity to conductivity and color. For the first time it made sense of chemistry.

On the other hand, the explanations given by quantum mechanics are based on the mathematics of complex functions of many variables. The physical interpretation of these functions is mysterious, to say the least. In fact, the interpretation is so radical that it has led many scientists to deny the existence of an objective world. (See Nelson's lectures [N1] for critical comments.)

Thus quantum mechanics is both practical and mysterious, the ultimate vindication of a mathematical picture of the world (if it is true). This book does not resolve the mysteries, but it will give a systematic account of the mathematics. This is in itself a fascinating story; it turns out that the possible types of motion of the quantum mechanical waves correspond to various properties of spectra of operators in Hilbert space.

The book is intended as a self-contained and rigorous introduction to non-relativistic quantum mechanics and the mathematics behind it. This is the theory underlying our understanding of matter on the atomic and molecular scale, and some of the physics will be presented, but the emphasis is on the mathematics: linear operator theory and partial differential equations.

The reader will need a reference on the physics of quantum mechanics. There are many texts; Messiah [Me] is authoritative. There are also a

number of books on the mathematics of quantum mechanics. The lectures of Amrein [A] are an elegant introduction. The book of Amrein, Jauch, and Sinha [AJS] is systematic and rigorous. The multiple volumes of Reed and Simon [RS1, RS2, RS3, RS4] contain a wealth of information. The text of Thirring [T] contains useful insights.

The reader should also consult texts on Hilbert space; Weidmann [W] has a good balance of theory and application. There are also several useful references on linear operator theory. The lectures of Nelson [N2] contain the basics. The book of Riesz and Nagy [RN] is a classic. The book of Kato [K] is a systematic account of perturbation theory.

## 1.2 The quantum scale

### 1.2.1 Planck's constant

Non-relativistic quantum mechanics is a physical theory. We begin with a deviation from mathematical tradition, actually writing numerical values, in order to show where this theory should play a role. Of course the answer is atomic and molecular and solid-state physics, but it is worth being reminded that this is also the study of quite ordinary matter in everyday experience. For the present we give no derivations or explanations, just numbers. Precision is not important; factors of 2 are chosen for later convenience.

Recall that physical quantities are usually expressed in consistent units of length $L$, mass $M$, and time $T$. The units of force are $ML/T^2$ and the units of energy are $ML^2/T^2$. For example in the meter, kilogram, second system the unit of force is the newton and the unit of energy is the joule. In the centimeter, gram, second system the unit of force is the dyne ($10^{-5}$ newton) and the unit of energy is the erg ($10^{-7}$ joule).

The characteristic sign of quantum mechanics is the appearance of *Planck's constant*

$$\hbar = 1.05 \times 10^{-27} \text{erg sec.} \tag{1.1}$$

This is actually the rationalized Planck's constant, that is, Planck's constant $h$ divided by $2\pi$. In general, we shall use the units that go with measuring radians instead of rotations. Thus we multiply frequencies by $2\pi$ to get angular frequencies, and similarly we divide wavelengths by $2\pi$ to get angular wavelengths.

The dimensions of Planck's constant are $ML^2/T$. This may be interpreted in various ways. Perhaps the simplest is $M \cdot L^2/T$, that is, mass times diffusion constant. Another is $ML^2/T^2 \cdot T$, energy times time. This allows conversions between energy and frequency. Still another is $ML/T \cdot L$,

momentum times length, which allows conversion between momentum and wave number.

It is interesting to see how something as small as Planck's constant determines properties of the world on the human scale. The article by Press and Lightman [14] contains a good account. Here are a few of the ideas.

### 1.2.2 Diffusion

In ordinary free motion distance is proportional to time, so the relevant measure is velocity with units $L/T$. In diffusive motion, the displacement is random, and on the average the displacement is only proportional to the square root of the time. Thus natural units for measuring the amount of diffusion are $L^2/T$. There are analogies between diffusion and quantum mechanics, so it is not surprising that a diffusion constant plays a role in quantum mechanics.

In quantum mechanics a particle of mass $m$ has diffusion constant

$$D = \frac{\hbar}{2m}. \tag{1.2}$$

Thus only masses on the molecular scale or smaller have a noticeable diffusion constant. On the atomic scale the typical mass is that of an electron. Then

$$m = 9.1 \times 10^{-28}\text{gm}, \tag{1.3}$$

and so

$$2D = \frac{\hbar}{m} = 1.16\text{cm}^2/\text{sec}. \tag{1.4}$$

This is actually a reasonable number on a human scale.

### 1.2.3 Speed

We can also use Planck's constant to associate a speed $v$ with a particle of charge $e$ by

$$v = \frac{Ke^2}{\hbar}. \tag{1.5}$$

Here $K$ is the constant that occurs in the Coulomb electrostatic force law $Ke^2/r^2$. In one system of units it is written as $1/(4\pi\epsilon_0)$; in another it is just 1. In any case, the units of $Ke^2$ are $ML^3/T^2$, so dividing by Planck's constant gives units $L/T$ of velocity.

For an electron $Ke^2 = 2.3 \times 10^{-19}$erg cm. This gives a velocity

$$v = 2.19 \times 10^8\text{cm/sec}. \tag{1.6}$$

The speed of light plays no role in the properties of bulk matter. The reason is that the speed of light is

$$c = 3 \times 10^{10} \text{cm/sec}, \tag{1.7}$$

and so the ratio of speeds is the *fine structure constant*

$$\alpha = \frac{v}{c} = \frac{e^2}{\hbar c} = \frac{1}{137}. \tag{1.8}$$

Thus the speed $v = \alpha c$, even for something as small as an electron, is non-relativistic.

### 1.2.4 Length

The ratio of these two numbers gives the Bohr radius

$$a = \frac{2D}{v} = \frac{\hbar^2}{mKe^2} = 0.53 \times 10^{-8} \text{cm}. \tag{1.9}$$

Thus the Bohr diameter $2a$ is about $1.06 \times 10^{-8}$ cm. A cube with this diameter has a volume of $1.2 \times 10^{-24}$ cm. Since the mass of a proton is about $1.7 \times 10^{-24}$ gm, the density of matter consisting of one proton for every such cube is 1.4 gm/ cm$^3$. Planck's constant is an essential ingredient in establishing the density of ordinary matter.

### 1.2.5 Energy

The natural unit of energy on the atomic scale is

$$R = \frac{1}{2}mv^2 = \frac{Ke^2}{2a} = \frac{1}{2}\frac{mK^2e^4}{\hbar^2} = \frac{1}{2}\alpha^2 mc^2 = 2.18 \times 10^{-11} \text{erg}. \tag{1.10}$$

Notice that while the energy unit may be written in terms of the fine structure constant and the speed of light, the factors of $c$ cancel, and this is a completely non-relativistic expression.

### 1.2.6 Compressibility

The typical bulk modulus (compressibility) of solid matter is of the order of its internal binding energy density, which gives a pressure

$$\frac{R}{(2a)^2} = 1.8 \times 10^{13} \text{dyne/cm}^2. \tag{1.11}$$

This is another number from everyday experience, at least from the experience of builders who expect structures to bear heavy compressive loads. (The typical shear modulus or tensile strength of solid matter is determined by molecular energies, and so is considerably smaller.)

### 1.2.7 Frequency

Planck's constant may also be used to associate an angular frequency $\omega$ with an energy, such as $2R$. In this case the result is

$$\omega = \frac{2R}{\hbar} = 4.15 \times 10^{16}/\text{sec}, \tag{1.12}$$

the frequency of ultraviolet light.

### 1.2.8 Other length scales

There are other length scales that arise from comparison with the speed of light.

The diffusion constant may be compared to the speed of light. This gives the angular *Compton wavelength*

$$\lambda\!\!\!^{-} = \frac{2D}{c} = \frac{\hbar}{mc} = \alpha a = 3.86 \times 10^{-11}\text{cm}. \tag{1.13}$$

Notice that this is considerably smaller than the Bohr radius.

On the other hand, there is an angular wavelength associated with the atomic units of angular frequency given by

$$\frac{c}{\omega} = \frac{c\hbar}{2R} = \frac{a}{\alpha} = 7.24 \times 10^{-7}\text{cm}. \tag{1.14}$$

This is about $1/\alpha = 137$ times the Bohr radius, so is a much larger distance. Light from atomic processes is on a much larger scale than atomic dimensions. This light is in the ultraviolet. Visible light generated by molecular processes is of even longer wavelength. In a sense, atoms are inherently invisible.

## 1.3 The Schrödinger equation

### 1.3.1 The equation

The idea that Schrödinger brought to quantum mechanics was to describe matter by a conservative linear wave equation. There is no way to derive

his equation; it is a physical law. However we shall see that the necessary presence of Planck's constant at least partially suggests the form of the equation.

In the following we shall consider waves moving in $\nu$ dimensional space. Of course in nature $\nu = 3$, but it is very useful to keep the extra generality; it helps put various formulas in a larger context.

The ingredients for a description of quantum motion are a mass parameter $m > 0$ and a real potential energy function $V(\mathbf{x})$ defined on $\mathbf{R}^\nu$. What is desired is a wave equation involving space and time variables. The ingredients in a wave equation are the time derivative, which has dimensions $1/T$ of frequency, and the space derivatives (gradient) $\nabla_{\mathbf{x}}$, which have dimensions $1/L$. The most natural second space derivative is $\nabla_{\mathbf{x}}^2 = \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}}$. This is the divergence of the gradient, that is, the Laplace operator. Its dimensions are $1/L^2$. The equation relates the action of these operators.

Here Planck's constant comes into play. With a mass $m$ comes a diffusion constant $D = \hbar/(2m)$. The corresponding differential operator $-D\nabla_{\mathbf{x}}^2$ has the dimensions of frequency. Similarly, the potential energy function $V(\mathbf{x})$ has the dimensions of energy, so $V(\mathbf{x})/\hbar$ also has the dimensions of frequency.

This suggests a wave equation relating the time derivative to the operator $-D\nabla_{\mathbf{x}}^2 + V(\mathbf{x})$. The obvious equation is the *diffusion equation*

$$\frac{\partial u}{\partial t} = D\nabla_{\mathbf{x}}^2 u - \frac{1}{\hbar} V(\mathbf{x}) u. \tag{1.15}$$

It is natural to think of the quantity $u$ as being some sort of density or concentration. This equation describes how the density changes with time.

For the diffusion equation we may define the flux $\mathbf{F} = -D\nabla_{\mathbf{x}} u$. This gradient vector field represents the flow from regions of high concentration to low concentration.

If we apply Gauss's theorem to a region $\Omega$ we obtain

$$\frac{d}{dt} \int_\Omega u \, d^\nu \mathbf{x} = -\int_{\partial\Omega} \mathbf{F} \cdot d\mathbf{S} - \frac{1}{\hbar} \int_\Omega V(\mathbf{x}) u \, d^\nu \mathbf{x} \tag{1.16}$$

This says that if there is a high concentration in the region, then the amount in the region decreases, due to the net flow out of the region represented by the first term, and also possibly due to the rate of destruction in the region represented by the second term.

The effect of the diffusion equation is to produce solutions that are increasingly uniform. The predominate effect on whatever initial structure is present is of damping or decay. This is a *dissipative* wave equation. Since structure is lost, it is only feasible to solve this equation forward in time.

Schrödinger was interested in an equation that described reversible mechanics rather than irreversible dissipation. He wanted oscillations instead of damping. He guessed the equation to be

$$i\frac{\partial \psi}{\partial t} = -D\nabla_{\mathbf{x}}^2\psi + \frac{1}{\hbar}V(\mathbf{x})\psi. \tag{1.17}$$

The inspiration was the factor of $i$. This made it into a *conservative* wave equation. The effect of changing the direction of time is simply the effect of complex conjugation, so this equation is equally good forward and backward in time.

### 1.3.2 Density and current

It is not obvious how to interpret the solution of the Schrödinger equation. The values of the wave function are complex. However the *density*

$$\rho = \psi^*\psi = |\psi|^2 \tag{1.18}$$

is real and in fact positive. In the standard interpretation of quantum mechanics $\rho$ is interpreted as a position probability density. However there is clearly other information in the wave function.

This information is contained in the *current*

$$\mathbf{J} = 2D\Im(\psi^*\nabla_{\mathbf{x}}\psi) = -iD(\psi^*\nabla_{\mathbf{x}}\psi - \nabla_{\mathbf{x}}\psi^*\psi). \tag{1.19}$$

This has the dimensions of a probability density times a velocity.

There is an important relation between the density and the current. It is the conservation law

$$\frac{\partial \rho}{\partial t} = -\nabla_{\mathbf{x}} \cdot \mathbf{J}. \tag{1.20}$$

This is proved by computing

$$\frac{\partial \psi^*\psi}{\partial t} = iD(\psi^*\nabla_{\mathbf{x}}^2\psi - \nabla_{\mathbf{x}}^2\psi^*\psi) = iD\nabla_{\mathbf{x}} \cdot (\psi^*\nabla_{\mathbf{x}}\psi - \nabla_{\mathbf{x}}\psi^*\psi). \tag{1.21}$$

If we apply the divergence theorem we obtain

$$\frac{d}{dt}\int_\Omega \rho\, d^\nu\mathbf{x} = -\int_{\partial\Omega} \mathbf{J} \cdot d\mathbf{S} \tag{1.22}$$

This says that the increase in probability for the region $\Omega$ is the flow into the region through the boundary $\partial\Omega$. This is a local conservation law.

If we take the limit as $\Omega$ approaches the whole space and assume that the boundary terms vanish, then we obtain

$$\frac{d}{dt}\int \rho\, d^\nu\mathbf{x} = 0. \tag{1.23}$$

This is a global conservation law for the total probability.

### 1.3.3 Osmotic and current velocity

Define the *current velocity* by

$$\mathbf{v}\rho = \mathbf{J} \tag{1.24}$$

and the *osmotic velocity* by

$$\mathbf{u}\rho = D\nabla_{\mathbf{x}}\rho. \tag{1.25}$$

It is easy to check that

$$-2iD\nabla_{\mathbf{x}}\psi/\psi = \mathbf{v} - i\mathbf{u}. \tag{1.26}$$

Therefore these velocity variables determine $\psi$ (up to a multiplicative constant).

Note that $\mathbf{v}$ changes sign under time reversal, while $\mathbf{u}$ keeps the same sign. This suggests that $\mathbf{v}$ resembles a fluid velocity, while $\mathbf{u}$ is more like a drift in a diffusion process.

Now introduce the complex velocity $\mathbf{w} = \mathbf{v} - i\mathbf{u}$. After some computation the Schrödinger equation may be written

$$-2iD\frac{1}{\psi}\frac{\partial\psi}{\partial t} + \frac{1}{2}\mathbf{w}^2 - iD\nabla_x \cdot \mathbf{w} = -\frac{1}{m}V(\mathbf{x}). \tag{1.27}$$

This gives

$$\left(\frac{\partial}{\partial t} + \mathbf{w}\cdot\nabla_x - iD\nabla_{\mathbf{x}}^2\right)\mathbf{w} = -\frac{1}{m}\nabla_x V(\mathbf{x}). \tag{1.28}$$

The imaginary part gives a variant of the current conservation equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}}\right)\mathbf{u} + \left(\mathbf{u}\cdot\nabla_{\mathbf{x}} + D\nabla_{\mathbf{x}}^2\right)\mathbf{v} = 0. \tag{1.29}$$

The real part gives the dynamical part of the Schrödinger equation

$$m\left(\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}}\right)\mathbf{v} + \left(\mathbf{u}\cdot\nabla_{\mathbf{x}} + D\nabla_{\mathbf{x}}^2\right)\mathbf{u}\right) = -\frac{1}{m}\nabla_x V(\mathbf{x}). \tag{1.30}$$

This is of the form mass times acceleration equals force. The first term in the acceleration is the usual acceleration term from fluid dynamics. The differential operator is the time derivative along the trajectory of the fluid particle moving with velocity $\mathbf{v}$. The second term is less familiar. The derivative is a stochastic derivative of the sort that arises when there is a drift $\mathbf{u}$ along with diffusion. This term is the contribution of quantum mechanics!

This form of writing the equation gives an indication of what to expect in the classical limit $\hbar \to 0$. Assume that in this limit $\rho$ and $\mathbf{v}$ have limiting values. Then $\mathbf{u} \to 0$ in this limit. So the limiting equation is just Newton's law of motion for a fluid particle moving in a gradient force field.

### 1.3.4 Momentum

Define the *momentum* operator by

$$\mathbf{P} = -i\hbar\nabla_{\mathbf{x}}. \tag{1.31}$$

Then

$$\psi^*\mathbf{P}\psi = m(\mathbf{v} - i\mathbf{u})\rho. \tag{1.32}$$

When we integrate this, we obtain

$$\int \psi^*\mathbf{P}\psi \, d^\nu\mathbf{x} = \int m\mathbf{v}\rho \, d^\nu\mathbf{x} = \int m\mathbf{J} \, d^\nu\mathbf{x}. \tag{1.33}$$

In the conventional interpretation of quantum mechanics this is the *expected momentum*.

Such quantities are naturally expressed in terms of inner products and norms. We define the *norm* $\|\psi\|$ by

$$\|\psi\|^2 = \int |\psi|^2 \, d^\nu\mathbf{x}. \tag{1.34}$$

(When taking the norm of a vector quantity we take the norm squared of the vector quantity before doing the integral.) For $\psi$ and $\phi$ with finite norm we define the *inner product* by

$$\langle\psi, \phi\rangle = \int \psi^*\phi \, d^\nu\mathbf{x}. \tag{1.35}$$

Thus for instance in the inner product notation the expression for the expected momentum is $\langle\psi, \mathbf{P}\psi\rangle$.

**Problems**

1. Why is $\int \mathbf{u}\rho \, d^\nu\mathbf{x} = 0$?
2. Show that $(d/dt)\int \mathbf{x}\rho \, d^\nu\mathbf{x} = \int \mathbf{v}\rho \, d^\nu\mathbf{x}$.
3. Show that $m(d/dt)\int \mathbf{v}\rho \, d^\nu\mathbf{x} = -\int \nabla_X V(\mathbf{x})\rho \, d^\nu\mathbf{x}$.

### 1.3.5 Energy

In addition to the conservation law for probability there is a conservation law for energy. The Schrödinger equation is usually written in energy units as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{x}}\psi + V(\mathbf{x})\psi. \tag{1.36}$$

This is also written as the operator equation

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi \tag{1.37}$$

where

$$H = -\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 + V(\mathbf{x}) = \frac{1}{2m}\mathbf{P}^2 + V(\mathbf{x}). \tag{1.38}$$

By applying the divergence theorem (in conditions in which the boundary terms are zero) we obtain

$$\langle\psi, H\psi\rangle = \frac{1}{2m}\|\mathbf{P}\psi\|^2 + \langle\psi, V(\mathbf{x})\psi\rangle = \langle H\psi, \psi\rangle. \tag{1.39}$$

This is the sum of two terms, corresponding to a kinetic energy and a potential energy.

We may write the conservation law for the total probability as

$$i\hbar\frac{d\|\psi\|^2}{dt} = \langle\psi, H\psi\rangle - \langle H\psi, \psi\rangle = 0. \tag{1.40}$$

This shows that the normalization $\|\psi\|^2 = 1$ can be maintained for all time.

The conservation law for the total energy is

$$i\hbar\frac{d\langle\psi, H\psi\rangle}{dt} = \langle\psi, H^2\psi\rangle - \langle H\psi, H\psi\rangle = 0. \tag{1.41}$$

Thus $\langle\psi, H\psi\rangle$ is also constant in time.

It is interesting to note that the expression for the energy density may be written

$$\frac{1}{2m}|\mathbf{P}\psi|^2 = (\frac{1}{2}m\mathbf{v}^2 + \frac{1}{2}m\mathbf{u}^2)\rho. \tag{1.42}$$

In the conventional interpretation of quantum mechanics the quantity

$$\frac{1}{2m}\|\mathbf{P}\psi\|^2 = \int \frac{1}{2m}|\mathbf{P}\psi|^2\, d^\nu\mathbf{x} = \int \frac{1}{2}m(\mathbf{v}^2 + \mathbf{u}^2)\rho\, d^\nu\mathbf{x} \tag{1.43}$$

is the *expected kinetic energy*. The quantity

$$\langle\psi, V(\mathbf{x})\psi\rangle = \int V(\mathbf{x})\rho\, d^\nu\mathbf{x} \tag{1.44}$$

is the *expected potential energy*. Their sum is of course the expected total energy. It is this quantity that is conserved.

## 1.4 The uncertainty principle

The expectation of the $j$th component of position is

$$\mu_{X_j} = \langle \psi, X_j \psi \rangle = \int x_j \rho \, d^\nu \mathbf{x}. \tag{1.45}$$

Its standard deviation is

$$\sigma_{X_j} = \|(X_j - \mu_{X_j})^2\| = \left( \int (x_j - \mu_{X_j})^2 \rho \, d^\nu \mathbf{x} \right)^{\frac{1}{2}}. \tag{1.46}$$

Similarly, the expectation of the $j$th component of momentum is

$$\mu_{P_j} = \langle \psi, P_j \psi \rangle = \int m v_j \rho \, d^\nu \mathbf{x}. \tag{1.47}$$

The standard deviation of the $j$th component of momentum is

$$\sigma_{P_j} = \|(P_j - \mu_{P_j})^2 \psi\| = \left( \int ((m v_j - \mu_{P_j})^2 + (m u_j)^2) \rho \, d^\nu \mathbf{x} \right)^{\frac{1}{2}}. \tag{1.48}$$

The famous *Heisenberg uncertainty principle* relates the second moments of momentum and position.

**Proposition 1** *For every $\psi$ we have*

$$\sigma_{X_j} \sigma_{P_j} \geq \hbar/2. \tag{1.49}$$

Proof: Integrate by parts to see that

$$\hbar/2 \int \rho \, d^\nu \mathbf{x} = -\hbar/2 \int (x_j - \mu_{X_j}) \frac{\partial \rho}{\partial x_j} \, d^\nu \mathbf{x} = - \int (x_j - \mu_{X_j}) m u_j \, d^\nu \mathbf{x}. \tag{1.50}$$

Apply the Schwarz inequality. It is amusing that one gets a bound involving only the osmotic velocity.

The significance of the Heisenberg uncertainty principle is that it is impossible to find a $\psi$ so that both the momentum and the position have small standard deviations. One application of this is to the situation when the total energy is the sum of a kinetic energy with a potential energy with a negative singularity. One want to show that the total energy cannot be too small. The kinetic energy always gives a positive contribution. If the kinetic energy is small, then the momentum must be small, so the position must have a large standard deviation. The argument is that the position cannot be concentrated near the singularity. So the energy cannot have a large

negative contribution from the potential energy, unless this contribution is compensated by a large positive contribution from the kinetic energy.

This argument is not valid. It is perfectly possible to have a probability distribution that has part concentrated close to the singularity, and another part that gives a large standard deviation. We shall see in the next section that a valid argument is possible, but it must use a stronger form of the uncertainty principle.

At this point the reader should be warned that in the orthodox interpretation of quantum mechanics the velocity fields $\mathbf{v}$ and $\mathbf{u}$ do not play a major role (nor does the current $\mathbf{J} = \mathbf{v}\rho$). The fundamental quantities are the operators, and the interpretation of these operators is through the spectral theorem.

It could be argued that $\mathbf{u}$ is a legitimate part of quantum mechanics, since it is derived from the density $\rho$, which in turn is something that can be obtained from position information. There is even a case to be made for $\mathbf{v}$, since the expectation of the momentum when the density is concentrated near a point $\mathbf{x}$ is approximately $m\mathbf{v}$ evaluated at $\mathbf{x}$. Nevertheless we henceforth abandon the use of these quantities.

## 1.5 Quantum stability

Quantum mechanics does not always resemble classical mechanics. The uncertainty principle in quantum mechanics makes quantum mechanics more stable than classical mechanics.

Let us look at the hydrogen atom where

$$H = \frac{1}{2m}\mathbf{P}^2 - \frac{Ke^2}{r}. \tag{1.51}$$

The first term is a kinetic energy term involving the mass $m > 0$ of the electron. The second term is a potential energy term. It represents the electrostatic potential energy of a proton with charge $e$ and an electron with charge $-e$ at a distance $r = |\mathbf{x}|$. (For simplicity we take the proton at the origin and take its mass to be infinite.) Notice that this potential energy becomes singular as the electron approaches the proton.

We shall show that in quantum mechanics this singularity is perfectly harmless. The argument uses a refinement of the Heisenberg uncertainty principle. Because of its immediate application, we call it the Hydrogen uncertainty principle. It says that

$$\|\mathbf{P}\psi\|\langle\psi, \frac{1}{r}\psi\rangle^{-1} \geq ((\nu - 1)/2)\hbar. \tag{1.52}$$

In physics we are of course interested in the case $\nu = 3$, so the factor on the right is just one.

The quantity

$$\langle \psi, \frac{1}{r}\psi \rangle^{-1} = (\int \frac{1}{r}\rho \, d^{\nu}\mathbf{x})^{-1} \tag{1.53}$$

is the *harmonic mean* of the radius, and is a measure of the spread of the position from the origin. The principle thus says that a small kinetic energy makes a large spread in the position, while a small spread in the position makes a large kinetic energy. The intuition for the hydrogen atom is that an electron too close to a proton gains a kinetic energy which kicks it away again.

Take the case $\nu = 3$ of physical interest. We prove that for all $\psi$ with $\|\psi\|^2 = 1$ the total energy

$$\frac{1}{2m}\|\mathbf{P}\psi\|^2 - \langle \psi, \frac{Ke^2}{r}\psi \rangle \geq -R = -\frac{mK^2e^4}{\hbar^2}. \tag{1.54}$$

We show that this follows from the Hydrogen uncertainty principle. The principle give a lower bound

$$\frac{\hbar^2}{2m}\langle \psi, \frac{1}{r}\psi \rangle^2 - Ke^2\langle \psi, \frac{1}{r}\psi \rangle. \tag{1.55}$$

This is a polynomial in $\langle \psi, (1/r)\psi \rangle$ which assumes its minimum at $1/a$, where $a = \hbar^2/(mKe^2)$ is the Bohr radius. Putting in this value gives the lower bound.

Now we give the proof of the Hydrogen uncertainty principle. Since $|\partial\psi/\partial r| \leq |\nabla_{\mathbf{x}}\psi|$, it is sufficient to prove the principle with just the radial derivative. Recall that the unit of volume in $\nu$ dimensions in polar coordinates involves the differential $r^{\nu-1}\,dr$. This factor will come in when we integrate by parts. Let $c$ be a real constant. Compute

$$0 \leq \|(\frac{\partial}{\partial r} + c)\psi\|^2 = \langle \psi, -\frac{1}{r^{\nu-1}}(\frac{\partial}{\partial r} - c)r^{\nu-1}(\frac{\partial}{\partial r} + c)\psi \rangle. \tag{1.56}$$

This works out to

$$\langle \psi, (-\frac{1}{r^{\nu-1}}\frac{\partial}{\partial r}r^{\nu-1}\frac{\partial}{\partial r} - (\nu-1)c\frac{1}{r} + c^2)\psi \rangle = \|\frac{\partial}{\partial r}\psi\|^2 - (\nu-1)c\langle \psi, \frac{1}{r}\psi \rangle + c^2. \tag{1.57}$$

Thus the right hand side is greater than or equal to zero for all real $c$. This is equivalent to the Hydrogen uncertainty principle.

We can also get the bound on the energy directly by taking $\nu = 3$ and $c = 1/a$, where $a$ is the Bohr radius. We see as a corollary that the only

function $\psi$ for which the bound is obtained satisfies

$$\left(\frac{\partial}{\partial r} + \frac{1}{a}\right)\psi = 0. \tag{1.58}$$

The solution is

$$\psi = C\exp(-\frac{r}{a}). \tag{1.59}$$

This is in fact the hydrogen ground state wave function.

In the classical limit $\hbar \to 0$ we have also $a \to 0$. The ground state collapses to a point, and the energy becomes negative infinite. It is important to have quantum mechanics; otherwise all matter would collapse under electrostatic attraction.

**Problems**

1. Show that the harmonic mean is less than the arithmetic mean: $1/\langle\psi, (1/r)\psi\rangle \le \langle\psi, r\psi\rangle$.

2. Show that the first moment is less than the second moment: $\langle\psi, r\psi\rangle \le \langle\psi r^2\psi\rangle^{1/2}$.

3. Show that the Hydrogen uncertainty principle gives the following version of the Heisenberg uncertainty principle in dimension 3:

$$\|\mathbf{P}\psi\|\langle\psi, r^2\psi\rangle^{1/2} \ge \hbar.$$

4. Define the probability

$$\Pr[r \le \epsilon] = \int_{r\le\epsilon} \rho\, d^3\mathbf{x}.$$

Show that $\hbar \Pr[r \le \epsilon] \le \epsilon\|\mathbf{P}\psi\|$.

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# Chapter 2

# Hilbert Space

We have seen that the wave functions (regarded as functions of the space variable) have a natural notion of inner product. Various quantum mechanical notions are defined in terms of this inner product. The space of all wave functions such that the corresponding norm is finite forms a Hilbert space.

This chapter defines the abstract notion of Hilbert space. It also introduces the concept of operator acting in Hilbert space. Particularly important are the bounded operators, which are defined on the whole space and are continuous. Some elementary properties of bounded operators are presented.

## 2.1 Definition

The mathematical setting for quantum mechanics is Hilbert space.

**Definition 1** *A* Hilbert space *is a vector space with complex scalars and with an inner product. It must be a complete metric space in the norm defined by the inner product.*

Let us emphasize the elements of this definition. A *vector space* (or *linear space*) is a set of elements (called vectors) together with a definition of addition of vectors and multiplication of vectors by scalars. These operations must satisfy the well known vector space axioms. We denote the sum of two vectors $\psi$ and $\phi$ by $\psi + \phi$ and the product of the complex number $z$ with the vector $\psi$ by $z\psi$.

An *inner product* is a function defined on ordered pairs of vectors and with scalar values. Normally the inner product of the vectors $\psi$ and $\phi$ is

denoted $\langle \psi, \phi \rangle$. It must satisfy the Hermitian symmetry condition

$$\langle \psi, \phi \rangle = \langle \phi, \psi \rangle^*. \tag{2.1}$$

Here $z^*$ denotes the complex conjugate of the complex number $z$. In addition it must be strictly positive on ordered pairs consisting of the same non-zero vector twice. The positivity condition is thus

$$\langle \psi, \psi \rangle > 0 \quad \text{for} \quad \psi \neq 0. \tag{2.2}$$

Finally it must be linear in one variable and conjugate linear in the other variable.

There is unfortunately a difference in the conventions of mathematics and physics about which variable is linear and which is conjugate linear. In physics the first variable is conjugate linear and the second variable is linear. In mathematics it is just the opposite. We adopt the physics convention. Thus

$$\langle z\psi, \phi \rangle = z^* \langle \psi, \phi \rangle, \tag{2.3}$$

$$\langle \psi, z\phi \rangle = z \langle \psi, \phi \rangle. \tag{2.4}$$

The advantage of this convention is that the function $\langle \psi, \cdot \rangle$ that sends $\phi$ into $\langle \psi, \phi \rangle$ is linear and takes its argument on the right, in accordance with usual convention for functions.

The *quadratic form* associated with the inner product is the function from vectors to scalars defined by assigning to the vector $\psi$ the value $\langle \psi, \psi \rangle$. This quadratic form is strictly positive except on the zero vector. The length or *norm* of a vector $\psi$ is defined by

$$\|\psi\| = \sqrt{\langle \psi, \psi \rangle}. \tag{2.5}$$

Thus the quadratic form is the square of the norm.

It is assumed that the reader knows the basic facts about inner products and norms. Perhaps the most basic computation is

$$0 \leq \|\psi + \phi\|^2 = \|\psi\|^2 + 2\Re\langle \psi, \phi \rangle + \|\phi\|^2. \tag{2.6}$$

We say that two vectors $\psi$ and $\phi$ are *orthogonal* (*perpendicular*) if $\langle \psi, \phi \rangle = 0$. We may also indicate that the vectors are orthogonal by writing $\psi \perp \phi$. Such vectors satisfy the *theorem of Pythagoras* $\|\psi + \phi\|^2 = \|\psi\|^2 + \|\phi\|^2$.

If $\psi$ and $\phi$ are arbitrary unit vectors, so that $\|\psi\| = 1$ and $\|\psi\| = 1$, then the basic computation gives $-\Re\langle \psi, \phi \rangle \leq 1$. It follows easily by scaling that for arbitrary vectors $\psi$ and $\phi$ we have the *Schwarz inequality*

$$\langle \psi, \phi \rangle \leq \|\psi\| \|\phi\|. \tag{2.7}$$

It is a remarkable fact about complex Hilbert space that the inner product may be expressed in terms of the quadratic form. The following proposition gives the explicit formula.

**Proposition 2** *The inner product may be expressed in terms of the quadratic form by the* polarization identity*:*

$$4\langle\psi,\phi\rangle = \langle\phi+\psi,\phi+\psi\rangle + i\langle\phi+i\psi,\phi+i\psi\rangle - \langle\phi-\psi,\phi-\psi\rangle - i\langle\phi-i\psi,\phi-i\psi\rangle. \tag{2.8}$$

The distance between two vectors $\psi$ and $\phi$ is defined to be $\|\psi-\phi\|$. This makes it possible to define the notion of convergence. The requirement that the Hilbert space $\mathcal{H}$ be *complete* means that every Cauchy sequence of vectors belonging to $\mathcal{H}$ converges to a limiting vector in the same Hilbert space $\mathcal{H}$ .

**Definition 2** *An* isomorphism *of Hilbert spaces is a linear transformation $W$ from one Hilbert space $\mathcal{H}$ onto another Hilbert space $\mathcal{K}$ that preserves the inner product:*

$$\langle W\psi, W\phi\rangle = \langle\psi,\phi\rangle. \tag{2.9}$$

*Such a transformation is also called a* unitary *operator.*

Note that by the polarization identity, if $W$ preserves the Hilbert space norm, then it automatically preserves the inner product.

The simplest concrete example of a Hilbert space is obtained by taking a set $J$ and defining $\ell^2(J)$ as the set of all functions $f$ from $J$ to the complex numbers such that $\sum_j |f(j)|^2 < \infty$. The inner product of $f$ and $g$ in this Hilbert space is just $\langle f,g\rangle = \sum_j f(j)^* g(j)$.

It will be shown that every Hilbert space is isomorphic to some $\ell^2(J)$. The *dimension* of the Hilbert space is the number of points in $J$. Thus all Hilbert spaces of the same dimension are isomorphic.

In an alternative approach one could dispense with the axioms for vector spaces and inner products and define a Hilbert space as a space with notions of sum and scalar multiplication and inner product that satisfy all the properties that hold true in $\ell^2(J)$. This approach would not be elegant, but it would give a good idea of the truth.

The Hilbert spaces used in quantum mechanics are either finite dimensional or have countable infinite dimension. In fact most problems are formulated in a Hilbert space of countable infinite dimension. Up to isomorphism there is only one Hilbert space of this dimension!

Here is an important example (or rather counter-example). Assume for the moment that $J$ is infinite. Consider the linear subspace of $\ell^2(J)$

consisting of all $f$ with finite support. This is an example of an inner product space that is not complete and hence not a Hilbert space. It is clear that every element of $\ell^2(J)$ is a limit of elements from this subspace, so this is actually an example of a dense linear subspace of the Hilbert space.

**Problems**

1. Say that $\phi_j$ for $j$ in some index set $J$ is is a family of mutually orthogonal vectors. Prove the theorem of Pythagoras $\| \sum_j \phi_j \|^2 = \sum_j \|\phi_j\|^2$ when $J$ is finite.

2. Prove it when $J$ is infinite. In particular, show that when the numerical sum on the right hand side is finite, then the vector sum $\sum_j \phi_j$ must converge.

## 2.2 Self-duality

It is an obvious consequence of the Schwarz inequality that for every $\psi$ in the Hilbert space $\mathcal{H}$ the function $\langle \psi, \cdot \rangle$ is a continuous linear complex function on $\mathcal{H}$. It is a consequence of completeness that every continuous linear complex function on $\mathcal{H}$ is of this form. A continuous linear complex function is said to be a member of the *dual space*, so this says that every Hilbert space is self-dual.

**Theorem 1** *Every Hilbert space is self-dual. If $L$ is a continuous linear complex function on a Hilbert space $\mathcal{H}$, then there exists a vector $\psi$ in $\mathcal{H}$ such that*

$$L(\phi) = \langle \psi, \phi \rangle. \tag{2.10}$$

Proof: Since $L$ is continuous and linear, there is a constant $M$ such that $|L(\phi)| \leq M\|\phi\|$ for all $\phi$ in $\mathcal{H}$. Define the complex function $I$ on $\mathcal{H}$ by

$$I(\psi) = \frac{1}{2}\|\psi\|^2 - \Re L(\psi). \tag{2.11}$$

Since

$$I(\psi) \geq \frac{1}{2}\|\psi\|^2 - M\|\psi\| \geq -\frac{1}{2}M^2, \tag{2.12}$$

$I$ is bounded below. Let $b$ be the infimum of $I$.

The crucial step in the proof is the identity:

$$I(\frac{\psi + \psi'}{2}) + \frac{1}{4}\|\psi - \psi'\|^2 = \frac{1}{2}I(\psi) + \frac{1}{2}I(\psi'). \tag{2.13}$$

Let $\psi_n$ be a sequence of vectors in $\mathcal{H}$ such that $I(\psi_n) \to b$. The above identity shows that

$$b + \frac{1}{4}\|\psi_n - \psi_m\|^2 \leq \frac{1}{2}I(\psi_n) + \frac{1}{2}I(\psi_m). \tag{2.14}$$

Thus $\psi_n$ is a Cauchy sequence and hence converges to some $\psi$ in $\mathcal{H}$. It is not difficult to see that $I(\psi) = b$.

The proof is completed by noting that where the minimum is assumed the differential in any direction $\phi$ must be zero. This says that

$$\Re\langle\psi, \phi\rangle - \Re L(\phi) = 0. \tag{2.15}$$

The same argument works for $i\phi$, so the imaginary part is also zero. This proves the theorem. Q.E.D.

Actually, the statement that the Hilbert space is self-dual is slightly misleading. For each $\psi$ the function $\langle\psi, \cdot\rangle$ gives an element of the dual space, and every element is obtained this way. Note however that $\langle z\psi, \cdot\rangle = z^*\langle\psi, \cdot\rangle$. Thus the correspondence between vectors and elements of the dual space is conjugate linear.

On the other hand, for each $\chi$ the function $\langle\cdot, \chi\rangle$ gives an element of the conjugate dual space. Furthermore $\langle\cdot, z\chi\rangle = z\langle\cdot, \chi\rangle$. The correspondence between vectors and elements of the conjugate dual space is linear.

Dirac introduced a notation that is sometimes convenient. The element of the Hilbert space $\phi$ is also denoted $|\ \phi\rangle$ and called a "ket." The element $\langle\psi, \cdot\rangle$ of the dual space corresponding to a vector $\psi$ is denoted $\langle\psi\ |$ and called a "bra." The complex number $\langle\psi, \phi\rangle$ is written $\langle\psi\ |\ \phi\rangle$ and called a "bracket." That a joke this feeble could persist in the physics literature is truly remarkable. Nevertheless, it is convenient to have a notation for elements of the dual space, and the Dirac notation does provide this.

Dirac actually used an extended notation in which some of the linear functionals are not continuous functionals on the Hilbert space and hence are not represented by vectors in the Hilbert space. We shall look at this situation during the discussion of generalized bases.

**Problems**

1. Give an example of a dense linear subspace of a Hilbert space and a continuous linear functional on this space that is not represented by a vector in the subspace.

2. Give an example of a dense linear subspace of a Hilbert space and a linear functional on this space that is not represented by a vector in the Hilbert space.

## 2.3 Projections

If $\mathcal{H}$ is a Hilbert space, a *linear subspace* is a subspace in the vector space sense. It is not necessarily a Hilbert space with respect to the inner product of $\mathcal{H}$, since it need not be complete. (However it may be a Hilbert space with a different inner product!)

It may be shown that a linear subspace $M$ of $\mathcal{H}$ is a Hilbert space with respect to the inner product of $\mathcal{H}$ if and only if it is a closed linear subspace. The following result is the *projection theorem* for such closed subspaces.

**Theorem 2** *Let $\mathcal{H}$ be a Hilbert space and $M$ be a closed linear subspace. Let $\chi$ be a vector in $\mathcal{H}$. Then there exists a vector $\psi$ in $M$ that is the orthogonal projection of $\chi$ onto $M$, that is,*

$$\langle \chi - \psi, \phi \rangle = 0 \tag{2.16}$$

*for all $\phi$ in $M$.*

Proof: Since $M$ is a closed subset of a complete metric space, it is itself a complete metric space. Thus $M$ is a Hilbert space. Define the linear function $L$ on $M$ by

$$L(\phi) = \langle \chi, \phi \rangle. \tag{2.17}$$

This is continuous, by the Schwarz inequality. Therefore by the self-duality of Hilbert space there is a vector $\psi$ in $M$ with

$$\langle \chi, \phi \rangle = \langle \psi, \phi \rangle \tag{2.18}$$

for all $\chi$ in $M$. This completes the proof.

Note that the function that is minimized in the proof of the self-duality theorem is

$$I(\psi) = \frac{1}{2}\|\psi\|^2 - \Re\langle \chi, \psi \rangle = \frac{1}{2}\|\psi - \chi\|^2 - \frac{1}{2}\|\chi\|^2. \tag{2.19}$$

Thus the orthogonal projection minimizes the distance to the vector $\chi$.

**Definition 3** *Let $M$ be a linear subspace of $\mathcal{H}$. Then $M^\perp$ is the closed linear subspace of all vectors in $\mathcal{H}$ that are orthogonal to $M$.*

The projection theorem above says that if $M$ is a closed linear subspace, then every vector may be written as the sum of a vector in $M$ and a vector in $M^\perp$.

In general if $M$ and $N$ are orthogonal closed subspaces, then we write $M \oplus N$ for the closed subspace consisting of all sums of vectors from the two subspaces. In this notation the projection theorem says that $\mathcal{H} = M \oplus M^\perp$.

**Lemma 1** *If $M$ is a closed linear subspace of $\mathcal{H}$, then $M^{\perp\perp} = M$.*

Proof: It is obvious that $M$ is contained in $M^{\perp\perp}$. On the other hand, if $\chi$ is a vector in $M^{\perp\perp}$, then $\chi$ has a projection $\psi$ onto $M$. Since $\chi - \psi$ is in $M^{\perp}$ and also in $M^{\perp\perp}$, it must be zero. Thus $\chi = \psi$ is in $M$. This shows that $M^{\perp\perp}$ is contained in $M$.

The closure of a linear subspace $M$ is denoted $\bar{M}$ and is a closed linear subspace. Note that the closure $\bar{M}$ satisfies $\bar{M}^{\perp} = M^{\perp}$. This gives the projection theorem in the following form.

**Theorem 3** *If $M$ is a linear subspace of $\mathcal{H}$, then $M^{\perp\perp} = \bar{M}$.*

**Corollary 1** *If $M$ is a linear subspace of $\mathcal{H}$, then $M$ is dense in $\mathcal{H}$ (that is $\bar{M} = \mathcal{H}$) if and only if $M^{\perp} = \{0\}$.*

**Problems**

1. Give an example of a linear subspace of a Hilbert space that is dense but not the whole space.

2. Give an example of two such linear spaces that have only the zero vector in common. (Hint: Let $g$ be in $\ell^2(\mathbf{N})$. For $0 < \epsilon < 1$ let $f^\epsilon(n) = (1-\epsilon)\sum_{m\le n}\epsilon^m g(n-m)$. Show that $f^\epsilon \to g$ in the $\ell^2$ norm as $\epsilon \to 0$. Show that $f^\epsilon = 0$ implies $g = 0$.)

## 2.4 Operators

Additional structure is needed to make Hilbert space interesting. An *operator* $A$ acting in $\mathcal{H}$ is a linear transformation from a linear subspace $D(A)$ of $\mathcal{H}$ to $\mathcal{H}$.

Two operators, $A$ acting in $\mathcal{H}$ and $B$ acting in $\mathcal{K}$, are *isomorphic* if there is a unitary operator $W$ from $\mathcal{H}$ to $\mathcal{K}$ such that $W$ takes $D(A)$ onto $D(B)$ and $WA\psi = BW\psi$ for all $\psi$ in $D(A)$. Then $A = W^{-1}BW$ is just a disguised form of $B$. We shall see that isomorphism of operators is an valuable concept.

A *densely defined* operator $A$ is an operator such that $D(A)$ is dense in $\mathcal{H}$. Let $A$ be a densely defined operator. The adjoint $A^*$ is the operator consisting of all $\psi$ in $\mathcal{H}$ such that there is a vector $A^*\psi$ in $\mathcal{H}$ with

$$\langle A^*\psi, \phi\rangle = \langle \psi, A\phi\rangle \tag{2.20}$$

for all $\phi$ in $D(A)$.

It follows from the fact that $D(A)$ is dense in $\mathcal{H}$ that the vector $A^*\psi$ is uniquely determined by $A$ and $\psi$.

If $A$ is an operator, then its domain may be given the *domain inner product*

$$\langle \psi, \phi \rangle_{D(A)} = \langle \psi, \phi \rangle + \langle A\psi, A\phi \rangle. \tag{2.21}$$

The associated norm is

$$\|\psi\|^2_{D(A)} = \|\psi\|^2 + \|A\psi\|^2. \tag{2.22}$$

Notice that $\|A\psi\| \leq \|\psi\|_{D(A)}$, so the operator $A$ is continuous from $D(A)$ to $\mathcal{H}$, provided that $D(A)$ is given the domain norm instead of the norm inherited from $\mathcal{H}$.

A *closed* operator is an operator such that $D(A)$ with the domain inner product is a Hilbert space.

The closed densely defined operators are a reasonable class of operators. The reason is the following (proofs to come later). If $A$ is densely defined, then $A^*$ is a closed operator. If $A$ is a closed operator, then $A^*$ is densely defined. If $A$ is a closed densely defined operator, then $A^{**} = A$.

In Dirac's notation the action of an operator $A$ on a ket $\mid \phi\rangle$ is written $A \mid \phi\rangle$ and is defined to be $\mid A\phi\rangle$. The action on a bra $\langle\psi\mid$ is written $\langle\psi \mid A$ and is $\langle A^*\psi \mid$. Thus it is consistent to write $\langle\psi \mid A \mid \phi\rangle$ for $\langle A^*\psi, \phi\rangle = \langle\psi, A\phi\rangle$.

## 2.5 Bounded operators

A linear transformation $A$ from a Hilbert space $\mathcal{H}$ to itself is said to be a *bounded operator* if there exists a constant $M$ such that $\|A\psi\| \leq M\|\psi\|$ for all $\psi$ in $\mathcal{H}$. The least such $M$ is called the *uniform norm* of $A$ and is written $\|A\|_\infty$. This norm is used so often that it is written as $\|A\|$ when the context is clear. Notice that the $\infty$ refers to the fact that this is a bound on the maximum size of the operator, and does not refer to the space on which the operator is acting, which could of course be $\ell^2$.

A bounded operator is closed and densely defined. It is not difficult to see that a linear operator defined on the Hilbert space is bounded if and only if it is continuous.

One special property of the norm is that it is related to multiplication (composition) of operators in a pleasant way. In fact, the general inequality that holds is $\|AB\| \leq \|A\|\|B\|$.

It is important to realize that there is more than one natural notion of convergence for bounded operators. A sequence $A_n$ is said to *converge in norm* (or *uniformly*) to $A$ if $\|A_n - A\| \to 0$ as $n \to \infty$. It is said to

*converge strongly* (or *pointwise*) if for every $\psi$ in $\mathcal{H}$ $A_n\psi \to A\psi$ in the $\mathcal{H}$ norm as $n \to \infty$. Since $\|A_n\psi - A\psi\| \leq \|A_n - A\|\,|\psi\|$, it is clear that norm convergence implies strong convergence. Norm convergence is clearly more desirable; we will usually have only strong convergence.

Self-duality plays an important role in Hilbert space theory. One example is with respect to the notion of adjoint operator of a bounded operator.

**Proposition 3** *Let $A$ be a bounded operator acting in $\mathcal{H}$. Then the adjoint operator $A^*$ is also bounded. For all $\psi$ and $\phi$ in $\mathcal{H}$ we have*

$$\langle \psi, A\phi \rangle = \langle A^*\psi, \phi \rangle. \tag{2.23}$$

Proof: Fix $\psi$. Then the function that sends $\phi$ to $\langle \psi, A\phi \rangle$ is continuous. Therefore there is a vector $A^*\psi$ given by the self-duality theorem.

We can see that $\|A^*\| \leq \|A\|$ from the calculation

$$\|A^*\psi\|^2 = \langle \psi, AA^*\psi \rangle \leq \|\psi\|\|AA^*\psi\| \leq \|\psi\|\|A\|\|A^*\psi\|. \tag{2.24}$$

For bounded operators it is not hard to check that $A^{**} = A$. It follows easily from this that $\|A^*\| = \|A\|$.

The notion of adjoint of an operator is related to the notion of orthogonal complement of a subspace.

**Proposition 4** *Let $M$ be a linear subspace of $\mathcal{H}$ that is invariant under a bounded operator $A$. Then $M^\perp$ is invariant under $A^*$.*

Proof: Assume that for every $\psi$ in $M$ we have also $A\psi$ in $M$. Let $\phi$ be in $M^\perp$. Then for every $\psi$ in $M$ we have $\langle A^*\phi, \psi \rangle = \langle \phi, A\psi \rangle = 0$. Thus $A^*\phi$ must be in $M^\perp$.

**Corollary 2** *Let $M$ be a linear subspace of $\mathcal{H}$ that is invariant under a bounded operator $A$ and its adjoint $A^*$. Then $M^\perp$ is invariant under $A$ and $A^*$.*

How is this used? Assume that $M$ is a closed linear subspace of $\mathcal{H}$. By the projection theorem $\mathcal{H} = M \oplus M^\perp$, where $M^\perp$ is the orthogonal complement of $M$ in $\mathcal{H}$. Both $M$ and $M^\perp$ are Hilbert spaces. If $A$ leaves both $M$ and $M^\perp$ invariant, then the study of $A$ in the Hilbert space $\mathcal{H}$ can be reduced to the study of two operators: the restriction of $A$ to $M$ and the restriction of $A$ to $M^\perp$.

Thus if $\chi$ is in $\mathcal{H}$, we may compute $A\chi$ by writing $\chi = \psi + \phi$, with $\psi$ in $M$ and $\phi$ in $M^\perp$. Then $A\psi$ is in $M$ and $A\phi$ is in $M^\perp$ and from these we recover $A\chi = A\psi + A\phi$.

**Problems**

1. Show that if $A$ and $B$ are bounded, then $(AB)^* = B^*A^*$.
2. Show that $A^*A$ is its own adjoint. (Assume $A$ is bounded.)
3. Show that $\|A\|^2 = \|A^*A\|$.
4. Let $M$ be a closed subspace. Define an operator $E$ by setting $E\chi = \psi$, where $\psi$ is the orthogonal projection of $\chi$ onto $M$. Show that $E^2 = E$.
5. Show that $E$ is bounded. What is its norm?
6. Show that $E^* = E$.
7. Express the projection onto $M^\perp$ in terms of $E$.
8. Let $A$ be a bounded operator. Then $M$ is invariant under $A$ if and only if $AE = EAE$.
9. Let $A$ be a bounded operator. Then $M$ is invariant under $A$ and $A^*$ if and only if $AE = EA$.

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# Chapter 3

# Function Spaces

This chapter introduces the standard concrete realization of a Hilbert space as an $L^2$ space. It also gives criteria for recognizing integral operators as bounded operators. This gives the world of reality that corresponds to the Platonic world of the chapter on Hilbert space.

## 3.1 Integration

Let $X$ be a set. We say that $X$ is a *measurable space* if there is given a vector space of real functions on $X$ with the following properties. The space should contain the constant functions. If $f$ is in the space, then so is $|f|$. If $f_n$ is a sequence of functions in the space, and $f_n \to f$ pointwise, then $f$ is in the space. The functions in this space are called real *measurable functions*.

Example: Let $J$ be a set. Take all functions to be measurable.

Example: Let $X$ be $\mathbf{R}^\nu$. Consider the smallest set of functions that contain the continuous functions and is closed under pointwise convergence. This is called the space of *Borel measurable* functions.

The notion of measurable set is a special case of the notion of measurable function. Let $f = 1_S$ be the indicator function of a subset $S$ of $X$. The subset $S$ is said to be measurable if the function $1_S$ is measurable.

The definition of a space of measurable functions ensures that the space is closed under numerous nonlinear operations beside the absolute value.

For example, if $f$ and $g$ are measurable, then so are the maximum $\max(f, g)$ and the minimum $\min(f, g)$. This is because $\max(f, g) = (f + g + |f - g|)/2$ and $\min(f, g) = (f + g - |f - g|)/2$.

In particular, if $f$ be a real measurable function then its positive and negative parts $f_+ = \max(f, 0)$ and $f_- = -\min(f, 0)$ are also measurable.

Also, if $f$ is measurable, then for each real $a$ the set where $f > a$ is measurable. It is sufficient to prove this when $a = 0$. However the pointwise limit as $n \to \infty$ of $\min(nf_+, 1)$ is the indicator function of the set where $f > 0$.

An easy consequence is that for each real $a$ and $b$ with $a < b$ the set where $a < f \leq b$ is measurable. (Subtract the indicator function of $b < f$ from that of $a < f$.)

If follows easily from this that if $f$ is measurable and $\phi$ is continuous, then the function $\phi(f)$ (the composition) is measurable. The reason is that for each $n$ the function $\sum_k \phi(k/n) 1_{\{k/n < f \leq (k+1)/n\}}$ is measurable. If $\phi$ is continuous, then for the limit as $n \to \infty$ of these functions is $\phi(f)$. (For each $x$ the value of $k/n$ that is relevant is within $1/n$ of $f(x)$, so the value of $\phi(k/n)$ is correspondingly close to $\phi(f(x))$.)

The conclusion of this line of reasoning is the following proposition.

**Proposition 5** *If $f$ is a measurable function and $\phi$ is a Borel measurable function, then the composition $\phi(f)$ is a measurable function.*

The proof is to note that Borel measurable functions may be obtained from continuous functions by repeated limits.

Finally, we note that the product of measurable functions is measurable. This follows from the fact that $fg = ((f + g)^2 - (f - g)^2)/4$.

An *integral* (or *measure* ) is a mapping that associates to every measurable function $f \geq 0$ a number $\int f \, d\mu$ with

$$0 \leq \int f \, d\mu \leq \infty. \tag{3.1}$$

It must satisfy the properties

$$\int (f + g) \, d\mu = \int f \, d\mu + \int g \, d\mu \tag{3.2}$$

and

$$\int af \, d\mu = a \int f \, d\mu \tag{3.3}$$

for $a \geq 0$. It must also satisfy the monotone convergence property that if $0 \leq f_n \uparrow f$ pointwise, then

$$\int f_n \, d\mu \uparrow \int f \, d\mu. \tag{3.4}$$

The usual notion of measure is a special case of the notion of integral. Let $f = 1_S$ be the indicator function of a subset $S$ of $X$. The subset $S$ is measurable if the function $1_S$ is measurable. The measure of the set is then $\mu(S) = \int 1_S \, d\mu$.

Let $f$ be a real measurable function. Then its positive and negative parts $f_+$ and $f_-$ are also measurable and since $f_+ \geq 0$ and $f_- \geq 0$, their integrals are defined. If at least one of these integrals is finite, then we may define

$$\int f \, d\mu = \int f_+ \, d\mu - \int f_- \, d\mu. \tag{3.5}$$

If both these integrals are $\infty$, then we have the indeterminate expression $\infty - \infty$, and the integral is not defined. (Notice that this definition is ruling out all "improper" integrals that are not absolutely convergent.)

It is a consequence of the axioms that the integral is order preserving, that is, if $f \leq g$, then

$$\int f \, d\mu \leq \int g \, d\mu. \tag{3.6}$$

Furthermore the more general monotone convergence theorem holds.

**Theorem 4** *Assume that $f_n \uparrow f$ pointwise and $-\infty < \int f_1 \, d\mu$. Then $\int f_n \, d\mu \uparrow \int f \, d\mu$. Similarly, assume that $g_n \downarrow g$ and $\int g_1 \, d\mu < +\infty$. Then $\int g_n \, d\mu \downarrow \int g \, d\mu$.*

There is one special class of integrals with particular significance. If $\int c \, d\mu = c$ for each constant $c$, then the integral is called an *expectation*. The measurable functions are called *random variables* and the measurable sets are called *events*. The points of the space $X$ are called outcomes. The measure of a measurable set of outcomes is called the *probability* of the event. Usually when we have this situation we refer to the integral or the measure as a *probability measure*.

A complex function is said to be measurable if its real and imaginary parts are measurable. The absolute value of a complex measurable function is a real measurable function.

If the real and imaginary parts of a complex measurable function have finite integrals, then the integral of the function is defined in the obvious way. It may also be shown that

$$\left| \int f \, d\mu \right| \leq \int |f| \, d\mu. \tag{3.7}$$

The standard example of an integral is when the measurable functions are Borel functions on $\mathbf{R}^\nu$ and the integral of a measurable function $f$ is the usual $\int f(\mathbf{x}) \, d^\nu \mathbf{x}$. This is usually called *Lebesgue measure*.

Here is another example of an integral. Let $\rho \geq 0$ be a measurable function with $\int \rho(\mathbf{x})\, d^\nu \mathbf{x} = 1$. Then the integral $\int f\, d\mu = \int f(\mathbf{x})\rho(\mathbf{x})\, d^\nu \mathbf{x}$ is the expectation with respect to the probability measure $\rho(\mathbf{x})\, d^\nu \mathbf{x}$. The function $\rho$ is called the density of the probability measure (with respect to Lebesgue measure).

Summation is a special case of integration. We can take a set $J$ and take the space of all functions on $J$ as the space of measurable function. In this case the integral is just $\sum_{j \in J} f(j)$. The measure in this case is called *counting measure*.

Again this leads to other interesting integrals. Let $p$ be a function on $J$ such that $\sum_j p(j) = 1$. Then $\int f\, d\mu = \sum_{j \in J} f(j)p(j)$ is an expectation. The probability measure $\mu$ is determined by the discrete density function $p$.

**Problems**

1. Find an example that shows that monotone convergence alone does not imply the integral of the limit is the limit of the integrals. (Hint: Some integrals will have to be infinite.)

## 3.2 Function spaces

We now introduce spaces of complex measurable functions.

The space $L^1(X, \mu)$ consists all complex measurable functions such that

$$\|f\|_1 = \int |f|\, d\mu < \infty. \tag{3.8}$$

The space $L^2(X, \mu)$ consists all complex measurable functions such that

$$\|f\|_2^2 = \int |f|^2\, d\mu < \infty. \tag{3.9}$$

The space $L^\infty(X, \mu)$ consists of all complex measurable functions such that there exists a bound $M$ with

$$|f| \leq M < \infty \tag{3.10}$$

except on a set of measure zero. The norm $\|f\|_\infty$ is defined as the smallest such bound.

It may be shown that if $f$ is measurable, then the following three conditions are equivalent: $\int |f|\, d\mu = 0$, $\int |f|^2\, d\mu = 0$, $f = 0$ except possibly on a set of measure zero. Such a function is called a *null* function.

In many situations there are functions that are not the zero function but are null functions. This can be a minor technical problem in Hilbert space reasoning, since it is awkward to have non-zero vectors of zero norm.

It is customary to get around this problem by a redefinition. Instead of considering these spaces as spaces of functions, consider abstract spaces. Two functions that differ by a null function determine the same element of this abstract space.

One case when this is not necessary is when the measure space is counting measure on some index set $J$. In this case, the spaces are written as $\ell^1(J)$, $\ell^2(J)$, and $\ell^\infty(J)$.

Here is an example which is at the other extreme. Choose a set of points $\mathbf{x}_j$ in $\mathbf{R}^\nu$ and a sequence of weights $p_j > 0$. For each Borel measurable function $f$ define the integral by $\int f\,d\mu = \sum_j p_j f(\mathbf{x}_j)$. Then every $f$ such that $f(\mathbf{x}_j) = 0$ for all $j$ is a null function. All these null functions determine the same zero vector in the Hilbert space. The values of $f$ at other points are completely irrelevant.

We are mainly interested in $L^2$, because it is a Hilbert space, but it has important relations with the other spaces. The first obvious remark is that a function that is in both $L^1$ and $L^\infty$ is in $L^2$.

The interaction of these spaces in partly due to the following elementary product rules. The first is that the product of an $L^\infty$ function with an $L^2$ is in $L^2$. The second is that the product of two $L^2$ functions is in $L^1$, which a consequence of the Schwarz inequality.

There are two special cases when there are inclusions. On a discrete measure space $\ell^1 \subset \ell^2 \subset \ell^\infty$. This is due to the fact that a convergent sequence is bounded. It goes the other way on a finite measure space, in that case $L^\infty \subset L^2 \subset L^1$. This follows from applying the product rules with one of the functions being the function that is 1 on the set of finite measure.

For our purposes the most important thing about $L^2(X, \mu)$ is that it is a Hilbert space. The inner product is

$$\langle f, g \rangle = \int f^* g\,d\mu. \tag{3.11}$$

Here $f^*$ denotes the function complex conjugate to $f$.

The completeness of $\ell^2(J)$ is not difficult to verify directly. However in general the completeness of $L^2(X, \mu)$ is not obvious. The difficulty arises from the fact that evaluation of a function at a point need not be a continuous function on the Hilbert space. A sequence of functions that is convergent in the sense of the norm need not converge at any fixed point of $X$. The completeness is a major theorem that is one of the most remarkable consequences of the theory of the Lebesgue integral.

The Hilbert space of greatest concern will be $L^2(\mathbf{R}^\nu, d^\nu x)$, where $x = (x_1, \ldots, x_\nu)$ are Cartesian coordinates on the Euclidean space $\mathbf{R}^\nu$ and $d^\nu x = dx_1 \cdots dx_\nu$. The elements of this space are the wave functions $\psi = f(x)$ with

$$\int |\psi|^2 d^\nu x < \infty. \tag{3.12}$$

It will be easy to fall into the habit of calling this space by the abbreviation $L^2$.

Another Hilbert space that will occur is gotten by taking a countable index set $J$, such as the natural numbers. This Hilbert space is usually referred to simply as $\ell^2$.

**Problems**

1. Give an example of a discontinuous function that differs from a continuous function by a null function.

2. Give an example of a discontinuous function that does not differ from a continuous function by a null function.

3. Give an example of a function that is in $L^1$ but not in $L^2$.

4. Give an example of a function that is in $L^2$ but not in $L^1$.

5. Give an example of a bounded function that is not in $L^2$.

6. Give an example of a function that is zero outside of a bounded set and which is not in $L^2$.

7. Give an example of a sequence of $f_n$ of functions in $L^2$ that converges pointwise but not in $L^2$.

8. Give an example of a sequence of $f_n$ of functions in $L^2$ that converges in $L^2$ but not pointwise.

9. Consider a space $L^2(X, \mu)$ and a measurable subset $S$ of $X$. Show that the subspace of functions in $L^2(X, \mu)$ that vanish off $X$ form a closed subspace. What is the orthogonal complement? What is the decomposition given by the projection theorem?

## 3.3 Convergence

The main theorem is about integration of complex functions is the *dominated convergence theorem*.

**Theorem 5** *Assume that $f_n \to f$ pointwise and and $|f_n| \leq g$ for some $g \in L^1$. Then $\int f_n \, d\mu \to \int f \, d\mu$.*

Proof: First we give the proof in the case when the functions $f_n$ are real functions. We have $-g \leq f_n \leq g$. Define the lower and upper functions $l_n = \inf_{m \geq n} f_m$ and $u_n = \sup_{m \geq n} f_m$. Then $-g \leq l_n \leq f_n \leq u_n \leq g$. Furthermore $l_n \uparrow f$ and $u_n \downarrow f$. By monotone convergence $\int l_n \, d\mu \to \int f \, d\mu$ and $\int u_n \, d\mu \to \int f \, d\mu$. Since $\int l_n \, d\mu \leq \int f_n \, d\mu \leq \int u_n \, d\mu$, it follows that $\int f_n \, d\mu \to \int f \, d\mu$.

When the functions $f_n$ are complex functions, then we can apply the previous argument to the real and imaginary parts.

**Corollary 3** *Assume that $f_n \to f$ pointwise and and $|f_n| \leq g$ for some $g \in L^1$. Then $\int |f_n - f| \, d\mu \to 0$, that is, $f_n \to f$ in $L^1$.*

Proof: Since $|f_n| \leq g$ and $|f| \leq g$, we have $|f_n - f| \leq 2g$. Therefore we may apply the dominated convergence theorem.

**Corollary 4** *Assume that $f_n \to f$ pointwise and and $|f_n| \leq g$ for some $g \in L^2$. Then $\int |f_n - f|^2 \, d\mu \to 0$, that is, $f_n \to f$ in $L^2$.*

Proof: Since $|f_n| \leq g$ and $|f| \leq g$, we have $|f_n - f|^2 \leq 4g^2$. Therefore we may apply the dominated convergence theorem.

**Problems**

1. Let $f_n(x) = \exp(-(x-n)^2)$. Is the limit of the integrals the integral of the limit? Discuss.

2. Let $g_n(x) = n^2 |x| \exp(-nx^2)$. Same question.

3. Let $h_n(x) = n^{-1/2} \exp(-x^2/(2n))$. Same question.

4. Let $f$ be in $L^2$ and assume that $\phi_n$ are bounded in $L^\infty$. Assume that $\phi_n \to \phi$ pointwise as $n \to \infty$. Show that $\phi_n f \to \phi f$ in $L^2$. What does this say about strong convergence of multiplication operators?

## 3.4 Integral operators

How does one recognize a bounded operator? Consider a Hilbert space $L^2(X, \mu)$. The most obvious operators are *integral operators*

$$Tf(x) = \int t(x,y) f(y) \, d\mu(y). \tag{3.13}$$

Of course when the Hilbert space is $\ell^2(J)$ these are actually matrix operators.

One can manipulate bounded integral operators much like one manipulates matrices. For instance, for a bounded integral operator

$$Tf(x) = \int t(x,y) f(y)\, d\mu(y), \tag{3.14}$$

the adjoint is

$$T^* f(x) = \int t(y,x)^* f(y)\, d\mu(y). \tag{3.15}$$

This is a kind of conjugate transpose.

A *Hilbert-Schmidt integral operator* is an integral operator for which the double integral

$$\|T\|_2^2 = \int |t(x,y)|^2\, d\mu(x) d\mu(y) < \infty. \tag{3.16}$$

**Proposition 6** *If an integral operator $T$ is Hilbert-Schmidt, then it is bounded from $L^2$ to $L^2$, and $\|T\|_\infty \le \|T\|_2$.*

Proof: Apply the Schwarz inequality to $\int |t(x,y)| \cdot |f(y)|\, d\mu(y)$.

We may also consider integral operators acting on $L^1$ or $L^\infty$. If

$$\int |t(x,y)|\, d\mu(x) \le K_1 < \infty \tag{3.17}$$

for all $y$, then $T$ is bounded as an operator from $L^1$ to $L^1$. If

$$\int |t(x,y)|\, d\mu(y) \le K_\infty < \infty \tag{3.18}$$

for all $x$, then $T$ is bounded as an operator from $L^\infty$ to $L^\infty$. The following is a result using the idea of *interpolation*. It says that if $T$ is bounded on $L^1$ and on $L^\infty$ then $T$ is bounded on $L^2$. The interpolated bound is the geometric mean of the two extreme bounds.

**Proposition 7** *If $T$ is an integral operator satisfying both of the above conditions, then $T$ is a bounded operator from $L^2$ to $L^2$, and $\|T\|_\infty \le \sqrt{K_1 K_\infty}$.*

Proof: Apply the Schwarz inequality to $\int |t(x,y)|^{1/2} \cdot |t(x,y)|^{1/2} |f(y)|\, d\mu(y)$.

**Problems**

1. Consider the Hilbert space $\ell^2(\{1,2\})$ and the operator with matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

   Find its Hilbert-Schmidt norm.

2. Find its uniform norm.

3. Consider the Hilbert space $\ell^2(\{1,2\})$ and the operator with matrix

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

   Find its Hilbert-Schmidt norm.

4. Find its uniform norm.

5. Consider the Hilbert space $L^2([0,1], dx)$ and the integral operator $Vf(x) = \int_0^x f(y)\, dy$. Find its Hilbert-Schmidt norm.

6. Find its uniform norm.

7. Is the range of this operator equal to $L^2$? Is it dense in $L^2$?

8. Consider the Hilbert space $L^2(\mathbf{R}, dx)$ and the integral operator $Af(x) = (1/2)\int_{-\infty}^{\infty} \exp(-|x-y|) f(y)\, dy$. Find its Hilbert-Schmidt norm.

9. Show that it is bounded.

10. Find its uniform norm.

11. Give an example of an operator with $\|A\| > 1$ but $\|A^2\| < 1$.

**Problems**

1. Assume that $A_n \to A$ and $B_n \to B$ in norm. Show that $A_n B_n \to AB$ in norm.

2. Assume that $A_n \to A$ in norm. Show that $A_n^* \to A^*$ in norm.

3. Assume that $A_n \to A$ and $B_n \to B$ strongly. Assume in addition that $\|A_n\| \le M$ for all $n$. Show that $A_n B_n \to AB$ strongly.

4. Assume that $A_n \to A$ strongly. Must it follow that $A_n^* \to A^*$ strongly?

5. Assume that $A_n \to A$ strongly. Must it follow that $\|A_n\| \to \|A\|$?
6. Is the norm limit of unitary operators necessarily unitary?
7. Is the strong limit of unitary operators necessarily unitary?

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# Chapter 4

# Bases

This chapter is about the structure of an isomorphism of a Hilbert space with an $L^2$ space. There is a special case when this is particularly simple: Every isomorphism of a Hilbert space with an $\ell^2$ space is obtained from an an orthonormal basis. In the general case the isomorphism may be thought of as arising from a sort of continuous basis.

While the material of this chapter may be illuminating, it will not play a major role in the following. The natural Hilbert space notion is that of isomorphism; the basis concept is secondary.

## 4.1 Discrete bases

**Definition 4** *A (discrete)* basis *of a Hilbert space $\mathcal{H}$ is an isomorphism $W$ from $\mathcal{H}$ to $\ell^2(S)$ for some index set $S$.*

**Theorem 6** *Let $W$ be a basis. Then there are vectors $\phi_j$ for $j$ in $S$ such that $W\psi(j) = \langle \phi_j, \psi \rangle$. Furthermore $\psi = \sum_j \langle \phi_j, \psi \rangle \phi_j$.*

Proof: The existence of $\phi_j$ follows from the self-duality. In fact $|W\psi(j)| \leq \sqrt{\sum_j |W\psi_j|^2} = \|\psi\|$.

Let $\chi = \sum_j \langle \phi_j, \psi \rangle \phi_j$. Then $W\psi = W\chi$, so since $W$ is an isomorphism, $\psi = \chi$.

**Theorem 7** *Every Hilbert space has a basis.*

Proof: Consider families $\phi_j$ of unit vectors that are mutually orthogonal indexed by some set $J$. Take a maximal such family.

Let $M$ be the closed linear subspace of consisting of all vectors $\phi = \sum_j f(j)\phi_j$ with $\sum_j |f(j)|^2 < \infty$.

We observe that $M = \mathcal{H}$. If this were not the case, then by the projection theorem the would be a unit vector $\phi$ orthogonal to $M$. This would contradict the maximality.

For $\psi$ in $\mathcal{H}$ define $W\psi_j = \langle \phi_j, \psi \rangle$. Then $W\psi$ is in $\ell^2(J)$. It is not difficult to see that $W$ is an isomorphism.

In Dirac's notation the value of the function $W\psi$ on $j$ is written $\langle j \mid \psi \rangle$ instead of $\langle \phi_j, \psi \rangle$. This amounts to denoting the continuous linear functional $\langle \phi_j, \cdot \rangle$ by $\langle j \mid$ in Dirac's scheme. Note that the notation suppresses the isomorphism and the basis vectors; only the index set survives.

If we also denote $\langle \chi, \phi_j \rangle$ by $\langle \chi \mid j \rangle$, then we get the traditional Dirac formula

$$\langle \chi \mid \psi \rangle = \sum_j \langle \chi \mid j \rangle \langle j \mid \psi \rangle. \tag{4.1}$$

## 4.2 Continuous bases

Continuous bases play an important role in many expositions of quantum mechanics. There are relatively few rigorous presentations. We give one possible formulation More information on may be found in the books by Berezanskii [B] and Van Eijndhoven and De Graaf [EG]. The paper [F] contains a useful summary.

**Definition 5** *A* continuous basis *of a Hilbert space $\mathcal{H}$ is an isomorphism $W$ from $\mathcal{H}$ to $L^2(X, \mu)$ for some measure space.*

**Proposition 8** *Consider a bounded operator $T$ from $L^2$ to $L^2$. Let $W$ be an isomorphism to another $L^2$ space and set $S = WTW^{-1}$ be the isomorphic operator. Then $T$ is a Hilbert-Schmidt integral operator if and only if $S$ is a Hilbert-Schmidt integral operator.*

Proof: It is sufficient to prove this proposition when one of the $L^2$ spaces is $\ell^2$. So assume that $S$ is an operator acting in $\ell^2$.

Let the isomorphism of $L^2$ with $\ell^2$ be given by the basis vectors $\phi_j$ in $L^2$. It is easy to check that the relation between the integral kernel $t$ and the matrix $s$ is

$$t(x, y) = \sum_{ij} s_{ij} \phi_i(x) \phi_j(y)^*. \tag{4.2}$$

and

$$s_{ij} = \int \int \phi_i(x)^* t(x, y) \phi_j(y) \, d\mu(x) d\mu(y). \tag{4.3}$$

This is of the form of the isomorphism between the $L^2$ space of functions $t(x,y)$ of two variables and the $\ell^2$ space of matrices $s_{ij}$ given by the doubly indexed basis $\phi_i(x)\phi_j(y)^*$. Thus

$$\int\int |t(x,y)|^2\, d\mu(x)d\mu(y) = \sum_i \sum_j |s_{ij}|^2. \tag{4.4}$$

Q.E.D.

In general we may define a *Hilbert-Schmidt* operator as an operator that is isomorphic to a Hilbert-Schmidt integral operator on some $L^2$ space. In view of the preceding result, every Hilbert-Schmidt operator on an $L^2$ space is automatically a Hilbert-Schmidt integral operator on the same $L^2$ space. Hilbert-Schmidt operators are easy to recognize!

Let $T$ be a bounded operator with zero nullspace and dense range. Let $\mathcal{K}$ be the range of $T$ and define $\|\psi\|_{\mathcal{K}} = \|T^{-1}\psi\|$. Then $\mathcal{K}$ is a Hilbert space.

Let $\mathcal{K}^*$ be the space of continuous linear functionals on $\mathcal{K}$. If $\phi$ is in $\mathcal{H}$, then the function that sends $\psi$ to the inner product $\langle\psi,\phi\rangle$ is continuous in the norm of $\mathcal{K}$. This is because

$$|\langle\psi,\phi\rangle| = |\langle T^*\psi, T^{-1}\phi\rangle| \le \|T^*\psi\|\|T^{-1}\phi\| = \|T^*\psi\|\|\phi\|_{\mathcal{K}}. \tag{4.5}$$

Thus $\psi$ defines an element of $\mathcal{K}^*$. Since $\mathcal{K}$ is dense in $\mathcal{H}$, this element is uniquely determined by $\phi$. Thus one is allowed to think of elements of $\mathcal{K}^*$ as generalized elements of $\mathcal{H}$. Of course the norm is different; it is easily seen that the norm of $\psi$ as an element of $\mathcal{K}$ is just $\|T^*\psi\|$.

**Theorem 8** *Let $W$ be a continuous basis. Let $T$ be a bounded operator with zero nullspace and dense range. Assume that $T$ is Hilbert-Schmidt. Then for almost every $x$ there is a vector $\phi_x$ in $\mathcal{K}^*$ such that for all $\psi \in \mathcal{K}$ we have*

$$W\psi(x) = \langle\phi_x,\psi\rangle. \tag{4.6}$$

Proof: Write

$$W\psi(x) = WTW^{-1}WT^{-1}\psi(x) = \int s(x,y)WT^{-1}\psi(y)\, d\mu(y). \tag{4.7}$$

Then $WTW^{-1}$ is Hilbert-Schmidt. Hence

$$|\rho(x)W\psi(x)| \le \left(\int |s(x,y)|^2\, d\mu(y)\right)^{1/2} \left(\int |W\psi(y)|^2\, d\mu(y)\right)^{1/2} = \|s_x\|_2\|T^{-1}\psi\|. \tag{4.8}$$

Now $\|s_x\|$ is finite for almost every $x$, by Fubini's theorem. Therefore for almost every $x$ the value $W\psi(x)$ is continuous for $\psi$ in $\mathcal{K}$. Q.E.D.

Example: Take the Hilbert space to be $\mathcal{H} = L^2$. Take $T$ to be a suitable Hilbert-Schmidt operator. If $f$ is in $\mathcal{H}$, then the $\mathcal{K}^*$ norm of $f$ is given by

$$\|f\|_{\mathcal{K}^*}^2 = \|T^* f\|^2 = \int \int f(x)^* k(x,y) f(y)\, d\mu(x) d\mu(y) \tag{4.9}$$

where

$$k(x,y) = \int t(x,z) t(y,z)^*\, d\mu(z). \tag{4.10}$$

Note that

$$|k(x,y)|^2 \le \int |t(x,z)|^2\, d\mu(z) \int |t(y,z)|^2\, d\mu(z) \tag{4.11}$$

is finite for almost every $x$ and $y$.

Now take $W$ to be the identity operator. Then $Wf(x) = \langle \delta_x, f \rangle = f(x)$ for almost all $x$. Thus we should expect that $\delta_x$ should be in $\mathcal{K}^*$ for almost all $x$. If we compute the norm using the above formula we see that

$$\|\delta_x\|_{\mathcal{K}^*}^2 = k(x,x) < \infty \tag{4.12}$$

for almost every $x$.

Example: For a more concrete example take the Hilbert space to be $\mathcal{H} = L^2(\mathbf{R}^\nu, d^\nu \mathbf{x})$. Let $g$ and $h$ be in $L^2$ and define

$$Tf(\mathbf{x}) = \int g(\mathbf{x}) h(\mathbf{x} - \mathbf{y})\, d^\nu(\mathbf{y}). \tag{4.13}$$

Thus $T$ is a convolution followed by a multiplication. If $f$ is in $\mathcal{H}$, then the $\mathcal{K}^*$ norm of $f$ is given by

$$\|f\|_{\mathcal{K}^*}^2 = \int \int f(\mathbf{x})^* g(\mathbf{x}) r(\mathbf{x} - \mathbf{y}) g(\mathbf{y})^* f(\mathbf{y})\, d^\nu \mathbf{x} d^\nu \mathbf{y}, \tag{4.14}$$

where

$$r(\mathbf{x}) = \int h(\mathbf{x} - \mathbf{z}) h(-\mathbf{z})\, d^\nu \mathbf{z}. \tag{4.15}$$

Note that the function $r$ is continuous and bounded. It is clear from this that the function of the $r$ convolution operator is to smooth the elements of $\mathcal{K}^*$, while the function of the $g$ multiplication operator is to produce decrease at infinity.

This norm works for all isomorphisms! Therefore the space may be larger than is needed for a particular isomorphism. The theorem has a useful generalization in which the norm is adapted to the isomorphism. This allows smaller spaces that give more accurate information about the nature of the vectors giving the isomorphism.

**Theorem 9** *Let $W$ be a continuous basis. Let $T$ be a bounded operator with zero nullspace and dense range. Let $R$ be a bounded operator such that $WRW^{-1}$ is multiplication by a measurable function $\rho$ on $X$ that is never zero. Assume that $RT$ is Hilbert-Schmidt. Then for almost every $x$ there is a vector $\phi_x$ in $\mathcal{K}^*$ such that for all $\psi \in \mathcal{K}$ we have*

$$W\psi(x) = \langle \phi_x, \psi \rangle. \tag{4.16}$$

One could take $R$ to be the identity operator, but in practice one wants to make a cleverer choice. The $R$ should combine with the $T$ in such a way that product is Hilbert-Schmidt even though the individual factors are not. (For instance, $R$ could be a convolution operator and $T$ could be a multiplication operator.)

Proof: Write

$$\rho(x)W\psi(x) = WRTW^{-1}WT^{-1}\psi(x) = \int s(x,y)WT^{-1}\psi(y)\, d\mu(y). \tag{4.17}$$

Then $WRTW^{-1}$ is Hilbert-Schmidt. Hence

$$|\rho(x)W\psi(x)| \le \left(\int |s(x,y)|^2\, d\mu(y)\right)^{1/2} \left(\int |WT^{-1}\psi(y)|^2\, d\mu(y)\right)^{1/2} = \|s_x\|_2 \|T^{-1}\psi\|. \tag{4.18}$$

Now $\|s_x\|$ is finite for almost every $x$, by Fubini's theorem. Therefore for almost every $x$ the value $W\psi(x)$ is continuous for $\psi$ in $\mathcal{K}$.

Example: Take the Hilbert space to be $\mathcal{H} = L^2(\mathbf{R}^\nu, d^\nu\mathbf{x})$. Let $g$ be in $L^2$ and $L^\infty$ and such that $g$ never vanishes. Let $R$ be multiplication by $g$. Let $h$ be in $L^2$ and $L^1$ and assume that its Fourier transform never vanishes. Let $T$ to be the convolution operator

$$Tf(\mathbf{x}) = \int h(\mathbf{x}-\mathbf{y})\, d^\nu(\mathbf{y}). \tag{4.19}$$

If $f$ is in $\mathcal{H}$, then the $\mathcal{K}^*$ norm of $f$ is

$$\|f\|^2_{\mathcal{K}^*} == \int\int f(\mathbf{x})^* r(\mathbf{x}-\mathbf{y}) f(\mathbf{y})\, d^\nu\mathbf{x} d^\nu\mathbf{y}, \tag{4.20}$$

where

$$r(\mathbf{x}) = \int h(\mathbf{x}-\mathbf{z})h(-\mathbf{z})\, d^\nu\mathbf{z}. \tag{4.21}$$

Note that the function $r$ is continuous and in $L^\infty$ and in $L^1$.

Now take $W$ to be the identity operator. Then $Wf(\mathbf{x}) = \langle \delta_\mathbf{x}, f\rangle = f(\mathbf{x})$ for almost all $\mathbf{x}$. Thus we should expect that $\delta_x$ should be in $\mathcal{K}^*$ for almost all $x$. If we compute the norm using the above formula we see that

$$\|\delta_\mathbf{x}\|^2_{\mathcal{K}^*} = r(\mathbf{x}). \tag{4.22}$$

for every $\mathbf{x}$.

Example: Take the Hilbert space to be $\mathcal{H} = L^2(\mathbf{R}^\nu, d^\nu\mathbf{x})$. Let $g$ be in $L^2$ and $L^\infty$ and and never vanishing. let $T$ be multiplication by $g$. Let $h$ be in $L^2$ and $L^1$ and with Fourier transform never vanishing. Let $R$ to be the convolution operator

$$Rf(\mathbf{x}) = \int h(\mathbf{x} - \mathbf{y})\, d^\nu(\mathbf{y}). \tag{4.23}$$

If $f$ is in $\mathcal{H}$, then the $\mathcal{K}^*$ norm of $f$ is

$$\|f\|^2_{\mathcal{K}^*} == \int\int |f(\mathbf{x})|^2\, |g(\mathbf{x})|^2 d^\nu\mathbf{x}. \tag{4.24}$$

This is just a weighted $L^2$ space. Note that $|g|^2$ is in $L^1$.

Now assume that $W$ is such that $WRW^{-1}$ is a multiplication operator, as in the theorem. The correct choice of $W$ is of course the Fourier transform. Then $Wf(\mathbf{k}) = \langle \phi_\mathbf{k}, f\rangle$ for almost all $\mathbf{k}$. We should expect that $\phi_\mathbf{k}$ should be in $\mathcal{K}^*$ for almost all $k$. Therefore they must be functions!

In fact for the Fourier transform the $\phi_\mathbf{k}$ are bounded functions given by $\phi_\mathbf{k}(\mathbf{x}) = \exp(i\mathbf{k}\cdot\mathbf{x})$. If we compute the norm using the above formula we see that

$$\|\phi_\mathbf{k}\|^2_{\mathcal{K}^*} = \int |\phi_\mathbf{k}(\mathbf{x})|^2\, |g(\mathbf{x})|^2 d^\nu\mathbf{x} \tag{4.25}$$

is finite.

In order to verify the hypotheses of the theorem in more complicated situations, the following result is useful.

**Proposition 9** *Let $S$ be a Hilbert-Schmidt operator and $B$ be a bounded operator. Then $SB$ and $BS$ are Hilbert-Schmidt operators.*

The way this is used is to take an operator $R_0$ for which it is easy to prove that $R_0T$ is Hilbert-Schmidt. (The $R_0$ might be a convolution operator and $T$ a multiplication operator.) If one can write the operator $R$ of actual interest as $R = BR_0$, where $B$ is bounded, then it follows that $RT$ is Hilbert-Schmidt. (In applications $R$ can be the resolvent of the operator of interest, and $R_0$ is the resolvent of a simpler operator.)

Finally, here is the Dirac notation. Again it suppresses part of the information. In Dirac's notation the value of the function $W\psi$ on $k$ is written $\langle k \mid \psi\rangle$ instead of $\langle \phi_k, \psi\rangle$. This amounts to denoting the linear functional $\phi_k$ by $\langle k \mid$ in the Dirac scheme. This is an example of a bra functional that does not come from a vector in the Hilbert space. The

corresponding conjugate linear functional $\mid k\rangle$ is given on $\chi$ by $\langle \chi \mid k\rangle = \langle k \mid \chi\rangle^*$. This gives the Dirac formula

$$\langle \chi \mid \psi\rangle = \int \langle \chi \mid k\rangle\langle k \mid \psi\rangle \, d\mu(k). \tag{4.26}$$

**Problems**

1. Let $\mathcal{H} = L^2(\mathbf{R}^\nu, d^\nu\mathbf{x})$. Let $R$ be a convolution operator acting in $\mathcal{H}$, so $Rf(\mathbf{x}) = \int h(\mathbf{x}-\mathbf{y})f(\mathbf{y})\, d^\nu\mathbf{y}$. Let $T$ be a multiplication operator $Tf(\mathbf{x}) = g(\mathbf{x})f(\mathbf{x})$. Find conditions on these operators that make $RT$ Hilbert-Schmidt. Find conditions on these operators that make $R$ and $T$ bounded. What are the resulting spaces $\mathcal{K}$ and $\mathcal{K}^*$?

2. In the context of the previous problem the Fourier transform is an isomorphism $W$ from $\mathcal{H}$ to a (different) $L^2$ space. Show that the convolution operator on $\mathcal{H}$ is isomorphic to a multiplication operator on $L^2$.

3. In this same context, find the elements of $\mathcal{K}^*$ that give the isomorphism.

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# Chapter 5

# Spectral Representations

In this chapter we look at the situation when an operator acting in a Hilbert space is isomorphic to a multiplication operator acting in an $L^2$ space. The classical example is translation invariant operators; the isomorphism is given by the Fourier transform. The Fourier transform is particularly important in quantum mechanics, because it permits an analysis of the solution of the free Schrödinger equation.

## 5.1 Multiplication operators

**Definition 6** *Consider the situation when the Hilbert space is $L^2(X, \mu)$. A* multiplication operator *is an operator defined by a complex measurable function $\alpha$ defined on $X$. The domain consists of all $f$ in $L^2$ such that $\alpha f$ is also in $L^2$. The operator is the transformation that sends $f$ to the product $\alpha f$.*

Notice that in the special case when the Hilbert space is $\ell^2(J)$, a multiplication operator is just an operator given by a diagonal matrix. So one should think of a multiplication operator as being diagonal, perhaps in some continuous sense.

**Proposition 10** *A multiplication operator is densely defined and closed. Its adjoint is the operator of multiplication by the complex conjugate $\alpha^*$.*

Proof: Let $\alpha$ define a multiplication operator. Let $f$ be in $L^2(X, \mu)$. Let $X_n$ be the set on which $|\alpha| \leq n$. Let $f_n = f$ on $X_n$ and 0 elsewhere. Then for each $n$ the function $f_n$ is in the domain of $\alpha$, and $f_n \to f$ as $n \to \infty$. This proves that the operator is densely defined.

The domain of the operator of multiplication by $\alpha$ with the graph norm is just $L^2(X, (1+|\alpha|^2)\mu)$. This is a Hilbert space, so the operator is closed.

In order to prove the statement about the adjoint, consider a pair $(u, v)$ in the graph of the adjoint. Then $\langle v, f\rangle = \langle u, \alpha f\rangle$ for all $f$ in $L^2$ such that $\alpha$ f is in $L^2$. Let $X_n$ be the set on which $|\alpha| \leq n$. Then for all $f$ in $L^2$ supported on $X_n$ we have $\langle v - \alpha^* u, f\rangle = 0$. Thus $v - \alpha u = 0$ on $X_n$. Since the union of the $X_n$ is all of $X$, it follows that $v - \alpha u = 0$. Q.E.D.

A multiplication operator is self-adjoint if and only if $\alpha = \alpha^*$, that is, the function is real. A multiplication operator is unitary if and only if $|\alpha| = 1$.

One special case is when the function $\alpha$ is in $L^\infty$. Then the corresponding multiplication operator is a bounded operator, and hence defines a continuous linear transformation defined on all of $L^2$.

For a sequence of bounded multiplication operators convergence of the functions in $L^\infty$ implies norm convergence of the corresponding operators.

The following proposition is fundamental.

**Proposition 11** *Assume that there is a bound $|\alpha_n| \leq M$ for all $n$ and that $\alpha_n \to \alpha$ pointwise as $n \to \infty$. Then the corresponding multiplication operators converge strongly.*

The proof is obvious: Apply the $L^2$ dominated convergence theorem.

**Problems**

1. Show that the norm of multiplication by $\alpha$ is the $L^\infty$ norm of $\alpha$. (Make the reasonable assumption that every set of infinite measure contains a subset of non-zero finite measure. This rules out certain peculiar situations that should not arise in practice.)

## 5.2 Spectral representations

**Definition 7** *Let $A$ be an operator from $D(A) \subset \mathcal{H}$ to $\mathcal{H}$. Then $A$ has a spectral representation if there exists a measure space $L^2(X, \mu)$ and an isomorphism $W$ from $\mathcal{H}$ to $L^2$ and a function $\alpha$ such that $A$ is related to the corresponding multiplication operator by $A = W^{-1}\alpha W$.*

Notice that this definition means in particular that the domain $D(A)$ must consist of all $\psi$ in $\mathcal{H}$ such that $\alpha W\psi$ is in $L^2$. For such $\psi$ we have $A\psi = W^{-1}\alpha W\psi$, which is in $\mathcal{H}$.

Let $A$ be an self-adjoint operator that has a spectral representation. Then the function $\alpha$ is a real function. Define the *unitary group* generated by $A$ to be $U_t = W^{-1}\exp(-it\alpha)W$.

Notice that for each $t$ the multiplication operator $\exp(-it\alpha)$ is multiplication by a function with absolute value one. Thus it is a unitary multiplication operator. Therefore for each $t$ the operator $U_t$ is unitary.

**Proposition 12** *Let $A$ have a spectral representation by a real function. Then the corresponding unitary group is strongly continuous: For each $\psi$ in $\mathcal{H}$ the function $U_t\psi$ with values in $\mathcal{H}$ is continuous in $t$.*

Proof: $U_t\psi = W^{-1}\exp(-it\alpha)W\psi$. Since $W\psi$ is in $L^2$, we see from the $L^2$ dominated convergence theorem that $\exp(-it\alpha)W\psi$ is continuous as a function from the reals to $L^2$.

**Proposition 13** *Let $A$ have a spectral representation by a real function. Then the abstract Schrödinger equation is satisfied: For each $\psi$ in $D(A)$ we have*

$$i\frac{dU_t\psi}{dt} = AU_t\psi. \tag{5.1}$$

Proof: Fix $t$ and consider the difference quotients

$$i(\exp(-i(t+h)\alpha) - \exp(-it\alpha))/h\, W\psi. \tag{5.2}$$

It is easy to see that the absolute value of the difference quotient is bounded by $|\alpha W\psi|$ which is in $L^2$. Therefore by the $L^2$ dominated convergence theorem the difference quotients converge in $L^2$ to

$$\alpha\exp(-it\alpha)W\psi. \tag{5.3}$$

Example: One important example is when the spectral representation is an isomorphism with $\ell^2$ given by a basis. Then

$$(W\psi)_j = \langle\phi_j, \psi\rangle = c_j. \tag{5.4}$$

The inverse $W^{-1}$ takes the coefficients and restores the vector $\psi$ by

$$\psi = \sum_j c_j\phi_j. \tag{5.5}$$

The equation $A\psi = W^{-1}\alpha W\psi$ takes the form

$$A\psi = \sum_j \alpha_j c_j\phi_j. \tag{5.6}$$

Thus the solution of the Schrödinger equation is obtained by multiplying the coefficients by the exponentiated values

$$U_t\psi = \sum_j \exp(-it\alpha_j)c_j\phi_j. \tag{5.7}$$

We now record how the spectral representation condition appears in the Dirac notation. Let $\psi$ be in the domain of $A$. The condition $\langle \chi, A\psi \rangle = \langle W\chi, \alpha W\psi \rangle$ may be written out in detail as

$$\langle \chi, A\psi \rangle = \int W\chi(k)^* \alpha(k) W\psi(k)\, d\mu(k). \tag{5.8}$$

The Dirac version of this is

$$\langle \chi \mid A \mid \psi \rangle = \int \langle \chi \mid k \rangle \alpha(k) \langle k \mid \psi \rangle\, d\mu(k). \tag{5.9}$$

In the discrete case it would be

$$\langle \chi \mid A \mid \psi \rangle = \sum_j \langle \chi \mid j \rangle \alpha_j \langle j \mid \psi \rangle. \tag{5.10}$$

**Problems**

1. Consider the example above when the isomorphism is given by an orthonormal basis. Develop a generalization in which the basis consists of orthogonal vectors in $\mathcal{H}$, not necessarily normalized to have length one. The $\ell^2$ space should be given by a discrete measure, but not necessarily counting measure. (This measure can be specified by specifying a positive weight for each point.)

## 5.3 Translation

One fundamental example of of a unitary operator is *translation*. Consider the Hilbert space $L^2(\mathbf{R}^\nu, d\mathbf{x}^\nu)$. For each vector $\mathbf{a}$ define translation by $\mathbf{a}$ according to

$$U_{\mathbf{a}} g(\mathbf{x}) = g(\mathbf{x} - \mathbf{a}). \tag{5.11}$$

One of the fundamental properties of $L^2$ is that translation is strongly continuous. That is, for each $f$ in $L^2$ the function that sends $\mathbf{a}$ to $U_{\mathbf{a}} f$ is continuous from $\mathbf{R}^\nu$ to $L^2$.

This may be proved by noting that it is true when $f$ is a function that is the indicator function of a rectangle. Since such functions are dense in $L^2$, it follows that it is true in general.

Translation has several important extensions and generalizations. The notion of convolution is one of them.

**Definition 8** *Let $f$ be in $L^1$ and $g$ be in $L^1$ or in $L^2$. The convolution of $f$ and $g$ is the function $f * g$ defined by*

$$f * g(\mathbf{x}) = \int f(\mathbf{y}) U_{\mathbf{y}} g(\mathbf{x})\, d\mathbf{y} = \int f(\mathbf{y}) g(\mathbf{x} - \mathbf{y})\, d\mathbf{y}. \tag{5.12}$$

Notice that the convolution is simply the average of the translates of the one of the functions with the other function. If one thinks of the integral as a sort of generalized sum, then it is plausible (and true) that the convolution satisfies

$$\|f * g\| \leq \int |f(\mathbf{y})| \|U_{\mathbf{y}} g\|\, d\mathbf{y} = \int |f(\mathbf{y})|\, d\mathbf{y}\, \|g\|. \tag{5.13}$$

(This works with either the $L^1$ or the $L^2$ norm.)

Another extension of translation is differentiation. Differentiation is defined by a limiting operation. The directional derivative along $\mathbf{a}$ is defined by

$$\frac{dU_{t\mathbf{a}}g}{dt} == -\mathbf{a} \cdot \nabla_x g \tag{5.14}$$

for all $g$ in $L^2$ for which the limit exists.

**Problems**

1. Show that translation is not norm continuous.
2. Show that if $f$ and $g$ are in $L^1$, then convolution is commutative: $f * g = g * f$.

## 5.4 Approximate delta functions

The next useful tool is the approximate $\delta$ function. This is a family of functions $\delta_\epsilon(\mathbf{x})$ indexed by $\epsilon > 0$. Each such function has integral one. Furthermore, we assume the homogeneity property $\delta_\epsilon(\mathbf{x}) = \epsilon^{-\nu} \delta_1(\mathbf{x}/\epsilon)$.

**Proposition 14** *$\delta_\epsilon * f \to f$ in $L^1$ and in $L^2$ as $\epsilon \to 0$.*

Proof: We have

$$\delta_\epsilon * f = \int \delta_\epsilon(\mathbf{y}) U_{\mathbf{y}} f\, d\mathbf{y}^\nu = \int \delta_1(\mathbf{z}) U_{\epsilon\mathbf{z}} f\, d^\nu \mathbf{z}. \tag{5.15}$$

It follows that

$$\|\delta_\epsilon * f - f\| \leq \int \delta_1(\mathbf{z}) \|U_{\epsilon\mathbf{z}} f - f\|\, d^\nu \mathbf{z}. \tag{5.16}$$

The integrand goes to zero pointwise by the continuity of translation. Therefore the integral goes to zero by the dominated convergence theorem. Q.E.D.

One suitable choice is the Gauss kernel

$$\delta_\epsilon(\mathbf{x}) = (2\pi\epsilon^2)^{-\nu/2} \exp(-\frac{\mathbf{x}^2}{2\epsilon^2}). \tag{5.17}$$

Another choice is the Poisson kernel

$$\delta_\epsilon(\mathbf{x}) = c_\nu \frac{\epsilon}{(\epsilon^2 + \mathbf{x}^2)^{(\nu+1)/2}} \tag{5.18}$$

where $c_\nu$ is the normalizing constant $\Gamma((\nu+1)/2)/\pi^{(\nu+1)/2}$. In this following we shall often use the Poisson kernel in dimension $\nu = 1$. This case has a particularly convenient partial fraction decomposition

$$\delta_\epsilon(x) = \frac{1}{\pi} \frac{\epsilon}{(\epsilon^2 + \mathbf{x}^2)} = \frac{1}{2\pi i} \left( \frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon} \right). \tag{5.19}$$

## 5.5 The Fourier transform

**Definition 9** *Let $f$ be in $L^1(\mathbf{R}^\nu, d^\nu\mathbf{x})$. Its Fourier transform is defined by*

$$\hat{f}(\mathbf{k}) = \int \exp(-i\mathbf{k}\cdot\mathbf{x}) f(\mathbf{x})\, d^\nu\mathbf{x}. \tag{5.20}$$

From the Hilbert space point of view we would like to view the Fourier transform as a sort of inner product of $\exp(i\mathbf{k}\cdot\mathbf{x})$ with $f(\mathbf{x})$. Of course the exponential is not in $L^2$. The traditional way is to think of the exponential as being in $L^\infty$ and $f$ as being in $L^1$, and this is correct. However these spaces are not Hilbert spaces.

One way of getting Hilbert spaces has been explored in the last chapter. Let $g$ be a bounded function in $L^2$ that never vanishes. Let $\mathcal{K}$ be the Hilbert space $L^2(\mathbf{R}^\nu, |g(\mathbf{x})|^{-2} d^\nu\mathbf{x})$ and $\mathcal{K}^*$ be the dual space $L^2(\mathbf{R}^\nu, |g(\mathbf{x})|^2 d^\nu\mathbf{x})$. The ordinary $L^2(\mathbf{R}^\nu, d^\nu\mathbf{x})$ inner product gives a pairing between $\mathcal{K}$ and $\mathcal{K}^*$. It follows from the Schwarz inequality that $\mathcal{K}$ is contained in $L^1$, and it is also clear that $L^\infty$ is contained in $\mathcal{K}^*$. So we may also think of the Fourier transform as a sort of inner product of $\exp(i\mathbf{k}\cdot\mathbf{x})$ in $\mathcal{K}^*$ with with $f(\mathbf{x})$ in $\mathcal{K}$.

What we would like in the end is an inversion formula of the form

$$f(\mathbf{x}) = \int \exp(i\mathbf{k}\cdot\mathbf{x}) \hat{f}(\mathbf{k}) \frac{d^\nu\mathbf{k}}{(2\pi)^\nu}. \tag{5.21}$$

Unfortunately it is not true in general that $\hat{f}$ is in $L^1$, so this integral need not converge absolutely. We would nevertheless like to recover $f$ from $\hat{f}$.

This is accomplished by using an approximate delta function. In the presence of the homogeneity property the Fourier transform of such a function satisfies $\hat{\delta}_\epsilon(\mathbf{k}) = \hat{\delta}_1(\epsilon\mathbf{k})$. We also require that the Fourier transform be in $L^1$ and satisfy $\hat{\delta}_\epsilon(\mathbf{k}) \geq 0$. The Gauss and Poisson kernels are both suitable. The Gauss kernel has Fourier transform

$$\hat{\delta}_\epsilon(\mathbf{k}) = \exp(-\epsilon^2\mathbf{k}^2/2). \tag{5.22}$$

The Poisson kernel has Fourier transform

$$\hat{\delta}_\epsilon(\mathbf{k}) = \exp(-\epsilon|\mathbf{k}|). \tag{5.23}$$

Notice that these Fourier transforms are remarkably simple and memorable.

Let $f$ be in $L^1$ and in $L^2$. Then it is easy to compute that

$$\langle f, \delta_\epsilon * f\rangle = \int \hat{\delta}_\epsilon(\mathbf{k})|\hat{f}(\mathbf{k})|^2 \frac{d^\nu\mathbf{k}}{(2\pi)^\nu}. \tag{5.24}$$

Let $\epsilon \to 0$. Then the $L^2$ convergence of the convolution by the approximate delta function shows that the left hand side converges to the square of the norm of $f$. The monotone convergence theorem shows that the right hand side converges to the square of the norm of $\hat{f}$. The conclusion is that for $f$ in $L^1$ and $L^2$ we have

$$\|f\|^2 = \int |f(\mathbf{x})|^2\, d^\nu\mathbf{x} = \int |\hat{f}(\mathbf{k})|^2 \frac{d^\nu\mathbf{k}}{(2\pi)^\nu}. \tag{5.25}$$

This shows that $\|f\|^2 = \|\hat{f}\|^2$ for $f$ in $L^1$ and $L^2$. Since such functions are dense in $L^2$, we may extend the definition of the Fourier transform to $L^2$ by continuity.

One way to do this is to take a sequence of functions $u_n$ in $L^2$ with $|u_n| \leq 1$ and $u_n \to 1$ as $n \to \infty$. Then for $f$ in $L^2$ we observe that $u_n f$ is in $L^1$ for each $n$. Furthermore, $u_n f \to f$ in $L^2$ as $n \to \infty$, by the $L^2$ dominated convergence theorem. Therefore the Fourier transform of $u_n f$ converges to the Fourier transform of $f$. The following definition summarizes the situation.

**Definition 10** *The* Fourier transform *gives an operator $F$ from $L^2$ to $L^2$ satisfying $\|Ff\| = \|f\|$. It is defined for $f$ in $L^1$ and $L^2$ by*

$$Ff(\mathbf{k}) = \int \exp(-i\mathbf{k}\cdot\mathbf{x}) f(\mathbf{x})\, d^\nu\mathbf{x} \tag{5.26}$$

*and extended to $L^2$ by continuity.*

In the same way, we may define an *inverse Fourier transform* from $L^2$ to $L^2$ satisfying $\|F^{-1}g\| = \|g\|$. It is defined for $g$ in $L^1$ and $L^2$ by

$$F^{-1}g(\mathbf{x}) = \int \exp(i\mathbf{k}\cdot\mathbf{x})g(\mathbf{k})\,\frac{d^\nu\mathbf{k}}{(2\pi)^\nu}. \tag{5.27}$$

In order to see that these are indeed inverses of each other, one can check that

$$\delta_\epsilon * f(\mathbf{x}) = \int \exp(i\mathbf{k}\cdot\mathbf{x})\hat{\delta}_\epsilon(\mathbf{k})Ff(\mathbf{k})\,\frac{d^\nu\mathbf{k}}{(2\pi)^\nu}. \tag{5.28}$$

Let $\epsilon \to 0$. We obtain $f = F^{-1}Ff$. We can also check in a similar way that $g = FF^{-1}g$. We have proved the fundamental *Plancherel theorem.*

**Theorem 10** *The Fourier transform $F$ defines an isomorphism of $L^2(\mathbf{R}^\nu, d^\nu\mathbf{x})$ with $L^2(\mathbf{R}^\nu, d^\nu\mathbf{k}/(2\pi)^\nu)$.*

The importance of the Fourier transform is that it gives a spectral representation for the unitary group of translations. Fix a vector $\mathbf{a}$. Then the spectral representation is

$$U_\mathbf{a}g = F^{-1}\exp(-i\mathbf{a}\cdot\mathbf{k})Fg. \tag{5.29}$$

As a consequence, the Fourier transform also gives a spectral representation for convolution operators. Averaging the formula above with $f$ gives the result

$$f * g = F^{-1}\hat{f}(\mathbf{k})Fg. \tag{5.30}$$

The Fourier transform also gives a spectral representation for differentiation. The usual limiting operation on the translation representation gives

$$\mathbf{a}\cdot\nabla_\mathbf{x}g = F^{-1}i\mathbf{a}\cdot\mathbf{k}Fg. \tag{5.31}$$

For the important case of the Laplace operator we differentiate twice and obtain

$$\nabla^2_\mathbf{x}g = F^{-1}(-\mathbf{k}^2)Fg. \tag{5.32}$$

**Problems**

1. Evaluate $\int_{-\infty}^{\infty}\sin^2(k)/k^2\,dk$ by using the fact that the Fourier transform preserves the $L^2$ norm.
2. Let $f(x) = 1/(x-i)$. Find $\hat{f}$.
3. Show that if $f$ is in $L^1$, then $\hat{f}$ is continuous.

4. Give an example of a function in $L^2$ whose Fourier transform is not continuous.

5. Give an example of a function in $L^1 \cap L^2$ whose Fourier transform is not in $L^1$.

6. Assume that $f$ is in $L^2$ and $\hat{f}$ is never zero. Show that the linear span of the translates $f_a$ is dense in $L^2$. (You may use the fact that a function in $L^1$ whose Fourier transform is zero is a null function.)

7. Describe the class of $f$ in $L^2$ such that both $f$ and $\hat{f}$ have compact support.

8. Show that if $f$ and $g$ are in $L^2$ and $f' = g$ almost everywhere, then $f$ need not have a Hilbert space derivative.

9. Give a practical sufficient condition on $f$ in $L^2$ that ensures that $\hat{f}$ is in $L^1$. Illustrate with an example.

## 5.6 Free motion

### 5.6.1 Diffusion

Now it is time to solve the Schrödinger equation. The most basic situation is that of free motion.

First let us treat the *diffusion equation*

$$\frac{\partial \psi}{\partial t} = D\nabla_{\mathbf{x}}^2 \psi. \tag{5.33}$$

The Fourier transform gives an representation of $\nabla_{\mathbf{x}}^2$ as multiplication by $-\mathbf{k}^2$.

The solution of the initial value problem is given in the Fourier transform representation by multiplication by $\exp(-Dt\mathbf{k}^2)$. This is bounded by one for all $t \geq 0$. The solution may be written

$$f(\mathbf{x}, t) = \int \exp(i\mathbf{k} \cdot \mathbf{x}) \exp(-Dt\mathbf{k}^2) \hat{f}(\mathbf{k}) \, \frac{d^\nu \mathbf{k}}{(2\pi)^\nu} \tag{5.34}$$

When $t > 0$ it is given back in the original representation by convolution with the Gaussian kernel

$$f(\mathbf{x}, t) = \delta_{\sqrt{2Dt}} * f(\mathbf{x}) = \int \left( \frac{1}{\sqrt{4\pi Dt}} \right)^\nu \exp(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4Dt}) f(\mathbf{y}) \, d^\nu \mathbf{y}. \tag{5.35}$$

Notice that as $t \to 0$ the kernel gets small everywhere except where it becomes concentrated near $\mathbf{x}$. On the other hand, as $t \to \infty$ it spreads out. It represents a *dissipation* that takes place forward in time.

### 5.6.2 Oscillation

Now we may turn to the Schrödinger equation. The corresponding solution is obtained by replacing $D$ by $iD$. The solution of the initial value problem is given in the Fourier transform representation by multiplication by $\exp(iDt\mathbf{k}^2)$. This has absolute value one for all $t$. The solution may be written

$$f(\mathbf{x},t) = U_t f(\mathbf{x}) = \int \exp(i\mathbf{k}\cdot\mathbf{x}) \exp(iDt\mathbf{k}^2) \hat{f}(\mathbf{k}) \, \frac{d^\nu \mathbf{k}}{(2\pi)^\nu} \tag{5.36}$$

This solution is of the form

$$U_t = F^{-1} \exp(iDt\mathbf{k}^2) F. \tag{5.37}$$

This is the composition of three unitary transformations. The first important conclusion is that $U_t$ is unitary.

When $t \neq 0$ it is given back in the original representation by convolution with the complex Gaussian kernel

$$\delta_{\sqrt{2iDt}}(\mathbf{x}) = \left(\frac{1}{\sqrt{4\pi i D t}}\right)^\nu \exp(i\frac{\mathbf{x}^2}{4Dt}). \tag{5.38}$$

Notice that this is not in $L^1$. As $t \to 0$ it becomes wildly oscillatory everywhere except near the origin.

For $t \neq 0$ we may write the solution as

$$f(\mathbf{x},t) = \int \left(\frac{1}{\sqrt{4\pi i D t}}\right)^\nu \exp(i\frac{|\mathbf{x}-\mathbf{y}|^2}{4Dt}) f(\mathbf{y}) \, d^\nu \mathbf{y} \tag{5.39}$$

and this makes sense for $f$ in $L^1$ and $L^2$. Again it approaches $f(\mathbf{x})$ as $t \to 0$. However notice that the reason is quite different. As $t \to 0$ the oscillations produce cancellations in the integral everywhere except near $\mathbf{x}$.

This equation differs from the diffusion equation in another way, in that reversing the direction of time is simply equivalent to taking a complex conjugate. The solution can run either forward or backward in time.

We can actually compute the large $t$ behavior of the solution.

**Theorem 11** *Let $U_t$ be the unitary operators giving the solution of the free Schrödinger equation. Define the unitary operators $V_t$ in terms of the Fourier transform by*

$$V_t f(\mathbf{x}) = \left(\frac{1}{\sqrt{4\pi i D t}}\right)^\nu \exp(i\frac{\mathbf{x}^2}{4Dt}) \hat{f}(\frac{\mathbf{x}}{2Dt}). \tag{5.40}$$

*Then for each initial condition $f$*

$$\|U_t f - V_t f\| \to 0 \tag{5.41}$$

*as $t \to \pm\infty$.*

Proof: This uses the explicit solution of the free Schrödinger equation. Expand the quadratic term in the exponent. Use the fact that the exponential of the sum is the product of the exponentials. Define

$$W_t f(\mathbf{y}) = \exp(i\frac{\mathbf{y}^2}{4Dt})f(\mathbf{y}). \tag{5.42}$$

Then we have

$$U_t f = V_t W_t f. \tag{5.43}$$

For each $f$ the function $W_t f$ approaches $f$ as $t \to \pm\infty$, by the $L^2$ dominated convergence theorem. Therefore

$$\|U_t f - V_t f\| = \|V_t W_t f - V_t f\| = \|W_t f - f\| \to 0 \tag{5.44}$$

as $t \to \pm\infty$. Q.E.D.

This theorem shows that for large time the solution is concentrated where $\mathbf{x}/(2Dt) = m\mathbf{x}/(\hbar t)$ is in the support of the Fourier transform. Thus the waves move with a velocity profile determined by this function. Since the parts of the wave with different wave numbers move at different velocities and are consequently separated in space, the free Schrödinger equation acts as a kind of filter.

In quantum mechanics it is customary to redefine the Fourier transform in terms of the momentum variable $\mathbf{p} = \hbar k$ by $\tilde{f}(\mathbf{p}) = \hat{f}(\mathbf{k})$. With this convention we can write the density for large time as

$$|f(\mathbf{x},t)|^2 \sim \left(\frac{1}{4\pi Dt}\right)^\nu |\hat{f}(\frac{\mathbf{x}}{2Dt})|^2 \sim \left(\frac{m}{2\pi\hbar t}\right)^\nu |\tilde{f}(\frac{m\mathbf{x}}{t})|^2. \tag{5.45}$$

This is exactly the kind of spreading that one would expect in a free expanding gas, perhaps the aftermath of an explosion.

Let $\Sigma$ be a region in momentum space. Consider the moving region $\Omega_t = \{\mathbf{x} \mid m\mathbf{x}/t \in \Sigma\}$ of position space. Then

$$\int_{\Omega_t} |f(\mathbf{x},t)|^2 \, d^\nu\mathbf{x} \sim \int_\Sigma |\tilde{f}(\mathbf{p})|^2 \, \frac{d^\nu\mathbf{p}}{(2\pi\hbar)^\nu}. \tag{5.46}$$

The amount of the wave function in the moving region is given by the corresponding amount of the Fourier transform of the wave function in

momentum region. This justifies an interpretation of the absolute square of the Fourier transform of the wave function as momentum density, at least for the case of free motion.

**Problems**

1. Take $\nu = 1$ and consider $H_0 = -(\hbar^2/(2m))d^2/dx^2$. Let $c > 0$. Use the representation $(H_0+c^2)^{-1}f = F^{-1}(p^2/(2m)+c^2)^{-1}Ff$ to express the action of this operator as a convolution. (Recall that $p = \hbar k$.)

2. Take $\nu = 3$ and $H_0 = -(\hbar^2/(2m))\nabla^2_{\mathbf{x}}$. Compute the same inverse as in the previous problem.

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# Chapter 6

# The Harmonic Oscillator

This section deals with the harmonic oscillator. For this special system the dynamics of classical and quantum mechanical systems are very close, and it is easy to do explicit computations. For this reason the harmonic oscillator may give a misleading picture of quantum mechanics. The symmetry does not persist in more general systems.

The harmonic oscillator is an important example in its own right. However the isotropic harmonic oscillator in several dimensions is useful for another reason; it gives a convenient way of introducing spherical harmonics. These are important for all rotationally invariant systems.

## 6.1 The classical harmonic oscillator

The classical harmonic oscillator has equations of motion $dx/dt = p/m$ and $dp/dt = -m\omega^2 x$. Here $m > 0$ is the mass and the angular frequency $\omega$ is defined in such a way that $m\omega^2 > 0$ is the spring constant. The energy

$$H = \frac{1}{2m}p^2 + \frac{m\omega^2}{2}x^2 \tag{6.1}$$

satisfies $dH/dt = 0$. Thus the orbits are ellipses in phase space with fixed energy $H = E$. The solutions are linear combinations of $x = x(0)\cos(\omega t) + p(0)/(m\omega)\sin(\omega t)$ and $p = -m\omega x(0)\sin(\omega t) + p(0)\cos(\omega t)$. This may also be written in terms of the energy and phase as $x = \sqrt{2E/(m\omega^2)}\cos(\omega t - \theta)$ and $p = -\sqrt{2mE}\sin(\omega t - \theta)$.

There is another type of solution of the classical oscillator that is time invariant. However it is a random solution. Fix the energy $E$ and consider the ellipse $H = E$. Take the probability measure on this ellipse that is

proportional to $dt = mdx/p$. This is obviously time invariant. Such a solution is an oscillator of fixed energy but random phase.

## 6.2 The one dimensional quantum harmonic oscillator

The harmonic oscillator Hamiltonian is

$$H = \frac{1}{2m}P^2 + \frac{m\omega^2}{2}x^2 = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2. \tag{6.2}$$

We think of the operator as acting in the space of $L^2$ functions of position; we sometimes refer to this as the *Schrödinger representation*.

It is convenient to introduce a dimensionless variable $s = \sqrt{(m\omega/\hbar)}x$. In this variable the Hamiltonian is

$$H = \hbar\omega\left(-\frac{1}{2}\frac{d^2}{ds^2} + \frac{1}{2}s^2\right) \tag{6.3}$$

acting in $L^2(\mathbf{R}, ds)$. We think of this as a variant of the Schrödinger representation.

The key to the problem is the following clever factorization. Define the *annihilation operator*

$$A = 1/\sqrt{2}\left(s + \frac{d}{ds}\right) \tag{6.4}$$

and the *creation operator*

$$A^* = 1/\sqrt{2}\left(s - \frac{d}{ds}\right) \tag{6.5}$$

and the *number operator*

$$N = A^*A = -\frac{1}{2}\frac{d^2}{ds^2} + \frac{1}{2}s^2 - \frac{1}{2}. \tag{6.6}$$

Then $H = \hbar\omega(N + 1/2)$, and so it is sufficient to study $N$. It is easy to check that $N$ has the Hermitian symmetry property $\langle N\psi, \phi\rangle = \langle \psi, N\phi\rangle$.

We look for eigenvectors of $N$. Let $\phi_0(s) = 1/\sqrt{\pi}\exp(-s^2/2)$. Then $A\phi_0 = 0$ and hence $N\phi_0 = A^*A\phi_0 = 0$. So $\phi_0$ is an eigenvector of $N$ with eigenvalue 0.

We have the commutation relation

$$AA^* = A^*A + 1. \tag{6.7}$$

It follows that

$$NA^* = A^*(N+1). \tag{6.8}$$

Define $\phi_n = A^{*n}\phi_0$. Then by induction

$$N\phi_n = n\phi_n. \tag{6.9}$$

It is also easy to check that $A\phi_n = n\phi_{n-1}$ for $n \geq 1$.

Since $N$ is Hermitian, these eigenvectors are mutually orthogonal. In order to see what they look like, it is convenient to change to another representation, in which the Hilbert space is $L^2(\mathbf{R}, (1/\pi)\exp(-s^2)\,ds)$. The operator of multiplication by $1/\sqrt{\pi}\exp(-s^2/2)$ is an isomorphism from this space to $L^2(\mathbf{R}, ds)$. This new representation is called the *Gaussian representation*.

In this new representation the operators become

$$A = 1/\sqrt{2}\frac{d}{ds} \tag{6.10}$$

and

$$A^* = 1/\sqrt{2}\left(2s - \frac{d}{ds}\right) \tag{6.11}$$

and

$$N = A^*A = -\frac{1}{2}\frac{d^2}{ds^2} + s\frac{d}{ds}. \tag{6.12}$$

The vector $\phi_0(s) = 1$. Therefore in this representation

$$\phi_n = A^{*n}\phi_0 \tag{6.13}$$

is a polynomial $h_n(s)$ of degree $n$. We call this a *Hermite polynomial* of degree $n$.

Back in the original representation the eigenvectors are Hermite polynomials times the Gaussian, that is $h_n(s)1/\sqrt{\pi}\exp(-s^2/2)$. We call these Hermite basis functions.

We would like to show that these eigenvectors form a basis. It is easy to see that every polynomial of degree $\leq n$ is a sum of Hermite polynomials of degree $\leq n$. So this reduces to show that the functions $p(s)\exp(-s^2/2)$, where $p(s)$ is a polynomial in $s$, are dense in $L^2$. This follows from the density theorems of a later section.

It is easy to check by induction that the norms of these basis vectors are given by $\|\phi_n\|^2 = n!$. Most treatments replace these by vectors of norm one, but we will not bother to do that. The price we pay is that the discrete measure is not counting measure, but instead weights each point by $1/n!$. Thus the square of the norm on $\ell^2$ must be taken to be $\sum |c_n|^2/n!$. The corresponding vector in $\mathcal{H}$ is given by $f = \sum_n c_n/n!\phi_n$ where $c_n = \langle \phi_n, f\rangle$. We summarize with the following theorem.

**Theorem 12** *Let $H$ be the harmonic oscillator Hamiltonian acting in $\mathcal{H}$. Then the Hermite basis functions provide an isomorphism $W$ from $\mathcal{H}$ to $\ell^2(\mathbf{N}, 1/n!)$ such that the action of $H$ is isomorphic to multiplication by $\hbar\omega(n + 1/2)$, where $n = 0, 1, 2, 3, \ldots$.*

Now we look at some special solutions of the Schrödinger equation for the harmonic oscillator. We begin with analogs of the time-dependent solutions. Let $z = (a + ib)/\sqrt{2}$ be a complex number. Define the *coherent state* $\phi_z$ to be proportional to $\exp(ibs)\exp(-(s-a)^2/2)$ in the Schrödinger representation. This is proportional to $\exp((a + ib)s)$ in the Gaussian representation. It is obviously an eigenvector of $A$ with eigenvalue $z$. If we expand this eigenvector in terms of Hermite basis functions as $\sum_n c_n/n!\phi_n$, we obtain from $A\psi = z\psi$ the recursion $\sum_n c_n/(n-1)!\phi_{n-1} = \sum_n zc_n/n!\phi_n$. Thus $c_{n+1} = zc_n$ and finally $c_n = z^n c_0$. We can arrange that the coherent state vector has norm one by taking $c_0 = \exp(-|z|^2/2)$. Thus the coefficients in the number representation are $c_n = z^n \exp(-|z|^2/2)$. Note that the numbers $|c_n|^2/n! = |z|^{2n}/n! \exp(-|z|^2)$ are a Poisson distribution with mean $|z|^2$. The expected energy is thus $\hbar\omega(|z|^2 + 1/2)$.

**Proposition 15** *The time evolution of a coherent state is given by*

$$U_t\phi_z = \exp(-i\omega t/2)\phi_{z\exp(-i\omega t)}. \tag{6.14}$$

Proof: The time evolution in terms of the coefficients is

$$\exp(-i\omega t(n + 1/2))c_n = \exp(-i\omega t/2)(z\exp(-i\omega t))^n c_0. \tag{6.15}$$

The first factor has no physical effect, since it is independent of $n$. Thus the effect of the time evolution is to replace $z$ by $z\exp(-it\omega)$. This replaces $a+ib$ by $(\cos(\omega t)-i\sin(\omega t))(a+ib)$. In particular $a$ is replaced by $a\cos(\omega t)+b\sin(\omega t)$ and $b$ is replaced by $-a\sin(\omega t)+b\cos(\omega t)$. These special solutions thus have a dynamics that is completely determined by the corresponding classical dynamics. If we use $\sqrt{\hbar\omega}z = (\sqrt{m\omega^2}x_0+i/\sqrt{m}p_0)/\sqrt{2}$ to translate back into physical variables we see that this is precisely the classical time evolution. Notice that $\hbar\omega|z|^2$ is the clasical energy.

There are also analogs of the time-independent solutions. However in quantum mechanics these are not random mixtures of other states. For each $n$ the Hermite basis function constructed above provides a solution of the form $\exp(-i\omega t(n + 1/2))\phi_n$. These are solutions of constant energy $E = \hbar\omega(n + 1/2)$. The only time dependence is a scalar multiple, and this does not enter into physical calculations. So from a physical point of view this is a constant solution. Such solutions are the analogs of the random phase solutions of the classical oscillator.

This interpretation may be understood by looking at the form of the wave function. This is a polynomial of degree $n$ times a Gaussian, so it has $n$ zeros. These zeros are difficult to interpret in terms of a classical picture. However one may average out the effect of the zeros by taking the inner product with a coherent state. This gives $|\langle \phi_n, \phi_z \rangle|^2/n! = |z|^{2n}/n! \exp(-|z|^2)$. As a function of $|z|^2$ this rises to a maximum at $|z|^2 = n$ and falls off rapidly after that. If we take $z$ real with $\hbar\omega|z|^2 = m\omega^2 x_0^2$, we see that the wave function is essentially confined to the region where $m\omega^2 x_0^2 \leq \hbar\omega n$. For large $n$ the constraint $\hbar\omega n$ has the same asymptotics as the energy $\hbar\omega(n + 1/2)$. So this is very close to the classical restriction.

## 6.3 The Fourier transform

The harmonic oscillator casts new light on the Fourier transform. We work in the Schrödinger representation with the dimensionless variables $s$. The Fourier transform variable is denoted $t$. The Fourier transform of $d/ds$ is $it$. Similarly, the Fourier transform of multiplication by $s$ is $id/dt$. It follows that the Fourier transform of the annihilation operator $s + d/ds$ is $i(t + d/dt)$ and the Fourier transform of the creation operator $(s - d/ds)$ is $-i(t - d/dt)$. This immediately leads to the following fundamental result.

**Theorem 13** *The Fourier transform of the Hermite basis function given by* $h_n(s)1/\sqrt{\pi}\exp(-s^2/2)$ *is equal to* $(-i)^n h_n(t)\sqrt{2}\exp(-t^2/2)$.

Thus by using this sort of basis both in the position space and in the wave number space, the action of the Fourier transform reduces to introducing a coefficient $(-i)^n$.

## 6.4 Density theorems

In showing that the Hermite basis functions are indeed a basis, we used a density theorem for polynomials. In this section we give the details of this and related results. The results are valid in the $\nu$ dimensional case, so we may as well present them in this generality.

If $f$ is in $L^1$, then its Fourier transform need not be in $L^1$, nor need it be in $L^2$. However it is in $L^\infty$. This is enough so that the formulas in the following proposition make sense. Recall that the approximate delta function $\delta_\epsilon$ is chosen so that both $\delta_\epsilon$ and its Fourier transform $\hat{\delta}_\epsilon$ are in $L^1$ for each $\epsilon > 0$.

**Proposition 16** *Let $f$ be in $L^1$. Then $f$ may be recovered from its Fourier transform by computing*

$$\delta_\epsilon * f(\mathbf{x}) = \int \exp(i\mathbf{k}\cdot\mathbf{x})\hat{\delta}_\epsilon(\mathbf{k})\hat{f}(\mathbf{k})\, d^\nu\mathbf{k}/(2\pi)^\nu \tag{6.16}$$

*and taking the $L^1$ limit $\delta_\epsilon * f \to f$ as $\epsilon \to 0$.*

Notice that it follows from this proposition that if $f$ in $L^1$ has a Fourier transform $\hat{f} = 0$, then $f$ is a null function.

The basic density result is given in the following proposition.

**Proposition 17** *Let $f$ be a function in $L^2$ that never vanishes. Then the linear space spanned by $\exp(-i\mathbf{k}\cdot\mathbf{x})f(\mathbf{x})$ for all $\mathbf{k}$ is dense in $L^2$.*

Proof: Let $g(\mathbf{x})$ in $L^2$ be orthogonal to all the $\exp(-i\mathbf{k}\cdot\mathbf{x})f(\mathbf{x})$. Then by the preceeding result the $L^1$ function $g(\mathbf{x})f(\mathbf{x})$ is zero.

Here is a corollary.

**Corollary 5** *Let $f$ be a function in $L^2$ that never vanishes and such that for each $\mathbf{k}$ the function $\exp(|\mathbf{k}\cdot\mathbf{x})|)f(\mathbf{x})$ is in $L^2$. Then the linear space consisting of $p(\mathbf{x})f(\mathbf{x})$ for all polynomials is dense in $L^2$.*

Proof: Expand the exponential in $\exp(i\mathbf{k}\cdot\mathbf{x})f(\mathbf{x})$. The partial sums converge in $L^2$, by the dominated convergence theorem.

The proposition also has the following $L^2$ Wiener theorem as a corollary.

**Corollary 6** *Let $f$ be a function in $L^2$ such that its Fourier transform $\hat{f}$ never vanishes. Then the linear space spanned by the translates $f_\mathbf{a}$ for all $\mathbf{a}$ is dense in $L^2$.*

Proof: This is the Fourier transform of the situation in the proposition.

## 6.5 The isotropic quantum harmonic oscillator

The remainder of this chapter is devoted to the isotropic harmonic oscillator. The only purpose for this is that it gives an efficient way of developing the theory of spherical harmonics. The reader who is content with the summary of this theory in the following chapter may omit or postpone the following material.

In this section we describe the quantum harmonic oscillator in $\nu$ dimensions. We confine the treatment to the rotationally symmetric isotropic

oscillator, since we are mainly interested in the results for their application to spherical harmonics. The results are parallel to the one-dimensional results, since the basis functions in $\nu$ dimensions are obtained by taking products of the one-dimensional basis functions.

The isotropic harmonic oscillator Hamiltonian in $\nu$ dimensions is

$$H = \frac{1}{2m}\mathbf{P}^2 + \frac{m\omega^2}{2}\mathbf{x}^2 = -\frac{\hbar^2}{2m}\nabla_{\mathbf{x}}^2 + \frac{m\omega^2}{2}\mathbf{x}^2. \tag{6.17}$$

Introduce dimensionless vector variables $\mathbf{s} = \sqrt{(m\omega/\hbar)}\mathbf{x}$. In these variables the Hamiltonian is

$$H = \hbar\omega\left(-\frac{1}{2}\nabla_{\mathbf{s}}^2 + \frac{1}{2}\mathbf{s}^2\right). \tag{6.18}$$

Define operator vectors

$$\mathbf{A} = 1/\sqrt{2}\,(\mathbf{s} + \nabla_{\mathbf{s}}) \tag{6.19}$$

and

$$\mathbf{A}^* = 1/\sqrt{2}\,(\mathbf{s} - \nabla_{\mathbf{s}}) \tag{6.20}$$

and the operator

$$N = \mathbf{A}^* \cdot \mathbf{A} = -\frac{1}{2}\nabla_{\mathbf{s}}^2 + \frac{1}{2}\mathbf{s}^2 - \frac{\nu}{2}. \tag{6.21}$$

Then $H = \hbar\omega(N + \nu/2)$, and so it is sufficient to study $N$.

We look for eigenvectors of $N$. Let $\phi_0(\mathbf{s}) = (1/\sqrt{\pi})^\nu \exp(-\mathbf{s}^2/2)$. Then $\mathbf{A}\phi_0 = 0$ and hence $N\phi_0 = \mathbf{A}^* \cdot \mathbf{A}\phi_0 = 0$. So $\phi_0$ is an eigenvector of $N$ with eigenvalue 0.

Let $A_j$ and $A_j^*$ be the $j$ components of $\mathbf{A}$ and $\mathbf{A}^*$ and define $N_j = A_j^* A_j$. Then $N = \sum_j N_j$. Furthermore we have the commutation relation

$$A_j A_j^* = A_j^* A_j + 1. \tag{6.22}$$

It follows that

$$N_j A_j^* = A_j^*(N_j + 1). \tag{6.23}$$

Hence by induction

$$N_j A_j^{*n}\phi_0 = n A_j^{*n}\phi_0. \tag{6.24}$$

It follows easily that if $n = \sum_j n_j$, then

$$N A_1^{*n_1}\cdots A_\nu^{*n_\nu}\phi_0 = n A_1^{*n_1}\cdots A_\nu^{*n_\nu}\phi_0. \tag{6.25}$$

Again there is a Gaussian representation in which the Hilbert space is defined with a weighted measure by $L^2(\mathbf{R}^\nu, (1/\pi)^\nu \exp(-\mathbf{s}^2)\, d^\nu\mathbf{s})$. The

operator of multiplication by $(1/\sqrt{\pi})^\nu \exp(-\mathbf{s}^2/2)$ is an isomorphism from this space to $L^2(\mathbf{R}^\nu, d^\nu \mathbf{s})$.

In this new representation the operators become

$$\mathbf{A} = 1/\sqrt{2}\nabla_{\mathbf{s}} \tag{6.26}$$

and

$$\mathbf{A}^* = 1/\sqrt{2}\,(2\mathbf{s} - \nabla_{\mathbf{s}}) \tag{6.27}$$

and

$$N = \mathbf{A}^* \cdot \mathbf{A} = -\frac{1}{2}\nabla_{\mathbf{s}}^2 + \mathbf{s} \cdot \nabla_{\mathbf{s}}. \tag{6.28}$$

Notice that $N$ is the sum of $-1/2$ times the Laplace operator with the Euler operator $r\partial/\partial r$, where $r^2 = \mathbf{s}^2$ is the radius. The vector $\phi_0(\mathbf{s}) = 1$. Therefore in this representation

$$A_1^{*n_1} \cdots A_\nu^{*n_\nu} \phi_0 \tag{6.29}$$

is a polynomial of degree $n = \sum_j n_j$ in $\nu$ variables. We continue to call this a *Hermite polynomial* in $\nu$ variables of degree $n$.

Thus back in the original representation the eigenvectors are Hermite polynomials times a multiple of $\exp(-\mathbf{s}^2/2)$.

**Proposition 18** *The dimension of the space $\mathcal{H}_n$ of Hermite polynomials in $\nu$ variables of degree $n$ is $d_n^\nu = \binom{n+\nu-1}{\nu-1}$.*

Proof: The dimension is the number of ways of writing $n = n_1 + \cdots + n_\nu$ with each $n_j \geq 0$. This is the number of occupation numbers when one maps an $n$ element set into a $\nu$ element set.

It can also be thought of as the number of ways of writing $n + \nu - 1 = n_1 + 1 + n_2 + 1 + \cdots + n_{\nu-1} + 1 + n_\nu$. This is the number of ways of choosing $\nu - 1$ places (where the 1s occur) from $n + \nu - 1$ places.

**Proposition 19** *The dimension of the space $\mathcal{H}_n$ of Hermite polynomials in $\nu$ variables of degree $n$ is related to the dimension of the space in $\nu - 1$ variables by the sum rule $d_n^\nu = \sum_{m=0}^n d_m^{\nu-1}$.*

Proof: For each $m$ with $n_1 + \cdots + n_{\nu-1} = m$, there is a unique $n_\nu = n - m$ with $n_1 + \cdots + n_\nu = n$.

## 6.6 Spherical harmonics

The spherical harmonics now appear as special cases of Hermite polynomials. We compute systematically with the operators $\mathbf{A}^2$ and $\mathbf{A}^{*2}$. The point is that these are rotation invariant by construction.

**Definition 11** *The space $\mathcal{A}_n$ of* solid spherical harmonics *of degree $n$ is defined to be the space of solutions to $\mathbf{A}^2 y = 0$ and $Ny = ny$ in the Gaussian representation.*

Thus according to this definition the space of solid spherical harmonics $\mathcal{A}_n$ of degree $n$ is a subspace of the space of Hermite polynomials $\mathcal{H}_n$ of degree $n$.

In the Gaussian representation the operators

$$\mathbf{A}^2 = \frac{1}{2}\nabla_{\mathbf{s}}^2 \tag{6.30}$$

and

$$N = -\frac{1}{2}\nabla_{\mathbf{s}}^2 + \mathbf{s}\cdot\nabla_{\mathbf{s}}. \tag{6.31}$$

So the condition for a solid spherical harmonic $y$ of degree $n$ is that $\nabla_{\mathbf{s}}^2 y = 0$ and $\mathbf{s}\cdot\nabla_{\mathbf{s}} y = ny$. In other words, it must be harmonic and homogeneous of degree $n$. Notice that everything in this definition is invariant under rotation.

The condition for being homogeneous of degree $n$ may also be written $r(\partial/\partial r)y = ny$, where $r^2 = \mathbf{s}^2$. It follows that $y = r^n Y$, where $Y$ is the restriction of the solid spherical harmonic to the sphere $r^2 = 1$. This leads to the definition of a *surface spherical harmonic* as the restriction of a solid spherical harmonic to the unit sphere. The surface spherical harmonic may be thought of a a function of the angular variables alone.

**Proposition 20** *Let $\mathcal{H}_n$ be the space of Hermite polynomials of degree $n$ in $\nu$ dimensions. Let $\mathcal{A}_n$ be the subspace of solid spherical harmonics. Then $\mathcal{H}_n = \mathcal{A}_n \oplus \mathbf{A}^{*2}\mathcal{H}_{n-2}$. Furthermore, $\mathbf{A}^{*2}$ is one-to-one from $\mathcal{H}_{n-2}$ into $\mathcal{H}_n$.*

Proof: We know that $\mathbf{A}^2$ sends $\mathcal{H}_n$ into $\mathcal{H}_{n-2}$ and the adjoint $\mathbf{A}^{*2}$ sends $\mathcal{H}_{n-2}$ into $\mathcal{H}_n$. Therefore this is just the statement that $\mathcal{H}_n$ is the sum of the nullspace of $\mathbf{A}^2$ with the range of its adjoint.

The last statement follows from the commutation relation $\mathbf{A}^2\mathbf{A}^{*2} = \mathbf{A}^{*2}\mathbf{A}^2 + 2(2N + \nu)$. It follows that

$$\langle \mathbf{A}^{*2}y, \mathbf{A}^{*2}y\rangle = \langle \mathbf{A}^2 y, \mathbf{A}^2 y\rangle + 2\langle y, (2N+\nu)y\rangle. \tag{6.32}$$

. Thus if $\mathbf{A}^{*2}y = 0$, then $\langle y, (2N+\nu)y\rangle = 0$ and so $y = 0$.

**Proposition 21** *The dimension of the space $\mathcal{A}_n$ of spherical harmonics in $\nu$ variables of degree $n$ is $a_n^\nu = \binom{n+\nu-2}{n} + \binom{n+\nu-3}{n-1}$.*

Proof: From the previous result $d_n^\nu = a_n^\nu + d_{n-2}^\nu$. Using Pascal's triangle we obtain

$$a_n^\nu = \binom{n+\nu-1}{n} - \binom{n+\nu-3}{n-2} \tag{6.33}$$

$$= \binom{n+\nu-2}{n} + \binom{n+\nu-2}{n-1} - \binom{n+\nu-3}{n-2} \tag{6.34}$$

$$= \binom{n+\nu-2}{n} + \binom{n+\nu-3}{n-1}. \tag{6.35}$$

Let us look at the first few values of $\nu$. For $\nu = 1$ the result is $d_p^1 = \binom{p-1}{p} + \binom{p-2}{p-1}$ which is 1 when $p = 0$ or $p = 1$, due to the curious fact that $\binom{-1}{0} = 1$. For $\nu = 2$ the result is $d_m^2 = \binom{m}{m} + \binom{m-1}{m-1}$. This is 1 for $m = 0$ and 2 for all $m \geq 1$. The most famous special case is the result for dimension three that $a_\ell^3 = (\ell+1) + \ell = 2\ell + 1$. It is worth remarking that for dimension four we have $a_k^4 = (k+1)^2$.

**Proposition 22** *The dimension of the space $\mathcal{A}_n$ of spherical harmonics in $\nu$ variables of degree $n$ is related to the dimension of the space in $\nu - 1$ variables by the sum rule $a_n^\nu = \sum_{m=0}^n a_m^{\nu-1}$.*

Proof: Since $a_n^\nu = d_n^\nu - d_{n-2}^\nu$ this follows from the sum rule for Hermite polynomials.

**Definition 12** *The $\ell$th* angular momentum subspace *$\mathcal{M}_\ell$ is defined to be the direct sum of the spaces $\mathbf{A}^{*2m}\mathcal{A}_\ell$ for $m = 0, 1, 2, 3 \ldots$.*

The angular momentum subspaces are also defined in terms of rotation invariant quantities. According to the following theorem they give a decomposition of the Hilbert space.

**Theorem 14** *The Hilbert space is a direct sum of the angular momentum subspaces: $\mathcal{H} = \oplus_{\ell=0}^\infty \mathcal{M}_\ell$.*

Proof: We know that the Hilbert space is the direct sum of the number subspaces: $\mathcal{H} = \oplus_{n=0}^\infty \mathcal{H}_n$. On the other hand, each number subspace $\mathcal{H}_n = \oplus_{\ell+2m=n} \mathbf{A}^{*2m}\mathcal{A}_\ell$. Therefore $\mathcal{H}_n = \oplus_{\ell=0}^\infty \oplus_m \mathbf{A}^{*2m}\mathcal{A}_\ell = \oplus_{\ell=0}^\infty \mathcal{M}_\ell$.

We can look more closely at the structure of the angular momentum spaces by looking at the summands $\mathbf{A}^{*2m}\mathcal{A}_\ell$.

**Proposition 23** *For each dimension $\nu$ and degree $\ell$ there are polynomials $f_m(r)$ of degree $2m$ in the radius $r$ such that the space $\mathbf{A}^{*2m}\mathcal{A}_\ell$ consists of $f_m(r)y$ with $y$ in $\mathcal{A}_\ell$. These radial polynomials satisfy the relation*

$$f_{m+1}(r) = 2r^2 f_m(r) - r\frac{\partial f_m(r)}{\partial r} + (2m + 2\ell + \nu) f_m(r). \tag{6.36}$$

Proof: We work in the Gaussian representation. Let $y$ be a solid spherical harmonic of degree $\ell$. The operator $\mathbf{A}^{*2}$ is given in the Gaussian representation by

$$\mathbf{A}^{*2} = 2r^2 - (r\frac{\partial}{\partial r} + N + \nu), \tag{6.37}$$

where $r^2 = \mathbf{s}^2$. The solid spherical harmonic is homogeneous of degree $\ell$, so it is of the form $y = r^\ell Y$, where $Y$ has only angular dependence. We proceed inductively. Let $f_m(r)$ be the radial polynomial of degree $2m$. The action of $\mathbf{A}^{*2}$ on $f_m(r)y$ is $2r^2 f_m(r)y - r\frac{\partial f_m(r)}{\partial r}y + (\ell + \ell + 2m + \nu)f_m(r)y$ which is $f_{m+1}(r)y$. Q.E.D.

We see from this result that the angular momentum subspaces $\mathcal{M}_\ell$ consist of radial functions times spherical harmonics of degree $\ell$. The basis functions for the radial functions are given by the polynomials discussed in the proposition; these are closely related to Laguerre polynomials.

## 6.7 Fourier transforms involving spherical harmonics

One useful consequence of the above results is the theory of Fourier transforms of the angular momentum subspaces. These consist of radial functions times solid spherical harmonic of degree $\ell$ for some $\ell = 0, 1, 2, 3, \ldots$.

When $\ell = 0$ we have radial functions. The Fourier transform of a radial function is radial. We call this the *radial Fourier transform*. This transform may be expressed in terms of Bessel functions by a formula depending on the dimension. The explicit expression is given in standard references [SW]. The most important special cases are dimension $\nu = 1$ and $\nu = 3$. The formulas for $\nu = 1$ is

$$\hat{f}(t) = \int_0^\infty 2\cos(tr)f(r)\,dr. \tag{6.38}$$

The formula for $\nu = 3$ is

$$\hat{f}(t) = 4\pi \int_0^\infty \frac{\sin(tr)}{t} f(r) r\,dr. \tag{6.39}$$

This leads to a useful trick for reducing the three dimensional radial Fourier transform to a one dimensional transform. Extend the radial functions $f(r)$ and $\hat{f}(t)$ to be even functions on the line. Then the three dimensional formula becomes

$$t\hat{f}(t) = 2\pi i \int_{-\infty}^\infty e^{-itr} r f(r)\,dr. \tag{6.40}$$

Each function in the subspace of $\mathbf{A}^{*2m}\mathcal{A}_\ell$ is taken by the Fourier transform into $(-i)^{(2m+\ell)}$ times the same function. If we fix the spherical harmonic in $\mathcal{A}_\ell$ and build the radial function by summing over $m$, we see that the Fourier transform of a radial function times a spherical harmonic is another radial function times the same spherical harmonic. In particular, the Fourier transform takes the angular momentum space into the corresponding angular momentum space.

**Theorem 15** *The $\nu$ dimensional Fourier transform of a radial function times a solid spherical harmonic of degree $\ell$ is $(2\pi i)^{-\ell}$ times the radial Fourier transform in dimension $\nu + 2\ell$ times the same solid spherical harmonic.*

Proof: We work in the Schrödinger representation. It is sufficient to check this for functions of the form $f_m(r)y\exp(-r^2/2)$ where $f_m(r)$ is the radial polynomial of degree $2m$. The Fourier transform is $(-i)^{2m+\ell}$ times the same radial polynomial of degree $2m$ times $y$ times $\exp(-r^2/2)$ times $(2\pi)^{\nu/2}$. On the other hand, the Fourier transform of $f_m(r)\exp(-r^2/2)$ in dimension $\nu + 2\ell$ is $(-i)^{2m}$ times the same radial polynomial times $\exp(-r^2/2)$ times $(2\pi)^{(\nu+2\ell)/2}$. The first result is obtained from the second result by multiplying by $(2\pi i)^{-\ell}$ and by $y$.

Example: The special case $\nu = 1$ and $\ell = 1$ is instructive. Let $f(r)$ be an even function. The solid spherical harmonic of degree one is just $r$. Therefore the Fourier transform of $rf(r)$ is obtained by taking the three dimensional radial Fourier $\hat{f}(t)$ of $f(r)$ and multiplying by $t$ and dividing by $2\pi i$. This is precisely the relation between one dimensional Fourier transforms of odd functions and three dimensional radial Fourier transforms given above.

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# Chapter 7

# The Hydrogen Atom

## 7.1 The Kepler problem

In classical mechanics the Kepler problem is

$$\frac{d\mathbf{x}}{dt} = \frac{\mathbf{p}}{m} \tag{7.1}$$

$$\frac{d\mathbf{p}}{dt} = -\frac{k}{r^2}\frac{\mathbf{x}}{r}, \tag{7.2}$$

where $r = |\mathbf{x}|$. The constant $m > 0$ is the mass and the parameter $k > 0$ is the proportionality constant in the force law. The energy is

$$H = \frac{1}{2m}\mathbf{p}^2 - \frac{k}{r}. \tag{7.3}$$

It is easy to check that $dH/dt = 0$.

The first step toward a solution is to use the rotational symmetry of the problem. Consider a constant vector $\mathbf{h}$ that is orthogonal to $\mathbf{x}$ and $\mathbf{p}$ at some time. Then since $d\mathbf{x}/dt$ is proportional to $\mathbf{p}$ and $d\mathbf{p}/dt$ is proportional to $\mathbf{x}$, it is easy to check that it remains orthogonal for all future time. It follows that $\mathbf{x}$ and $\mathbf{p}$ always lie in the same plane.

Since the motion lies in a plane, we may introduce polar coordinates $r$ and $\theta$ in this plane. Write $\mathbf{x} = r\mathbf{n}$, where $\mathbf{n}$ is the unit vector in the direction of $\mathbf{x}$. Then the first equation gives

$$\mathbf{p} = m\left(\frac{dr}{dt}\mathbf{n} + r\frac{d\theta}{dt}\mathbf{t}\right), \tag{7.4}$$

where $\mathbf{t} = d\mathbf{n}/d\theta$ is a unit vector in the plane which is orthogonal to $\mathbf{n}$. Note that $d\mathbf{t}/d\theta = -\mathbf{n}$.

Define the planar angular momentum $h$ as the area $\mathbf{x} \wedge \mathbf{p}$ of the plane determined by $\mathbf{x}$ and $\mathbf{p}$. Then since $d\mathbf{x}/dt$ is proportional to $\mathbf{p}$ and $d\mathbf{p}/dt$ is proportional to $\mathbf{x}$, it follows that $h$ is constant. If one works out what $h$ is in polar coordinates the result is $h = mr^2 d\theta/dt$. Therefore the second equation may be written

$$\frac{d\mathbf{p}}{d\theta} = -\frac{mk}{h}\mathbf{n}. \tag{7.5}$$

This integrates to

$$\mathbf{p} = \frac{mk}{h}\mathbf{t} + \mathbf{c}, \tag{7.6}$$

where $\mathbf{c}$ is a constant vector. We may characterize the orbit by the equation

$$(\mathbf{p} - \mathbf{c})^2 = (mk/h)^2. \tag{7.7}$$

The momentum vector lies in a circle with center $\mathbf{c}$ in the plane of the motion!

The angular momentum $\mathbf{x} \wedge \mathbf{p}$ may be recomputed using this solution. Measure the angle $\theta$ of $\mathbf{t}$ from the direction of $\mathbf{c}$. The calculation gives $h = r(mk/h + \mathbf{n} \wedge \mathbf{c}) = r(mk/h + \mathbf{t} \cdot \mathbf{c}) = r(mk/h + |\mathbf{c}| \cos\theta)$. This is the equation of a conic section.

We can now compute the energy $E$. It is simplest to compute the energy at the point of the orbit when $\mathbf{x}$ is in the direction of $\mathbf{c}$, so that $\mathbf{c} \cdot \mathbf{t} = 0$. Then

$$2mE = \mathbf{p}^2 - 2mk/r = (mk/h)^2 + \mathbf{c}^2 - 2(mk/h)^2 = \mathbf{c}^2 - (mk/h)^2. \tag{7.8}$$

It is easy to see that the conic section is an ellipse, parabola, hyperbola depending on whether $E < 0$, $E = 0$, or $E > 0$. We have obtained the following result.

**Theorem 16** *Fix the energy $E$. The allowed orbits of the Kepler problem in momentum space are circles*

$$(\mathbf{p} - \mathbf{c})^2 = c^2 - 2mE \tag{7.9}$$

*lying in angular momentum planes $\mathbf{h} \cdot \mathbf{p} = 0$.*

Assume that $E < 0$. We may express the momentum circle in terms of the energy as

$$\mathbf{p}^2 - 2\mathbf{c} \cdot \mathbf{p} + 2mE = 0. \tag{7.10}$$

Change variables by setting $\mathbf{z} = \mathbf{p}/\sqrt{-2mE}$. The equation becomes

$$\mathbf{z}^2 - 2\mathbf{a} \cdot \mathbf{z} - 1 = 0, \tag{7.11}$$

where $\mathbf{a}$ is the center of the circle in the $\mathbf{z}$ space. Each orbit in momentum space with fixed negative energy corresponds to such a circle (lying in the plane determined by the angular momentum).

What do these circles have in common? The way to see is to linearize this equation by a change of variable. The equation determining the plane is $\mathbf{h} \cdot \mathbf{z} = 0$ which is already linear, so we want to leave this alone.

Place the momentum plane in a space of one more dimension (say four instead of three). Let $\mathbf{e}$ be the unit basis vector in the new dimension. Then the change of variable $\mathbf{z} = \bar{\mathbf{z}} + \mathbf{e}$ gives the equation in the form

$$\bar{\mathbf{z}}^2 - 2(\mathbf{a} - \mathbf{e}) \cdot \bar{\mathbf{z}} = 0, \tag{7.12}$$

Now make the non-linear change of variable by the *inversion* $\bar{\mathbf{z}} = 2\bar{\mathbf{w}}/|\bar{\mathbf{w}}|^2$. We get the linear equation

$$1 - (\mathbf{a} - \mathbf{e}) \cdot \bar{\mathbf{w}} = 0, \tag{7.13}$$

Finally, introduce a new variable $\mathbf{w}$ by $\bar{\mathbf{w}} = \mathbf{w} - \mathbf{e}$. The final form is $(\mathbf{a} - \mathbf{e}) \cdot \mathbf{w} = 0$. This is the equation of a $\nu$ dimensional subspace passing through through the origin in $\nu + 1$ dimensional space. This may be combined with the equations $\mathbf{h} \cdot \mathbf{w} = 0$ which determine a three dimensional subspace passing through the origin. The intersection of these two subspaces is a plane passing through the origin. Everything up to this point is linear.

The only trouble is that we must see the effect of the constraint $\mathbf{e} \cdot \mathbf{z} = 0$. Since $\mathbf{e} \cdot \mathbf{z} = (\mathbf{w}^2 - 1)/|\bar{\mathbf{w}}|^2$, this works out to $\mathbf{w}^2 = 1$. This is the equation of the $\nu$ dimensional sphere in $\nu + 1$ dimensional space. Each solution corresponds to a plane passing through the origin intersecting this sphere, that is, to a great circle on the sphere.

The geometry of this change of variables is just a stereographic projection from the north pole $e$. The variable $\bar{\mathbf{z}} = \mathbf{z} - \mathbf{e}$ is proportional to the variable $\bar{\mathbf{w}} = \mathbf{w} - \mathbf{e}$, but $\mathbf{z}$ lies in the equatorial plane $\mathbf{e} \cdot \mathbf{z} = 0$ while $\mathbf{w}$ lies in the sphere $\mathbf{w}^2 = 1$.

**Theorem 17** *Fix a negative value of the energy. Consider* $\mathbf{z}$ *in the space* $\mathbf{R}^\nu$ *of normalized momenta. Introduce a unit vector in a new dimension, so that* $\mathbf{e} \cdot \mathbf{z} = 0$. *Consider the Kepler momentum circles given by the equations* $(\mathbf{z} - \mathbf{a})^2 = \mathbf{a}^2 + 1$ *and* $\mathbf{h} \cdot \mathbf{z} = 0$. *Then the change of variable given by the stereographic projection transforms them to the great circles on the three sphere* $\mathbf{w}^2 = 1$ *in* $\mathbf{R}^{\nu+1}$. *The corresponding equations are* $(\mathbf{a} - \mathbf{e}) \cdot \mathbf{w} = 0$ *and* $\mathbf{h} \cdot \mathbf{w} = 0$.

This shows that there is a remarkable $\nu + 1$ dimensional symmetry to the Kepler problem. There is a beautiful discussion of this in an article

by Milnor [12]. (There is also an amusing connection between the Kepler problem and the harmonic oscillator problem [11].) We shall see that the higher dimensional symmetry persists in the quantum mechanical treatment of the hydrogen atom problem.

## 7.2 Spherical harmonics

Spherical harmonics play a role when there is rotational symmetry. Here we review the theory, relying on the results of the chapter on the isotropic harmonic oscillator for most of the proofs.

The *solid spherical harmonics* of degree $n$ are the polynomials $y$ in $\nu$ variables that are solutions of the Laplace equation $\nabla_{\mathbf{x}}^2 y = 0$ and of the Euler equation $\mathbf{x} \cdot \nabla_{\mathbf{x}} y = ny$.

The *surface spherical harmonics* of degree $n$ are the restrictions $Y$ of the solid spherical harmonics of degree $n$ to the sphere $\mathbf{x}^2 = 1$. We think of the surface spherical harmonics as functions of the angular variables. One can always recover the corresponding solid spherical harmonics by $y = r^n Y$, where $r = |\mathbf{x}|$ is the radius.

The dimension of the space of spherical harmonics of degree $n$ in $\nu$ dimensions is denoted $a_n^\nu$. This quantity satisfies the sum rule $a_n^\nu = \sum_{m=0}^n a_m^{\nu-1}$.

We now march through the first few cases, beginning with $\nu = 1$. The only solid spherical harmonics in one variable are multiples of 1 and $x$, in degrees 0 and 1 respectively. Thus $d_0^1 = d_1^1 = 1$ and $d_n^1 = 0$ for $n \geq 2$. The surface spherical harmonics are 1 and $\pm 1$. They correspond to the notions of even and odd *parity*.

For $\nu = 2$ the solid spherical harmonics of degree $m$ are linear combinations of $(x + iy)^m$ and $(x - iy)^m$. Thus $d_0^2 = 1$ while $d_m^2 = 2$ for all $m \geq 1$. The surface spherical harmonics of degree $m$ are linear combinations of $\exp(im\phi)$ and $\exp(-im\phi)$. An alternate description is as linear combinations of the even parity $\cos(m\phi)$ and the odd parity $\sin(m\phi)$. In quantum mechanics $\pm m$ is called the *magnetic quantum number*.

For $\nu = 3$ the story is more complicated. The dimension of the space of spherical harmonics of degree $\ell$ is $d_\ell^3 = 2\ell + 1$. For $\ell = 0$ the solid spherical harmonics are multiples of 1. For $\ell = 1$ they are linear combinations of $z, (x + iy), (x - iy)$, or alternatively of $x, y, z$. For $\ell = 2$ they are spanned by $3z^2 - r^2, z(x + iy), z(x - iy), (x + iy)^2, (x - iy)^2$. Another basis would be $2z^2 - x^2 - y^2, zx, zy, x^2 - y^2, 2xy$. For $\ell = 3$ the basis vectors may be taken to be $5z^3 - 3zr^2, (5z^2 - r^2)(x + iy), (5z^2 - r^2)(x - iy), z(x + iy)^2 z(x - iy)^2, \text{and}(x + iy)^3$. . Notice how they are built up out of polynomials in $z$ and $r^2$ times spherical harmonics in $x$ and $y$. (This is the reason for the sum rule.) One can go on this way systematically building basis vectors.

The corresponding surface spherical harmonics are obtained by restricting to $r^2 = x^2 + y^2 + z^2 = 1$ and making the substitutions $z = \cos\theta$ and $x + iy = \sin\theta \exp(i\phi)$. There are beautiful pictures of these in chemistry books. In quantum mechanics $\ell$ is called the *azimuthal quantum number*.

For $\nu = 4$ the dimension of the space of spherical harmonics of degree $k$ is given by the sum rule. Since $\sum_{\ell=0}^{k}(2\ell+1) = (k+1)^2$ this gives the result $d_k^4 = (k+1)^2$. We shall see that for the Hydrogen problem $k+1$ is the *principal quantum number*.

The fundamental result about spherical harmonics is the following.

**Theorem 18** *Consider the space $L^2(S_{\nu-1})$ of functions on the $\nu-1$ unit sphere in $\nu$ dimensions. Let $\mathcal{A}_\ell$ be the finite dimensional subspace of surface spherical harmonics of degree $\ell$. Then each subspace $\mathcal{A}_\ell$ is rotation invariant, and there is a direct sum decomposition $L^2(S_{\nu-1}) = \oplus_\ell \mathcal{A}_\ell$ representing every $L^2$ function on the sphere as a sum of spherical harmonics.*

We may write the Laplace operator in polar form as

$$\nabla_{\mathbf{x}}^2 = \frac{1}{r^{\nu-1}}\frac{\partial}{\partial r} r^{\nu-1}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_S, \tag{7.14}$$

where $\Delta_S$ is the Laplacian on the sphere. We have the following fundamental result.

**Proposition 24** *Let $Y$ be a surface spherical harmonic of degree $\ell$. Then $Y$ is an eigenfunction for the angular Laplacian with*

$$\Delta_S Y = -\ell(\ell+\nu-2)Y. \tag{7.15}$$

Proof: Let $y = r^\ell Y$ be the corresponding solid spherical harmonic. Then $\nabla_{\mathbf{x}}^2 y = 0$ gives $\ell(\ell+\nu-2)Y + \Delta_S Y = 0$. Q.E.D.

This result is applicable to the problem of finding eigenfunctions for Schrödinger operators of

$$H = \nabla_{\mathbf{x}}^2 + v(r) \tag{7.16}$$

with rotational symmetry. Write the eigenfunction $\phi$ as $f(r)Y$, where $Y$ is a spherical harmonic of degree $\ell$. Then the equation $H\phi = E\phi$ gives the radial equation

$$\frac{1}{r^{\nu-1}}\frac{\partial}{\partial r} r^{\nu-1}\frac{\partial}{\partial r} f(r) + \frac{\ell(\ell+\nu-2)}{r^2} f(r) + v(r)f(r) = Ef(r). \tag{7.17}$$

Thus every eigenfunction $f(r)$ of this radial equation gives rise to a $d_\ell^\nu$ dimensional space of eigenfunctions $\phi = f(r)Y$ of the original problem. This multiplicity of eigenvalues is called the *degeneracy* associated with rotational symmetry. Thus when $\nu = 3$ the rotational degeneracy is $2\ell+1$.

## 7.3 The quantum hydrogen atom

The Hamiltonian for the Hydrogen atom is

$$H = \frac{1}{2m}\mathbf{P}^2 - \frac{Ke^2}{r}. \tag{7.18}$$

Here $r = |\mathbf{x}|$ is the distance from the fixed proton with charge $e$. The electron has mass $m$ and charge $-e$. The potential energy is thus $-Ke^2/r$, where $K$ is the proportionality constant in the electrostatic force law. (The value of $K$ depends on the system of units.)

We let the dimension $\nu > 1$ of space be variable, but we are of course most interested in the case $\nu = 3$. This problem is spherically symmetric, so it is not surprising that the spherical harmonics in dimension $\nu$ would play a role. The surprise is that the analysis involves spherical harmonics in dimension $\nu + 1$.

Fix $E < 0$. We wish to solve the eigenvalue equation $H\psi = E\psi$. The first task is to transform this to momentum variables.

**Lemma 2** *The Fourier transform of* $1/|\mathbf{x}|$ *is* $\gamma/|\mathbf{k}|^{\nu-1}$*, where the constant gamma is given by* $\gamma = 1/\pi \cdot (2\pi)^\nu/\omega_{\nu-2} = 2/(\nu-1) \cdot (2\pi)^\nu/\omega_\nu$.

In this expression $\omega_\nu$ is the volume of the unit sphere $S_\nu$ contained in $\nu + 1$ dimensional space. Thus for instance $\omega_0 = 2$, $\omega_1 = 2\pi$, $\omega_2 = 4\pi$, $\omega_3 = 2\pi^2$, and $\omega_4 = 8\pi^2/3$. There is a general recursion relation $\omega_\nu = 2\pi/(\nu-1) \cdot \omega_{\nu-2}$. (Do not confuse the volume of the sphere with the volume $\Omega_\nu = \omega_{\nu-1}/\nu$ of the $\nu$ dimensional ball.)

Proof: Since $1/|\mathbf{x}|$ is a function of radius, by rotational symmetry its Fourier transform is also a function of radius. Since $1/|\mathbf{x}|$ transforms under a scale change of $1/a$ by a factor of $a$, its Fourier transform transforms under a scale change of $a$ by a factor of $a/a^\nu$. Thus the Fourier transform is identified as a multiple of $1/|\mathbf{k}|^{\nu-1}$.

It remains to find the multiple $\gamma$. Take the inner product of $1/|\mathbf{x}|$ with $(2\pi)^{-\nu/2}\exp(-\mathbf{x}^2/2)$. By the Plancherel theorem this is the same as the inner product of $\gamma/|\mathbf{k}|^{\nu-1}$ with the Fourier transform $\exp(-\mathbf{k}^2/2)$. One can evaluate these integrals in polar coordinates and thus obtain the stated value of $\gamma$. Q.E.D.

It follows from this lemma and the change of variable $\mathbf{p} = \hbar\mathbf{k}$ that in the Fourier transform representation the Hydrogen atom eigenvalue equation is

$$\frac{\mathbf{p}^2}{2m}f(\mathbf{p}) - Ke^2\gamma \int \frac{\hbar^{\nu-1}}{|\mathbf{p}-\mathbf{p}'|^{\nu-1}} f(\mathbf{p}') \frac{d^\nu \mathbf{p}'}{(2\pi\hbar)^\nu} = Ef(\mathbf{p}). \tag{7.19}$$

Let $\mathbf{z} = \mathbf{p}/\sqrt{-2mE}$. The equation may be written

$$(\mathbf{z}^2 + 1)g(\mathbf{z}) = \frac{4\eta}{\omega_\nu(\nu-1)} \int \frac{1}{|\mathbf{z} - \mathbf{z}'|^{\nu-1}} g(\mathbf{z}')\, d^\nu \mathbf{z}', \tag{7.20}$$

where $\eta = \hbar/a_0(-2mE)^{-1/2}$ and $a_0 = \hbar^2/(mKe^2)$ is the Bohr radius.

Now introduce the extra dimension and make the variable changes. First is the shift $\mathbf{z} = \bar{\mathbf{z}} + \mathbf{e}$, where $\mathbf{e}$ in the unit vector in this new dimension. This gives

$$\bar{\mathbf{z}}^2 h(\bar{\mathbf{z}}) = \frac{4\eta}{\omega_\nu(\nu-1)} \int \frac{1}{|\bar{\mathbf{z}} - \bar{\mathbf{z}}'|^{\nu-1}} g(\bar{\mathbf{z}}')\, d^\nu \bar{\mathbf{z}}'. \tag{7.21}$$

This says that the left hand side is a harmonic function in $\nu+1$ dimensions.

Next comes the inversion $\bar{\mathbf{z}} = 2\bar{\mathbf{w}}/|\bar{\mathbf{w}}|^2$. It is not difficult to compute that that distances are distorted according to the formula $|\mathbf{z} - \mathbf{z}'| = 2|\mathbf{w} - \mathbf{w}'|/(|\bar{\mathbf{w}}||\bar{\mathbf{w}}'|)$. Thus the $\nu$ dimensional volume element is distorted by a factor of $2^\nu/|\bar{\mathbf{w}}|^{2\nu}$.

Let $\psi(\bar{\mathbf{w}}) = h(\bar{\mathbf{z}})/|\bar{\mathbf{w}}|^{\nu+1}$. This Kelvin transform of the left hand side is also a harmonic function! The equation becomes

$$\psi(\bar{\mathbf{w}}) = \frac{2\eta}{\omega_\nu(\nu-1)} \int \frac{1}{|\bar{\mathbf{w}} - \bar{\mathbf{w}}'|^{\nu-1}} \psi(\bar{\mathbf{w}}')\, d\bar{\mathbf{w}}'. \tag{7.22}$$

Finally, let $\bar{\mathbf{w}} = \mathbf{w} - \mathbf{e}$. We get the final integral equation

$$\phi(\mathbf{w}) = \frac{2\eta}{\omega_\nu(\nu-1)} \int_{S_\nu} \frac{1}{|\mathbf{w} - \mathbf{w}'|^{\nu-1}} \phi(\mathbf{w}')\, d\mathbf{w}'. \tag{7.23}$$

This is an equation for a function on the unit sphere in $\mathbf{R}^{\nu+1}$.

The preceding equation defines an entension of the function $\phi(\mathbf{w})$ to the unit ball in $\mathbf{R}^{\nu+1}$. This extended function is harmonic in the interior of the ball.

Now let $p(\mathbf{w}, \mathbf{w}') = (1 - \mathbf{w}^2)/|\mathbf{w} - \mathbf{w}'|^{\nu+1}$ be the Poisson kernel for the unit ball in $\mathbf{R}^{\nu+1}$.

**Lemma 3** *The Greens's function and the Poisson kernel are related by*

$$\left(\mathbf{w} \cdot \nabla_{\mathbf{w}} + \frac{\nu-1}{2}\right) \frac{1}{|\mathbf{w} - \mathbf{w}'|^{\nu-1}} = \frac{\nu-1}{2} p(\mathbf{w}, \mathbf{w}'). \tag{7.24}$$

This converts our equation to the form

$$\left(\mathbf{w} \cdot \nabla_{\mathbf{w}} + \frac{\nu-1}{2}\right) \phi(\mathbf{w}) = \frac{\eta}{\omega_\nu} \int_{S_\nu} p(\mathbf{w}, \mathbf{w}') \phi(\mathbf{w}')\, d\mathbf{w}' \tag{7.25}$$

valid for $|\mathbf{w}| < 1$. The next lemma shows how to pass to the limit $|\mathbf{w}| = 1$.

**Lemma 4** *Consider a function $\phi$ defined on the unit sphere. Define a function in the interior of the unit ball by*

$$\phi(\mathbf{w}) = \int_{S_\nu} p(\mathbf{w}, \mathbf{w}')\phi(\mathbf{w}')\, d\mathbf{w}'/\omega_\nu. \tag{7.26}$$

*Then $\phi$ is the harmonic function in the interior of the unit ball $|\mathbf{w}| < 1$ that has boundary value $\phi$ on the unit sphere $|\mathbf{w}| = 1$.*

Proof: It is clear that $p(\mathbf{w}, \mathbf{w}') \geq 0$ and approaches zero rapidly when $\mathbf{w}$ approaches a point on the sphere other than $\mathbf{w}'$. Thus to show that it acts like an approximate delta function, we must show that the integral

$$\int_{S_\nu} p(\mathbf{w}, \mathbf{w}')\, d\mathbf{w}'/\omega_\nu = 1 \tag{7.27}$$

for $|\mathbf{w}| < 1$.

The integral may be calculated by the following trick. Take $\mathbf{w}$ and $\mathbf{w}'$ on the unit sphere. Let $r < 1$. By the mean value property for harmonic functions [SW]

$$\int_{S_\nu} p(r\mathbf{w}', \mathbf{w})\, d\mathbf{w}'/\omega_\nu = p(0, \mathbf{w}') = 1. \tag{7.28}$$

Then note that $p(r\mathbf{w}', \mathbf{w}) = p(r\mathbf{w}, \mathbf{w}')$. Q.E.D.

Now let $\phi$ be the solution of the eigenvalue equation. We see that

$$\left(\mathbf{w} \cdot \nabla_{\mathbf{w}} + \frac{\nu - 1}{2}\right) \phi(\mathbf{w}) = \eta\phi(\mathbf{w}). \tag{7.29}$$

This $\phi$ is not only harmonic but homogeneous of degree $k = \eta - (\nu - 1)/2$. It follows that $\phi$ is a spherical harmonic. Since $k = 0, 1, 2, 3, \ldots$ are the only possible values, we obtain that $\eta = k + (\nu - 1)/2$ is an eigenvalue of the operator on the left hand side with multiplicity $a_k^{\nu+1}$, the dimension of the space of spherical harmonics.

Notice that when $\nu = 3$ this says that $\eta = k + 1$ is an eigenvalue of the operator on the left hand side with multiplicity $(k + 1)^2$. The number $n = k + 1$ is the principle quantum number.

Now recall that $\eta = \hbar/a_0(-2mE)^{-1/2}$. Thus $\eta = n$ gives

$$E = -\frac{\hbar^2}{2ma_0^2}\frac{1}{n^2} = -\frac{mK^2e^4}{2\hbar^2}\frac{1}{n^2}. \tag{7.30}$$

This is the famous formula for the Hydrogen energy levels.

The treatment of the quantum mechanical Hydrogen atom with higher dimensional symmetry goes back to V. Fock in 1935. Much more is known about the symmetry of the hydrogen atom; the positive part of the spectrum may also be treated this way [1]. (There is also an interesting direct connection with the quantum harmonic oscillator [3].)

**Problems**

1. Let $E$ be the Euler operator and $\Delta$ be the Laplace operator. Show that $\Delta E - E\Delta = 2\Delta$.

2. Show that if $g$ is harmonic, then $Eg$ is harmonic.

## 7.4 The Hydrogen degeneracy

Now we fix the physical dimension $\nu = 3$. For a spherical symmetric problem in three dimensions one expects a multiplicity or degeneracy of eigenvalues of $a_\ell^3 = 2\ell + 1$. This $\ell$ is the azimuthal quantum number. Recall that $a_\ell^3 = \sum_{m=0}^{\ell} a_m^2$ where $m$ is the magnetic quantum number.

Due to spherical symmetry in four dimensions get $a_k^4 = (k+1)^2 = n^2$ degeneracy, where $n = k + 1$ is the principal quantum number. Recall that $a_k^4 = \sum_{\ell=0}^{k} a_\ell^3 = \sum_{\ell=0}^{k}(2\ell + 1)$ where $\ell$ is the azimuthal quantum number.

We have seen that the eigenvalue is $-R\frac{1}{(k+1)^2} = -R\frac{1}{n^2}$ where $R = mK^2e^4/(2\hbar^2)$.

The actual situation is complicated by the fact that the electron has *spin*. For our present purposes this simply means that the Hilbert space comes in two identical copies, so that all eigenvalues have a multiplicity two due to spin. Thus in the presence of spin a general spherically symmetric problem will have eigenvalues with degeneracies $2(2\ell+1)$, while the Hydrogen atom problem with its extra symmetry will have degeneracies $2n^2$.

Here is a table of $(n, \ell)$ states for the Hydrogen atom. Each entry in a column with angular momentum $\ell$ corresponds to $2(2\ell + 1)$ states. Thus the numbers corresponding to an entry in the first four columns are 2, 6, 10, 14. Each row corresponds to a state of degeneracy $2n^2$. Thus the sum for the first four rows are 2, 8, 18, and 32. This is displayed in Table 1.

## 7.5 The periodic table

The Hydrogen atom problem is the beginning of an understanding of the entire periodic table of the elements. The elements are numbered by a

| | | | | | |
|---|---|---|---|---|---|
| (1,0) | | | | | |
| (2,0) | (2,1) | | | | |
| (3,0) | (3,1) | (3,2) | | | |
| (4,0) | (4,1) | (4,2) | (4,3) | | |
| (5,0) | (5,1) | (5,2) | (5,3) | (5,4) | |
| (6,0) | (6,1) | (6,2) | (6,3) | (6,4) | (6,5) |

Table 7.1: $(n,\ell)$ table of Hydrogen states.
Each entry represents $2(2\ell+1)$ states.
Each row has $2n^2$ states of energy $-R/n^2$.

variable $Z$ called *atomic number*. An neutral atom of element $Z$ consists of a nucleus with charge $Ze$ (which we take to be fixed) and $Z$ electrons, each of charge $-e$. So we need to understand the behavior of a system of $Z$ particles (the electrons). The correct procedure is to take a wave function that depends on the coordinates (position and spin) of all the electrons.

The most important new effect in such a multi-electron system is *Fermi statistics*. This says that the wave functions must be anti-symmetric with respect to exchange of the coordinates of a pair of particles.

One consequence of the Fermi statistics is the *Pauli exclusion principle*. This says that a basis for the multi-electron system may be obtained from one-electron wave functions for the individual electrons; however no one-electron basis function can appear twice. (The reason is that the multi-electron wave functions are anti-symmetrized products, so that a repeated factor must be equal to its negative.)

In particular, for a system of $Z$ electrons with no mutual interaction the lowest energy eigenfunction is obtained from the first $Z$ one-electron energy eigenfunctions by anti-symmetrization.

There are two kinds of electrostatic forces, an attractive force between each electron and the nucleus and a repulsive force between each pair of electrons. If we neglect the repulsive force, then we have $Z$ one-electron problems, each of which is essentially the same problem as the Hydrogen atom. Thus by the Pauli exclusion principle the multi-electron ground state should correspond to the first $Z$ Hydrogen states. Recall that these states come in groups of $2 \cdot n^2$ states with the same energy. The states fill up in order of increasing $n$.

In fact there is electron-electron repulsion, and this makes the problem very difficult. However one can make some heuristic guesses about the electronic configurations based on the following remarks.

The first remark is one can approximate the problem by a problem in which one outer electron experiences the force due to the nucleus and an

average force due the the other electrons. The nucleus has charge $Ze$ and the other $Z-1$ electrons have total charge $-(Z-1)e$, so the outer electron should find itself in orbit about a spread-out positive charge of $e$. So in this approximation the situation is very much like the Hydrogen problem. The state of lowest $n$ compatible with the exclusion principle should determine the ground state of the atom.

There is however, an important difference. For the Hydrogen problem the energy level depends only on the principal quantum number $n$. For the present problem it also depends on the angular momentum quantum number $\ell$. The reason is that when $\ell$ is small, the wave function has a significant part that is concentrated near the nucleus, inside the orbits of the other electrons. Thus the effect of the nuclear charge $Ze$ is not completely compensated by the the charge $-(Z-1)e$ of the other electrons. The outermost electron with small $\ell$ experiences a stronger attractive force and has a lower energy. Thus the lowest energy state of the atom should come when the $n$ and $\ell$ for the outer electron are both small.

What combination of $n$ and $\ell$ should be minimized? The empirical facts are fairly well summarized in the $n+\ell$ rule. (Recall that $0 \leq \ell \leq n-1$.) This rule says that to find the next one-electron state that is filled in building up the ground state of the multi-electron atom, first minimize $n+\ell$. Then minimize $n$.

This rule allows a prediction of the properties of the outer electrons in the periodic table. In the first version the table is listed by increasing $Z$. Each entry is characterized by listing the values of $n$ and of $\ell$. The $Z$ that have a given value of $n$ and $\ell$ are grouped in one entry. The number of elements that correspond to an entry in one of the columns is given by $2(2\ell+1)$, that is, by 14, 10, 6, 2 for angular momentum 3,2,1,0. These are listed in Table 2. Notice that in this arrangement each row has decreasing

| | | | |
|---|---|---|---|
| | | | (1,0) |
| | | | (2,0) |
| | | (2,1) | (3,0) |
| | | (3,1) | (4,0) |
| | (3,2) | (4,1) | (5,0) |
| | (4,2) | (5,1) | (6,0) |
| (4,3) | (5,2) | (6,1) | (7,0) |

Table 7.2: $(n,\ell)$ table of elements from $n+\ell$ rule.
Each entry represents $2(2\ell+1)$ elements.

$\ell$ values.

In the conventional periodic table the final $\ell = 0$ values are grouped

with the following decreasing sequence of values of $\ell \geq 1$. Thus the number of elements that goes with an entry in one of the columns is 2, 14,10, 6. The totals that go with the first six rows are thus 2, 8, 8, 18, 18, 32. This is shown in Table 3.

| | | | |
|---|---|---|---|
| (1,0) | | | |
| (2,0) | | | (2,1) |
| (3,0) | | | (3,1) |
| (4,0) | | (3,2) | (4,1) |
| (5,0) | | (4,2) | (5,1) |
| (6,0) | (4,3) | (5,2) | (6,1) |
| (7,0) | (5,3) | | |

Table 7.3: $(n, \ell)$ values in periodic table of elements.
Each entry represents $2(2\ell + 1)$ elements.
Arrangement is $\ell = 0, 3, 2, 1$.

If we put in the atomic numbers in this order we get something very close to the periodic table from chemistry. The first two columns are the 2 $\ell = 0$ states. The next column replaces the 14 columns corresponding to $\ell = 3$. The next 10 columns are the $\ell = 2$ states. The final 6 columns are the $\ell = 1$ states. One should compare this ideal table with the actual periodic table; they are almost the the same. With careful inspection one can see the patterns of three and even four dimensional spherical harmonics in the properties of the chemical elements. The full glory is seen in Table 4.

| | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | | | | | | | | | | | | | | | | | |
| 3 | 4 | | | | | | | | | | | | 5 | 6 | 7 | 8 | 9 | 10 |
| 11 | 12 | | | | | | | | | | | | 13 | 14 | 15 | 16 | 17 | 18 |
| 19 | 20 | | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
| 37 | 38 | | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 |
| 55 | 56 | 57–70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 |
| 87 | 88 | 89–102 | | | | | | | | | | | | | | | | |

Table 7.4: $Z$ values in ideal periodic table of elements.
Arrangement is $\ell = 0, 3, 2, 1$.

There is another terminology for the angular momentum values $\ell = 0, 1, 2, 3$ that came from spectrographic history and is now standard in chemistry. The numbers are replaced by the letters s, p, d, f. (The first three letters are not in any particular sequence, but come from empirical

classifications of of spectral lines as sharp, principal, and diffuse.) Thus an $s$ state is spherically symmetric, a $p$ state transforms under rotation like an ordinary vector, and $d$ and $f$ states are more complex spherical harmonics.

The actual names of the elements are of course also determined by history. Cultured individuals are not expected to know the entire table by heart, but they should perhaps memorize the first 18 entries: Hydrogen, Helium; Lithium, Beryllium; Boron, Carbon, Nitrogen, Oxygen, Fluorine, Neon; Sodium, Magnesium; Aluminum, Silicon, Phosphorus, Sulfur, Chlorine, Argon. The first 54 entries are listed in Table 5.

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| H | He | | | | | | | | | | | | | | | | |
| Li | Be | | | | | | | | | | | B | C | N | O | F | Ne |
| Na | Mg | | | | | | | | | | | Al | Si | P | S | Cl | Ar |
| K | Ca | SC | Ti | V | Cr | Mn | Fe | Co | Ni | Cu | Zn | Ga | Ge | As | Se | Br | Kr |
| Rb | Sr | Y | Zr | Nb | Mo | Tc | Ru | Rh | Pd | Ag | Cd | In | Sn | Sb | Te | I | Xe |

Table 7.5: First 54 elements in the periodic table of elements.
Arrangement is $\ell = 0, 2, 1$.

In summary, the rich patterns of chemistry are determined by numbers arising in the mathematics of spherical harmonics.

1. The dimension of the space of one-dimensional spherical harmonics of degree $p$ is 1 when $p = 0$ and 1 when $p = 1$ and 0 for $p \geq 2$.

2. The dimension of the space of two-dimensional spherical harmonics of degree $m$ is 1 when $m = 0$ and $1 + 1 = 2$ for $m \geq 1$.

3. The dimension of the space of three-dimensional spherical harmonics of degree $\ell$ is $1 + \sum_{m=1}^{\ell} 2 = 2\ell + 1$.

4. The dimension of the space of four-dimensional spherical harmonics of degree $k$ is $\sum_{\ell=0}^{k}(2\ell + 1) = (k + 1)^2$.

All of these numbers are doubled due to spin. In the Hydrogen problem the symmetry is four dimensional, so the multiplicity of eigenvalues is $2(k+1)^2$. The four dimensional symmetry comes from a steoregraphic projection that relates the three-dimensional momentum space to a three dimensional sphere in four dimension space. By a miracle the problem turns out to be rotation invariant in four dimensions.

In more complicated atoms the symmetry is only three dimensional, so the multiplicities that are most apparent are $2(2\ell + 1)$. However enough of the four dimensional symmetry remains that the pattern can still be detected in the periodic table.æ

# Part II

# Self-adjoint Operators

# Chapter 8

# The spectral theorem

This chapter is devoted to the spectral theorem. We first prove the theorem for unitary operators and then deduce the theorem for self-adjoint operators as a consequence. The first result is that a unitary operator is isomorphic to a multiplication operator acting in $L^2$, where the multiplication is by a function of absolute value one. The second result says that a self-adjoint operator is isomorphic to multiplication by a real function. The passage from the first to the second result is obtained by observing that a self-adjoint operator may always be expressed as a function of a unitary operator.

There are many proofs of the spectral theorem. All of them require some sort of approximation argument. However there are many variants to the argument and many stages at which the argument can be applied. One can work directly with the self-adjoint operator [K, 9], one can work with the resolvent [N2], one can work with the unitary Cayley transform [vN] (as we do), or one can work with the unitary group. There is a very interesting approach using the resolvent and contour integration [L].

## 8.1 Difference approximations

Our main interest is the spectral theorem for self-adjoint operators. However we begin with some remarks meant to motivate the approach in terms of unitary operators.

The first thing to notice is that when a self-adjoint operator $A$ has a spectral representation, then the Schrödinger equation has a nice solution in terms of unitary operators. However even if there is a spectral representation, one may not know very explicitly what it is. Therefore it would be desirable to get at a solution without using the spectral representation.

One such strategy for solving the Schrödinger equation is by the use of *difference methods*. We shall assume that there is a spectral representation and explore the convergence of the difference methods.

Let $\psi(t) = U_t\psi$ be the solution of the abstract Schrödinger equation

$$i\frac{d\psi(t)}{dt} = A\psi(t). \tag{8.1}$$

Assume that we want to solve the equation by a finite difference method. One can approximate the equation by the *forward difference* approximation

$$i(\psi(t+h) - \psi(t)) = hA\psi(t). \tag{8.2}$$

This has solution

$$\psi(t+h) = (1 - ihA)\psi(t). \tag{8.3}$$

The obvious attempt to find a solution of the differential equation is

$$U_t\psi = \lim_{n\to\infty} \left((1 - i(t/n)A)\right)^n \psi. \tag{8.4}$$

However the conditions for convergence are going to be very delicate when $A$ is unbounded. Even though $U_t$ is unitary, the approximating operators are not even continuous. This method is thus delicate theoretically and useless in practice.

One can do much better with the *backward difference* approximation

$$i(\psi(t+h) - \psi(t)) = hA\psi(t+h). \tag{8.5}$$

This has solution

$$\psi(t+h) = (1 + ihA)^{-1}\psi(t). \tag{8.6}$$

which is expressed in terms of a bounded operator It is not difficult to verify that the solution of the differential equation is

$$U_t\psi = \lim_{n\to\infty} \left((1 + i(t/n)A)^{-1}\right)^n \psi. \tag{8.7}$$

However it is irritating that one is trying to approximate a unitary operator by operators that are not unitary.

Perhaps best of all is the *forward-backward difference* approximation

$$i(\psi(t+h) - \psi(t)) = hA(\psi(t+h) + \psi(t))/2. \tag{8.8}$$

This has solution

$$\psi(t+h) = (1 - (i/2)hA)(1 + (i/2)hA)^{-1}\psi(t). \tag{8.9}$$

which is continuous. We have

$$U_t\psi = \lim_{n\to\infty} \left((1 - (i/2)(t/n)A)(1 + (i/2)(t/n)A)^{-1}\right)^n \psi. \tag{8.10}$$

This time the approximating operators are unitary.

We thus see that there are several operators that are related to the abstract Schrödinger equation. There is the operator $A$ that defines the equation. There is the unitary group $U_t = \exp(-itA)$ that gives the solution. The unitary group may be approximated by the backward difference method. This uses bounded operators of the form $(1 - ihA)^{-1}$, where $h$ is real. Such an operator are called a *resolvent* operator of $A$. Finally the unitary group may be approximated by the forward-backward difference method. This uses unitary operators of the form $U = (1 - i(h/2)A)(1 + i(h/2)A)^{-1}$, where $h$ is real. Such an operator is called a *Cayley transform* of $A$.

The strategy for proving the spectral theorem is now clear. Start with a self-adjoint operator $A$. Consider its Cayley transform $U$. The integer powers $U^n$ define an unitary dynamics that approximate the dynamics of the Schrödinger equation. Work with this dynamics to prove a spectral theorem for the unitary operator. Then recover the spectral theorem for the self-adjoint operator by the inverse of the Cayley transform.

One could also attempt to use the true Schrödinger dynamics to prove the spectral theorem. The trouble with this is that one then has to solve the Schrödinger equation without use of a spectral representation. This can be done by showing directly that the approximate dynamics converge to the true dynamics, but this approach is slightly more technical.

## 8.2 Spectral theorem for unitary operators

We now investigate the structure of unitary operators from a Hilbert space to itself. This is the sort of operator we expect to encounter in quantum mechanical time evolution. The fundamental result is the spectral theorem.

The strategy may be understood by looking at the case when there is a basis of eigenvectors, so that the unitary operator $U$ satisfies $U\phi_j = e^{i\theta_j}\phi_j$. Let $\psi = \sum_j c_j\phi_j$ be an arbitrary vector. Then

$$\langle\psi, U^n\psi\rangle = \sum_j \exp(in\theta_j)|c_j|^2 = \int_0^{2\pi} e^{in\theta}\, d\mu(\theta), \tag{8.11}$$

where $d\mu(\theta) = \sum_j |c_j|^2\delta(\theta - \theta_j)\, d\theta$. In this case the measure associated with the operator $U$ and the vector $\psi$ is concentrated on those eigenvalues such that $\psi$ has a non-zero component in the eigenvector direction.

Not every unitary operator has a basis of eigenvectors in the Hilbert space. Correspondingly, not every spectral measure $\mu$ is discrete. However the above example suggests that one attempt to get at the measure $\mu$ by expressing its integral with trigonometric functions $e^{in\theta}$ directly in terms of Hilbert space quantities. The following proposition shows that this can be accomplished in general. The proof of the proposition will follow from the two lemmas immediately below.

**Proposition 25** *Let $U$ be a unitary operator from $\mathcal{H}$ to itself. Let $\psi$ be a (unit) vector in $\mathcal{H}$. Then there exists a (probability) measure $\mu$ on the unit circle such that*

$$\langle \psi, U^n \psi \rangle = \int_0^{2\pi} e^{in\theta} \, d\mu(\theta). \tag{8.12}$$

In order to prove this result we must first characterize the functions of the form $u_n = \langle \psi, U^n \psi \rangle$. Let $u$ be a function from the integers to the complex numbers. Then $u$ is said to be of *positive type* if for every sequence $a$ of complex numbers with finite support

$$\sum_m \sum_n a_m^* u_{n-m} a_n \geq 0. \tag{8.13}$$

Notice that if $u$ is of positive type, then in particular for each $n$ the 2 by 2 matrix

$$\begin{pmatrix} u_0 & u_n \\ u_{-n} & u_0 \end{pmatrix} \tag{8.14}$$

is positive. As a consequence $u_0 \geq 0$, $u_{-n} = u_n^*$, and $|u_n| \leq u_0$.

**Lemma 5** *Let $U$ be a unitary operator and $\psi$ be a vector in $\mathcal{H}$. Then $u_n = \langle \psi, U^n \psi \rangle$ is a positive type function of the integer variable $n$.*

Proof: Let $U$ be a unitary operator and $\psi$ be a vector in $\mathcal{H}$. Then $U^* = U^{-1}$ and so

$$\langle U^m \psi, U^n \psi \rangle = \langle \psi, U^{m^*} U^n \psi \rangle = \langle \psi, U^{n-m} \psi \rangle. \tag{8.15}$$

Then

$$0 \leq \| \sum_n a_n U^n \psi \|^2 = \langle \sum_m a_m U^m \psi, \sum_n a_n U^n \psi \rangle = \sum_m \sum_n a_m^* \langle \psi, U_{n-m} \psi \rangle a_n. \tag{8.16}$$

**Lemma 6** *Let $u$ be a function of positive type. Then there exists a unique measure $\mu$ on the unit circle such that*

$$u_n = \int_0^{2\pi} e^{in\theta} \, d\mu(\theta). \tag{8.17}$$

Proof: A *trigonometric polynomial* is a function of the form $p(e^{i\theta}) = \sum c_n e^{in\theta}$, a polynomial in positive and negative powers of $e^{i\theta}$. It is a function on the unit circle. We associate to each such polynomial the complex number $L(p) = \sum c_n u_n$. This is clearly linear.

If the polynomial is real, then $c_{-n} = c_n^*$. Since also $u_{-n} = u_n^*$, it follows that $L(p)$ is real.

A lemma of Fejér and Riesz (see below) says that if a trigonometric polynomial satisfies $p(e^{i\theta}) \geq 0$, then there exists another trigonometric polynomial $q(e^{i\theta})$ such that $p(e^{i\theta}) = |q(e^{i\theta})|^2$. Set $q(e^{i\theta}) = \sum_n a_n e^{in\theta}$. It then follows from the positive type condition that $L(p) = L(|q|^2) = \sum_m \sum_n a_m^* a_n u_{n-m} \geq 0$.

To each trigonometric polynomial $p(e^{i\theta})$ we have associated the number $L(p)$. This assigns positive numbers to positive polynomials. It follows that the operation preserves order. It also send constant polynomials to the corresponding constant times $u_0$. In particular, if $-c \leq p(e^{i\theta}) \leq c$, then $-cu_0 \leq L(p) \leq cu_0$. In other words this is a continuous linear functional on trigonometric polynomials, with the norm of uniform convergence. It is well known (for example from the Stone-Weierstrass approximation theorem) that trigonometric polynomials on the circle are dense in the continuous functions on the circle. It follows that this is a continuous linear functional on the continuous functions. It is a well-known theorem of Riesz that every such functional determines a measure (that is, an integral in the sense we have discussed). So we have $L(p) = \int_0^{2\pi} p(e^{i\theta})\, d\mu(\theta)$, where the integration is over the circle. Q.E.D.

Remark: The claim is that the integral satisfies all the properties of the integral, including the monotone convergence theorem. In particular, the original functional $L$ defined on the continuous functions must satisfy the monotone convergence theorem. It is natural to ask why this should always be so. This is explained by Dini's theorem, a result about continuous functions on a compact space. The theorem says that monotone pointwise convergence of continuous functions to a continuous function implies uniform convergence. Of course this in turn implies convergence of the functionals.

In the above proof we used the lemma of Fejér and Riesz.

**Lemma 7** *If the trigonometric polynomial $p(e^{i\theta})$ is positive, then there exists another trigonometric polynomial polynomial $q(e^{i\theta})$ such that $p(e^{i\theta}) = |q(e^{i\theta})|^2$.*

Proof: This is a result about trigonometric polynomials, which may be thought of as ordinary polynomials in $z$ and $z^{-1}$, where the complex number $z$ is restricted to the unit circle $|z| = 1$. We may as well assume

in the proof that $p(z) > 0$ for $|z| = 1$, since the hypothesis as stated is a limiting case.

We now look at these polynomials without the restriction that $|z| = 1$. The reality condition translates to the condition $p(z) = p(1/z^*)^*$. Now assume that $p(z)$ is of degree $k$ in $z$ and $1/z$. Then $r(z) = z^k p(z)$ is of degree $2k$ in $z$. Furthermore $r(z) = z^{2k} r(1/z^*)^*$. From this it is clear that for every root $a$ of $r(z)$, there is a corresponding root $1/a^*$. Since $p(z)$ has no roots on the unit circle, neither does $r(z)$. Hence the roots of $r(z)$ occur in pairs. This gives the representation

$$r(z) = b \prod_i (z - a_i)(z - 1/a_i^*). \tag{8.18}$$

This converts into a representation

$$p(z) = c \prod_i (z - a_i)(1/z - a_i^*). \tag{8.19}$$

In order to have $p(z) > 0$ for $|z| = 1$ we must have $c > 0$. Therefore we may take $q(z) = \sqrt{c} \prod_i (z - a_i)$. When we restrict to the unit circle, we may use $1/z = z^*$, and so $p(z) = q(z)q(z)^* = |q(z)|^2$. Q.E.D.

**Theorem 19** *Let $U$ be a unitary operator from $\mathcal{H}$ to itself. Then there exists a measure space and associated Hilbert space $L^2(X, \mu)$ of square-integrable functions, an isomorphism $W$ from $\mathcal{H}$ to $L^2$, and a measurable function $\upsilon$ with $|\upsilon| = 1$ such that $U = W^{-1} \upsilon W$. Every unitary operator is isomorphic to a multiplication operator (multiplication by a function with modulus one).*

Proof: For a unit vector $\psi$ in $\mathcal{H}$ let $\mathcal{H}_\psi$ be the closed linear subspace generated by $U^n \psi$ for integer $n$. Then $U$ restricted to $\mathcal{H}_\psi$ is a unitary operator. The first part of the proof is to prove a spectral representation for this restricted operator.

Since $U$ is unitary, for every trigonometric polynomial $q(e^{i\theta})$ with $p(e^{i\theta}) = q(e^{i\theta})^* q(e^{i\theta})$ we have $p(U) = q(U)^* q(U)$. Therefore for every trigonometric polynomial $q(e^{i\theta})$ we have

$$\|q(U)\psi\|^2 = \langle \psi, q(U)^* q(U) \psi \rangle = \int_0^{2\pi} q(e^{i\theta})^* q(e^{i\theta}) \, d\mu(\theta) = \int_0^{2\pi} |q(e^{i\theta})|^2 \, d\mu(\theta). \tag{8.20}$$

Therefore if $q(U)\psi = 0$, then $q(e^{i\theta}) = 0$ for all $\theta$ except for a set of $\mu$ measure zero. Therefore $q(e^{i\theta})$ is a nul function and may be identified with zero in the space $L^2(S, \mu)$ of square-integrable functions on the circle.

It follows that we may define an unitary operator $W_\psi$ from $\mathcal{H}_\psi$ to $\mathrm{L}^2(S, d\mu)$ by $W_\psi q(U)\psi = q(e^{i\theta})$. (Note that in particular $W_\psi \psi = 1$.) Furthermore it is easy to check that $W_\psi U q(U)\psi = e^{i\theta} W_\psi q(U)\psi$. It follows by continuity that $W_\psi U\chi = e^{i\theta} W_\psi \chi$ for all $\chi$ in $\mathcal{H}_\psi$. That is, we have a spectral representation for the part of $U$ in the subspace $\mathcal{H}_\psi$.

The second part of the proof is to piece together these spectral representations for subspaces into a spectral representation for the entire space. Consider families $\psi_j$ of vectors such that $\mathcal{H}_{\psi_j}$ are mutually orthogonal. Take a maximal such family.

Let $M$ be the closed linear subspace of consisting of all vectors $\phi = \sum_j \phi_j$ where $\phi_j$ is in $\mathcal{H}_{\psi_j}$.

**Lemma 8** *Let $U$ be a unitary operator from $\mathcal{H}$ to itself. Let $M$ be a closed linear subspace of $\mathcal{H}$ that is invariant under $U$ and $U^{-1}$. Then $M^\perp$ is invariant under $U$ and $U^{-1}$.*

By use of the lemma we see that $M = \mathcal{H}$. If this were not the case, then by the projection theorem there would be a unit vector $\psi$ orthogonal to $M$. Then we could construct another closed linear subspace $\mathcal{H}_\psi$. This would contradict the maximality.

Now take as many copies $S_j$ of the unit circle as there are vectors $\psi_j$. Let $X$ be the disjoint union of the $S_j$. Each point $x$ in $X$ is determined by a pair $(\theta, j)$. For each $j$ the measure $\mu_j$ is the measure determined by $U$ and $\psi_j$. Define the measure $\mu$ to be the measure that restricts to $\mu_j$ on the $j$th circle. Define the function $\upsilon$ by $\upsilon(x) = \upsilon(\theta, j) = e^{i\theta}$.

Now for every $\phi$ in $\mathcal{H}$ we define

$$W\phi(x) = W\phi(\theta, j) = W_{\psi_j}\phi_j(\theta). \tag{8.21}$$

It is easy to check that for each $x = (\theta, j)$ in $X$ we have

$$WU\phi(x) = W_{\psi_j} U\phi_j(\theta) = e^{i\theta} W_{\psi_j}\phi_j(\theta) = \upsilon(x) W\phi(x). \tag{8.22}$$

Thus we have found the required spectral representation. Q.E.D.

The construction in the proof of the theorem gives a measure, but does not tell much about whether the measure is point or continuous. It is important to note that in either case certain functions that are are very different may define the same member of $L^2$. In particular, when the measure consists only of masses at certain points, then the values of functions matter only at these points. In this case one is essentially dealing with a space $\ell^2$, even though the construction might not immediately suggest it.

Our construction gave the space $X$ as a disjoint union of circles, but the nature of the $L^2$ spaces obtained depend very much on the measures

on these circles. It is essential to realize that the actual nature of the space $X$ depends on the particular proof method and is largely irrelevant. On the other hand, the fact that the range of the multiplication operator is contained in the unit circle is essential for it to be unitary.

**Problems**

1. Let $U$ be a unitary operator such that $U$ has a basis of eigenvectors. Take the $\psi_j$ in the proof of the spectral theorem to be the corresponding eigenvectors. Describe the measure $\mu$ and function $v$ given by the proof of the spectral theorem.

2. Let $U$ be a unitary operator such that $U$ has a countable basis of eigenvectors $\phi_j$. Assume that each eigenvalue has multiplicity one. Take the $\psi$ in the proof of the spectral theorem to be $\psi = \sum_j c_j \phi_j$ where all the coefficients are non-zero. Describe the measure $\mu$ and function $v$ given by the proof of the spectral theorem.

3. Let the Hilbert space be $L^2(S, d\theta)$, where $S$ is the unit circle, and let $U_a$ be rotation by the angle $a$. In order to stay within the framework of the previous problem, take $a$ to be an irrational multiple of $2\pi$. Let $\psi$ be a function whose Fourier coefficients never vanish. Find the measure $\mu$ and function $v$ given by the proof of the spectral theorem.

4. Let the Hilbert space be $L^2(\mathbf{R}, dx)$ and let $U_a$ be translation by $a$. Let $\psi$ be a function whose Fourier transform never vanishes. Find the measure $\mu$ and function $v$ given by the proof of the spectral theorem.

## 8.3 Graphs

In this section we use the *Pauli matrices* to manipulate linear graphs. The first Pauli matrix is just an interchange.

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{8.23}$$

The second one involves a change of sign and an interchange. There is also a conventional factor of $i$, which serves to make its square equal to one. (This factor will play no role in our considerations, since we will be applying the matrix only to subspaces.)

$$\sigma_2 = i \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{8.24}$$

The third one involves only a change of sign.

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{8.25}$$

Consider the direct sum Hilbert space $\mathcal{H} \oplus \mathcal{H}$. This consists of all ordered pairs $(\psi, \phi)$ with the obvious vector space operations. The inner product is

$$\langle (\psi, \phi), (\psi', \phi') \rangle = \langle \psi, \psi' \rangle + \langle \phi, \phi' \rangle. \tag{8.26}$$

The Pauli matrices act on the direct sum Hilbert space in a natural way. They each define a unitary operator whose square is one.

**Definition 13** *A* graph *is a linear subspace of* $\mathcal{H} \oplus \mathcal{H}$.

If $A$ is a graph, then we may apply the Pauli matrices to the pairs in the graph to get a new graph. Thus we define the *inverse* $A^{-1}$ as $\sigma_1 A$. The *negative inverse* $-A^{-1}$ is $\sigma_2 A$. Finally the *negative* $-A$ is $\sigma_3 A$.

Notice that taking the closure of a graph commutes with each of these three operations, for instance $\bar{A}^{-1} = (A^{-1})^{-}$.

If $A$ is a graph, then its *domain* $D(A)$ consists of all $\psi$ in $\mathcal{H}$ such that there exists a $\phi$ in $\mathcal{H}$ with $(\psi, \phi)$ in $A$. Its *range* $R(A)$ consists of all $\phi$ in $\mathcal{H}$ such that there exists a $\psi$ in $\mathcal{H}$ with $(\psi, \phi)$ in $A$.

If $A$ is a graph, then its *nullspace* $N(A)$ consists of all $\psi$ in $\mathcal{H}$ such that $(\psi, 0)$ is in $A$. This is obviously a subset of the domain $D(A)$. The corresponding subset of $R(A) = D(A^{-1})$ is $N(A^{-1})$.

It is worth noting that if $A$ is closed as a subspace of $\mathcal{H} \oplus \mathcal{H}$, then $N(A)$ and $N(A^{-1})$ are also closed as subspaces of $\mathcal{H}$.

**Definition 14** *An* operator *is a graph such that the only pair of the form* $(0, \phi)$ *in the graph is* $(0, 0)$. *When a pair* $(\psi, \phi)$ *is in a graph* $A$ *that is an operator, then we write* $A\psi = \phi$.

Notice that $A$ is an operator if and only if $N(A^{-1})$ consists only of the zero vector.

**Problems**

1. Show that an operator has a closed graph if and only if its domain with the graph norm is a Hilbert space.

2. Must the closure of the graph of an operator be the graph of an operator?

## 8.4 Adjoints

**Definition 15** *The* adjoint *graph $A^*$ is defined to be $(\sigma_2 A)^\perp = \sigma_2 A^\perp$.*

Notice that it does not matter whether we take the orthogonal complement before or after applying the unitary operator.

It is easy to check that $(\sigma_1 A)^\perp$ is $-A^* = (-A)^*$. Also $(\sigma_3 A)^\perp$ is $A^{*-1} = A^{-1*}$.

**Theorem 20** *The closure of the graph and the adjoint are related by $\bar{A}^* = A^*$ and $\bar{A} = A^{**}$.*

Proof: Since $\bar{A}^\perp = A^\perp$, we have $\bar{A}^* = A^*$. Similarly, from the projection theorem we have $\bar{A} = A^{\perp\perp}$. This gives $\bar{A} = A^{**}$. Q.E.D.

One main reason for the introduction of the adjoint concept is that it gives information about ranges, that is about finding solutions of equations.

**Proposition 26** *We have the relations $N(A^*) = R(A)^\perp$ and $N(\bar{A}) = R(A)^{*\perp}$.*

There is a dual result for domains.

**Proposition 27** *We have the relations $N(A^{*-1}) = D(A)^\perp$ and $N(\bar{A}^{-1}) = D(A^*)^\perp$.*

Notice that $A$ is an operator if and only if $N(A^{-1})$ consists only of the zero vector. Therefore $A^*$ is an operator if and only if $D(A)$ is dense. Similarly $\bar{A}$ is an operator if and only if $D(A^*)$ is dense.

From this it is easy to see that the class of densely defined closed operators is a particularly nice class. If $A$ is densely defined and closed, then so is $A^*$, and $A^{**} = A$.

The most important classes of graphs are skew-adjoint, self-adjoint, and unitary. It is amusing that these correspond exactly to the Pauli matrices $\sigma_1$, $\sigma_2$, and $\sigma_3$.

**Definition 16** *We define a graph $A$ to be* skew-adjoint *if $(\sigma_1 A)^\perp = -A^* = A$.*

**Definition 17** *We define a graph $A$ to be* self-adjoint *if $(\sigma_2 A)^\perp = A^* = A$.*

**Definition 18** *We define a graph $U$ to be* unitary *if $(\sigma_3 A)^\perp = A^{-1*} = A$.*

**Proposition 28** *A unitary graph is an operator.*

Proof: Let $U$ be a unitary graph. Assume that $(0, \phi)$ is in $U$. Then $(0, \phi)$ is orthogonal to $\sigma_3(0, \phi) = (0, -\phi)$, so $\phi$ is orthogonal to $\phi$, and $\phi$ must be zero. Q.E.D.

It is not difficult to check that a unitary operator as defined here is the same notion as before: an isomorphism of the Hilbert space onto itself.

**Problems**

1. Show that a self-adjoint graph that is an operator is the same as a self-adjoint operator as previously defined.

## 8.5 Spectral theorem for self-adjoint operators

The Pauli matrices are two-by-two unitary matrices with eigenvalues $\pm 1$. Therefore they are all unitarily equivalent. Thus, for instance, we may find a unitary operator $\tau$ such that

$$\tau\sigma_2 = \sigma_3\tau. \tag{8.27}$$

Let $A$ be a self-adjoint graph, and define $U = \tau A$. It follows that

$$U = \tau A = \tau A^* = \tau\sigma_2 A^\perp = \sigma_3\tau A^\perp = \sigma_3 U^\perp = U^{*-1}. \tag{8.28}$$

Let us look more explicitly at the form of this relation. Take for instance

$$\tau = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ 1 & -i \end{pmatrix} \tag{8.29}$$

Then if $(\psi, \phi)$ is in the graph of $A$, the corresponding element of the graph of $U$ is a multiple of $(\psi + i\phi, \psi - i\phi)$. In other words, $U(\psi + i\phi) = (\psi - i\phi)$.

We may solve this equation by $(1 - U)\psi = i(1 + U)\phi$. We see that the self-adjoint graph $A$ is an operator if and only if $U$ has no eigenvectors with eigenvalue $-1$.

The spectral theorem for unitary operators now immediately gives the spectral theorem for self-adjoint operators.

**Theorem 21** *Let $A$ be a self-adjoint operator from $\mathcal{H}$ to itself. Then there exists a measure space $L^2(X, \mu)$ and an isomorphism $W$ from $\mathcal{H}$ to $L^2$ and a real measurable function $\alpha$ such that $A = W^{-1}\alpha W$. Every self-adjoint operator is isomorphic to a multiplication operator (multiplication by a real function).*

Proof: Define the unitary operator $U$ by

$$U(\psi + iA\psi) = \psi - iA\psi \tag{8.30}$$

as above. Since $A$ is an operator, $-1$ is not an eigenvalue of $U$. Then

$$A\psi = -i(1+U)^{-1}(1-U)\psi. \tag{8.31}$$

By the spectral theorem for unitary operators, $U$ is isomorphic to multiplication by some $\upsilon$ with $|\upsilon| = 1$. It follows that $A$ is isomorphic to multiplication by $\alpha$ given by $\alpha = -i(1+\upsilon)^{-1}(1-\upsilon)$. Q.E.D.

Notice that all this proof amounts to is to note that if $A$ is a self-adjoint operator, then the Cayley transform $U = (1 - i(h/2)A)(1 + i(h/2)A)^{-1}$ is unitary, and so the spectral theorem for unitary operators applies. As long as $h \neq 0$ one can solve for $A$ in terms of $U$.

One immediate consequence is that the unitary group $U_t = \exp(-itA)$ giving the Schrödinger time evolution is defined. Furthermore, it is also easy to see (now that the spectral theorem is available) that the approximate unitary dynamics $U^n$ given by the Cayley transform converges strongly to the exact dynamics $U_t$ as $n \to \infty$ and $h \to 0$ with $nh \to t$.

**Problems**

1. Show that the Cayley transform $U = (1 - iA)(1 + iA)^{-1}$ may be expressed in terms of the resolvent as $U = 2(1 + iA)^{-1} - 1$.

2. Let $A$ be a self-adjoint operator such that $A$ has a basis of eigenvectors. Take the $\psi_j$ in the proof of the spectral theorem to be the corresponding eigenvectors. Describe the measure $\mu$ and function $\alpha$ given by the proof of the spectral theorem.

3. Let $A$ be a self-adjoint operator such that $A$ has a countable basis of eigenvectors $\phi_j$. Assume that each eigenvalue has multiplicity one. Take the $\psi$ in the proof of the spectral theorem to be $\psi = \sum_j c_j\phi_j$ where all the coefficients are non-zero. Describe the measure $\mu$ and function $\alpha$ given by the proof of the spectral theorem.

4. Let $\mathcal{H} = L^2(\mathbf{R}, dx)$ and $A = -id/dx$. Find the Cayley transform $U$ as an integral operator.

5. Let $A$ be a self-adjoint operator. Define $U = (1 - i(h/2)A)(1 + i(h/2)A)^{-1}$. Let $U_t = \exp(-itA)$. Show that for each $\psi$ the vectors $U^n\psi$ converge to $U_t\psi$ as $n \to \infty$ and $h \to 0$ with $nh \to t$.

6. State and prove a spectral theorem for self-adjoint graphs.

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# Chapter 9

# Functions of self-adjoint operators

This chapter is devoted to complex functions of a self-adjoint operator. The most important are the resolvent and the unitary group. By the spectral theorem, these are families of operators isomorphic to multiplication operators on $L^2$.

One important application is to the energy operator $H$ of quantum mechanics. If this is a self-adjoint operator, then the corresponding unitary group $\exp(-itH/\hbar)$ solves the Schrödinger equation.

The spectral theorem plays an important role in the interpretation of quantum mechanics. For an arbitrary unit vector and self-adjoint operator, it gives a realization of the operator as a random variable on a probability space determined by the operator and by the vector.

In the case of the energy operator, the realization as a random variable is independent of time. This random variable specifies for the solution how much probability is associated with each set of energies.

## 9.1 Functional calculus

The spectral theorem says that a self-adjoint operator has the representation

$$A = W^{-1}\alpha W. \tag{9.1}$$

(As usual we write $\alpha$ both for the function and the corresponding multiplication operator.) Consider a complex Borel function $f$ defined on the line (or at least on the range of $\alpha$). It is natural to attempt to define an

arbitrary complex Borel function $f(A)$ of a self-adjoint operator $A$ by

$$f(A) = W^{-1} f(\alpha) W. \tag{9.2}$$

This turns out to be a good definition. It is not immediately obvious that it is independent of the spectral representation, but that is in fact the case [N2]. We shall see why this is so in the discussion below.

One of the most important functions is the *resolvent* $(A - z)^{-1}$. This is certainly defined for all $z$ that are not real, and in this case it is obvious that this is a bounded operator with bound $\|(A - z)^{-1}\| \leq 1/|\Im z|$. The resolvent is obviously well defined independent of the spectral resolution.

The complement of the set where the resolvent is defined as a bounded operator is called the *spectrum*. The spectrum is always a closed set. We have seen that the spectrum of a self-adjoint operator $A$ is real. It is clear from the spectral theorem that the spectrum is the essential range of the representing function $\alpha$. Therefore in defining functions $f(A)$ we only need to worry about $f$ being defined on the spectrum. In particular, the resolvent $(A - z)^{-1}$ is defined whenever $z$ is not in the spectrum of $A$ and it satisfies the bound $\|(A-z)^{-1}\| \leq 1/d(z)$, where $d(z)$ is the distance to the spectrum. Notice that $d(z) \leq |\Im z|$, so this is a generalization of the bound given in the preceding paragraph.

The Cayley transform that we have been considering is closely related to the resolvent; in fact for each real $h \neq 0$

$$U = (1 - i(h/2)A)(1 + i(h/2)A)^{-1} = -1 + (4i/h)(A - 2i/h)^{-1}. \tag{9.3}$$

If $f$ is a complex Borel function defined on the spectrum of $A$, then $f(A) = h(U)$, where $h(u) = f((2i/h)(1 - u)/(1 + u))$. So in order to show that $f(A)$ is independent of the spectral representation, it is enough to show that $h(U)$ is independent of the spectral representation.

This is certainly true for polynomials in positive and negative powers of $U$. Now observe that if $h_n$ is a sequence of functions bounded by a fixed constant for which $h_n(U)$ is uniquely defined, and $h_n \to h$ pointwise, then $h_n(U) \to h(U)$ strongly, and so $h(U)$ is uniquely defined. By repeated limiting operations we may obtain in this way all bounded complex Borel functions $h$ on the circle.

This shows the uniqueness of the definition of $f(A)$, at least for bounded functions $f$. However if $f$ is not bounded, but $f(A)\psi$ is defined, then there is a sequence of bounded functions $f_n$ that converges to $f$ pointwise and such that $f_n(A)\psi$ converges to $f(A)\psi$. This shows that even in this case $f(A)$ is uniquely defined.

One useful class of functions of $A$ consists of the functions that have values 0 or 1. Let $1_S$ be the function that is 1 on the Borel set $S$ (a

subset of the real line) and 0 on its complement. Then $1_S(A)$ is called the spectral projection of $A$ corresponding to the set $S$. It is an orthogonal projection onto a closed subspace of the Hilbert space. This subspace should be thought of as the part of the Hilbert space where $A$ has values in $S$.

**Problems**

1. What is the spectrum of $1_S(A)$? Consider all cases.

2. Consider the restriction of $A$ to the range of $1_S(A)$. Show that the spectrum of this restricted operator is contained in the closure of $S$.

3. Give an example where it is not contained in $S$.

## 9.2 Some useful functions

It is nice to be able to define arbitrary functions of a self-adjoint operator, but certain functions are particularly important. Perhaps the most important are the resolvent and the unitary group. From the resolvent one can construct approximate delta functions, and with these one can approximate a wide class of functions.

If $A$ is a self-adjoint operator, then we may define the *approximate delta function operator* for $\epsilon > 0$ by

$$\delta_\epsilon(A-a) = \frac{1}{\pi}\frac{\epsilon}{(A-a)^2+\epsilon^2} = \frac{1}{2\pi i}\left((A-a-i\epsilon)^{-1} - (A-a+i\epsilon)^{-1}\right). \tag{9.4}$$

The last equation is important because it says that the approximate delta function is defined by the resolvent $(A-z)^{-1}$ for $z$ not real.

**Proposition 29** *If $f$ is bounded and continuous, then $f(A)$ is determined by*

$$\int f(A)\psi = \lim_{\epsilon\to 0}\int f(a)\delta_\epsilon(A-a)\psi\, da. \tag{9.5}$$

Proof: If $f$ is bounded and continuous, then

$$\int f(a)\delta_\epsilon(\alpha(x)-a)\, da \to f(\alpha(x)) \tag{9.6}$$

as $\epsilon \to 0$ pointwise. The result follows from the $L^2$ dominated convergence theorem.

**Corollary 7** *The unitary group is expressed in terms of the resolvent by*

$$\int \exp(-itA)\psi = \lim_{\epsilon \to 0} \int \exp(-ita)\delta_\epsilon(A-a)\psi \, da. \tag{9.7}$$

It is also possible to go from the resolvent to the unitary group. The resolvent is given by a time integral. The integral goes over positive time or negative time depending on whether $z$ is in the upper or lower half plane.

**Proposition 30** *The resolvent is given in terms of the unitary group by*

$$(A-z)^{-1}\psi = \int_0^{\pm\infty} i \exp(itz) \exp(-itA)\psi \, dt \tag{9.8}$$

*for* $\pm z > 0$.

The delta function is given by the jump in the resolvent between the lower and upper half plane. Thus in order to get the delta function we need to integrate over all time.

**Corollary 8**

$$\delta_\epsilon(A-a)\psi = \int_{-\infty}^{\infty} \exp(iat) \exp(-\epsilon|t|) \exp(-itA)\psi \, \frac{dt}{2\pi}. \tag{9.9}$$

**Problems**

1. Let $f$ be a bounded piecewise continuous function with right and left hand limits at the points of discontinuity. How must $f$ be defined at the points of discontinuity so the formula for $f(A)$ in terms of the approximate delta function remains valid?

2. Under what circumstances does the result of the previous problem give a formula for spectral projections in terms of the approximate delta function?

3. Show that the strong limit as $\epsilon \to 0$ of $\pi\epsilon\delta_\epsilon(A-a)$ is the projection onto the eigenspace where $A = a$.

## 9.3 Random variables

Let $A$ be a self-adjoint operator. Then by the spectral theorem there is an isomorphism $W$ from $\mathcal{H}$ to $L^2(X,\mu)$. Under this isomorphism $A$ is isomorphic to multiplication by a real function $\alpha$.

Let $\psi$ be a unit vector in the Hilbert space $\mathcal{H}$. Then $W\psi$ is a function on $X$ such that

$$\int |W\psi(x)|^2 \, d\mu(x) = 1. \tag{9.10}$$

Thus $|W\psi(x)|^2 \, d\mu(x)$ is a probability measure. A measurable function on a space with a probability measure is called a *random variable*. Thus $\alpha$ is a random variable.

Take $f$ to be a bounded Borel measurable function. Then $f(\alpha)$ is a bounded random variable. The expectation of this random variable is

$$\langle \psi, f(A)\psi \rangle = \int f(\alpha(x)) |W\psi(x)|^2 \, d\mu(x). \tag{9.11}$$

This last equation is a remarkable correspondence between Hilbert space and probability expressions.

These considerations show that a unit vector and an arbitrary self-adjoint operator gives rise to a random variable. Of course, two non-commuting random variables will not give rise to random variables defined on the same probability space.

In quantum mechanics some self-adjoint operators may give rise to random variables having physical significance. One example is the energy operator $H$. Since the time development of $\psi$ is given by the energy operator as $\exp(-itH/\hbar)\psi$, the probability measure does not depend on time. The distribution of $H$ gives the amount of probability corresponding to each set of energy values, and this amount does not change with time.

We may write the expectation of a function of a random variable in terms of a measure on the reals, the *distribution* of the random variable. If $f$ is bounded and measurable, then we obtain

$$\langle \psi, f(A)\psi \rangle = \int f(a) \, d\nu(a). \tag{9.12}$$

The measure $\nu$ is uniquely determined by the unit vector and the self-adjoint operator. It is supported on the spectrum of the operator. A special case of the above formula is

$$\langle \psi, 1_S(A)\psi \rangle = \nu(S). \tag{9.13}$$

This is interpreted as the probability that $A$ is in $S$. It is clear that calculating the distribution $\nu$ must be one of the fundamental goals of quantum mechanics.

It is perhaps useful at this point to summarize the basic principles of quantum mechanics. A *state* of a system is determined by a unit vector $\psi$

in the Hilbert space $\mathcal{H}$. Two vectors determine the same state if they are multiples of each other. (Thus what is important is not the vector, but the one dimensional subspace, or *ray*, determined by the vector. The collection of all these subspaces is actually a projective space rather than a vector space.)

An *observable* is determined by a self-adjoint operator. The fundamental equation is that the expectation of a real measurable function of the operator is given (when the relevant integral converges absolutely) by

$$\langle \psi, f(A)\psi \rangle. \tag{9.14}$$

In particular, when $f$ has values only zero or one, this is the probability that $A$ has value in the set where $f$ is one.

We may summarize this as follows.

**Dogma 1** *States are determined by unit vectors in Hilbert space. Observables are given by self-adjoint operators. In every state each observable has a well-defined probability distribution.*

It is not clear how seriously to take the preceding dogma. Certainly the mathematics is correct; in every state a self-adjoint operator has an associated probability distribution. On the other hand, there is a bewildering variety of self-adjoint operators, most of which correspond to no conceivable physical experiment. Which ones should be taken seriously? This requires a serious analysis of actual measurement procedures, which will not be attempted here.

It may be that the only observables of interest are the momentum observables, and possibly the energy. In an electron scattering experiment counters are set up at various angles, and these measure the momenta of the outcoming electrons. The details of the interaction are not directly observed, but are inferred from the results of the scattering experiment. In observing the emission of light from electrons passing from one bound state to another, the spectral lines are predicted from the eigenvalues of the energy operator. The probability predictions give by the dogma of quantum mechanics seem to be relevant. However ultimately what is measured is the momentum of the emitted light.

## 9.4 Constructing spectral representations

Now that we have the spectral theorem for self-adjoint operators, we may construct spectral representations in a somewhat more convenient manner.

**Theorem 22** *Let $A$ be a self-adjoint operator from $\mathcal{H}$ to itself. Then there exists a measure space $L^2(X, \mu)$ and an isomorphism $W$ from $\mathcal{H}$ to $L^2$ and a real function $\alpha$ such that $U = W^{-1}\alpha W$. The space $X$ may be taken to be a disjoint union of copies of the reals. The measure $\mu$ may be taken so as to restrict to a probability measure on each copy. The function $\alpha$ may be taken to be the identity function on each copy.*

Remark: The probability measure $\nu_j$ on the $j$th copy is the distribution of the $A$ with respect to a vector $\psi_j$. Once we have constructed these distribution measures the proof can go almost exactly as for the unitary case.

Proof: For a unit vector $\psi$ in $\mathcal{H}$ let $H_\psi$ be the closed linear subspace generated by the $\exp(-itA)\psi$. This linear subspace is invariant also invariant under the resolvents of $A$ and hence under $f(A)$ for each bounded continuous function of $A$.

Let $\nu$ be the distribution of $A$ with respect to the unit vector $\psi$. Note that

$$\langle \psi, f(A)\psi \rangle = \int f(a)\, d\nu(a). \tag{9.15}$$

In particular

$$\langle \psi, |f(A)|^2\psi \rangle = \int |f(a)|^2\, d\nu(a). \tag{9.16}$$

Therefore if $f(A)\psi = 0$, then $f(a) = 0$ for all $z$ except for a set of $\nu$ measure zero. Therefore $f(a)$ may be identified with zero in the space $L^2(\mathbf{R}, \nu)$.

It follows that we may define a unitary operator $W_\psi$ from $\mathcal{H}_\psi$ to $\mathrm{L}^2(\mathbf{R},\, \nu)$ by $W_\psi f(A)\psi = f$. Furthermore it is easy to check that $W_\psi f(A)\phi = f(a)W_\psi\psi$.

Now consider families $\psi_j$ of vectors such that $\mathcal{H}_{\psi_j}$ are mutually orthogonal. Take a maximal such family. Let $M$ be the closed subspace of consisting of all vectors $\phi = \sum_j \phi_j$ where $\phi_j$ is in $\mathcal{H}_{\psi_j}$. By use of essentially the same argument as for the construction used for a single unitary operator we see that $M = \mathcal{H}$.

Now take as many copies $\mathbf{R}_j$ of the real line as there are are vectors $\psi_j$. Let $X$ be the disjoint union of the $\mathbf{R}_j$. Each point $x$ in $X$ is a pair $(a, j)$ with $a$ real. Define the function $\alpha$ by $\alpha(x) = a$.

Now for every $\phi$ in $\mathcal{H}$ we define

$$W\phi(x) = W_{\psi_j}\phi_j(a). \tag{9.17}$$

It is easy to check that

$$Wf(A)\phi(x) = W_{\psi_j}f(A)\phi_j(a) = f(a)W_{\psi_j}\phi_j(a) = f(\alpha(x))W\phi(x). \tag{9.18}$$

This completes the proof.

This result says that the points of $X$ may be labeled by the $a$ that are in the spectrum of $A$ and by an extra parameter $j$. The extra parameter is always necessary when the $A$ is an operator with multiplicity.

In general the points in the space $X$ used for a spectral representation may be labeled by a sequence of numbers belonging to the spectra of a commuting family of self-adjoint operators. This fact is heavily exploited in the Dirac formalism.

**Problems**

1. Let $A$ be a self-adjoint operator such that $A$ has a basis of eigenvectors. Take the $\psi_j$ in the proof of the spectral theorem to be the corresponding eigenvectors. Describe the measure $\mu$ and function $\alpha$ given by the proof of the spectral theorem.

2. Let $A$ be a self-adjoint operator such that $A$ has a countable basis of eigenvectors $\phi_j$. Assume that each eigenvalue has multiplicity one. Take the $\psi$ in the proof of the spectral theorem to be $\psi = \sum_j c_j \phi_j$ where all the coefficients are non-zero. Describe the measure $\mu$ and function $\alpha$ given by the proof of the spectral theorem.

3. Let $A = -d^2/dx^2$ acting in $L^2$ of the line. Find a spectral representation (as in the proof of the spectral theorem) that uses precisely two vectors $\psi$.

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# Chapter 10

# The Heisenberg Commutation Relations

This chapter is devoted to the analysis of the non-commuting operators that characterize quantum mechanics.

These operators may be analyzed in terms of the unitary groups (Weyl relations) or in terms of the self-adjoint operators (Heisenberg relations). We shall take the former course. The analysis in terms of the unbounded self-adjoint operators is more delicate but is certainly possible [4, 13, Pu].

## 10.1 Quantum automorphisms

There is another basic principle of quantum mechanics that describes the mechanism of transformation (in space or in time). Let $A$ be a self-adjoint operator, representing an observable. (It may of course be a function of another self-adjoint operator.) Let $\psi$ be a unit vector representing a state. Assume that the integral representing $\langle \psi, A\psi \rangle$ is absolutely convergent. Then

$$\langle \psi, A\psi \rangle \tag{10.1}$$

is the expectation of $A$ in the state $\psi$. (When $A$ has values zero or one, this is of course a probability.) We wish to see how this expression is transformed.

Let $U$ be a unitary operator, representing the transformation. Then as a mathematical identity

$$\langle U\psi, AU\psi \rangle = \langle \psi, U^*AU\psi \rangle. \tag{10.2}$$

This fundamental equation shows that there are two ways to interpret the change. In the *Schrödinger picture* the state is changed from $\psi$ to $U\psi$. In the *Heisenberg picture* the observable is changed from $A$ to $U^*AU^{-1}$. In either picture the change is given by specifying the unitary operator.

There is one amendment to this story. Recall that the state determines the vector $\psi$ only up to a scalar multiple. Thus the automorphisms of the states may be somewhat more general than the unitary operators that give automorphisms of the vectors. In fact, it turns out that sometimes it is useful to take operators $U$ that are anti-unitary rather than unitary. These are operators that satisfy $U(z\psi) = z^*U(\psi)$, with a complex conjugate on the scalar multiple. The most important example of such an operator is time reversal in quantum mechanics. For the simple case of the scalar Schrödinger equation this is given by complex conjugation of the wave function. Notice that this operation gives a solution of the equation that is obtained from the Schrödinger equation by reversing the direction of time.

This story on the automorphisms of quantum mechanics has been the subject of extensive study, and there is a useful survery by Simon [15].

Thus we have another dogma of quantum mechanics.

**Dogma 2** *The transformations in quantum mechanics are given by unitary (or anti-unitary) operators. They may be thought of in the Schrödinger picture as transforming the states or in the Heisenberg picture as transforming the observables.*

The transformations are often embedded in a one-parameter group of unitary transformations. This allows the transformations to be written in infinitesimal form. Consider for instance the time translation given by $U_t = \exp(-itH/\hbar)$. We have the Schrödinger equation

$$i\hbar \frac{dU_t\psi}{dt} = HU_t\psi. \tag{10.3}$$

If we compute the time derivative of the expectation of $A$ we obtain

$$\frac{d}{dt}\langle U_t\psi, AU_t\psi\rangle = \frac{i}{\hbar}\langle U_t\psi, [H,A]U_t\psi\rangle, \tag{10.4}$$

where $[H,A] = HA - AH$ is the commutator of $H$ and $A$. The interpretation of such formulas involve delicate considerations of domains of unbounded operators, but they provide an important way of thinking about quantum mechanics.

## 10.2 Heisenberg and Weyl relations

We now understand the action of a single self-adjoint operator or of a commuting family of such operators. But this is not enough to charactize quantum mechanics.

We would like to find an operator theory characterization of the Hilbert space framework that is used for the Schrödinger equation. For this we shall need non-commuting operators. For simplicity we begin with the case $\nu = 1$ of one dimensional space.

We have the momentum operator

$$P = -i\hbar \frac{d}{dx} \tag{10.5}$$

and the position operator

$$Q = x. \tag{10.6}$$

The relation between these two operators may be expressed in intrinsic Hilbert space terms by the famous *Heisenberg commutation relation*

$$[P, Q] = PQ - QP = -i\hbar. \tag{10.7}$$

Unfortunately, both $P$ and $Q$ are unbounded operators with domains that are not the entire Hilbert space. Therefore it is a delicate matter to interpret the expressions in this commutation in a rigorous way.

Fortunately, there are other formulations of the commutation relations, obtained by taking functions of each of these operators. In particular, they generate unitary groups. One is the *translation group*

$$\exp(-iaP/\hbar) f(x) = f(x - a), \tag{10.8}$$

and the other is the *boost group* consisting of multiplication operators

$$\exp(-ibQ/\hbar) f(x) = \exp(-ibx/\hbar) f(x). \tag{10.9}$$

Notice that the translation group acts on functions of position $Q$ by

$$\exp(iaP/\hbar) g(Q) \exp(-iaP/\hbar) = g(Q + a). \tag{10.10}$$

This is simply saying that the translation group acts in a reasonable way on position.

Similarly, the boost group acts on functions of momentum by

$$\exp(ibQ/\hbar) g(P) \exp(-ibQ/\hbar) = g(P + b). \tag{10.11}$$

Notice that this says that the momentum is increased (boosted) by the appropriated amount.

It may be that the formuation in terms of the boost transformations is more fundamental. The fundamental symmetries of non-relativistic quantum mechanics come from Galilean transformations. These are translations in space, translations in time, rotations in space, and boosts in space-time. The amount of a boost is given by a velocity change $v$. We may write the above equation as

$$\exp(ivmQ/\hbar)g(P)\exp(-ivmQ/\hbar) = g(P + mv). \tag{10.12}$$

From this we see that the generator of boosts is actually $mQ$. The relation between the generators of translations and boosts is given by a variant of the Heisenberg relation

$$PmQ - mQP = -im\hbar. \tag{10.13}$$

This is a characteristic feature of the action of Galilean transformations in quantum mechanics; there is a parameter $m$ that occurs in the commutation relations that parametrizes the way that the transformations act on Hilbert space.

Still another form of the commutation relations is the *Weyl relation* that relates the two groups. This is

$$\exp(-ibQ/\hbar)\exp(-iaP/\hbar) = \exp(-iaP/\hbar)\exp(-ibQ/\hbar)\exp(-iab/\hbar) \tag{10.14}$$

This relation is somewhat curious, in that the Galilean transformations of translation in space and boosting commute. However this equation says that the correspoinding unitary operators in quantum mechanics do not commute. The resolution of the difficulty is to remember that in quantum mechanics the states are determined only up to scalar multiples. The extra term $\exp(-iab/\hbar)$ is a scalar multiple, and has no effect on the actual state.

The relation between the Heisenberg relation and the Weyl relation is an instance of the relation between a Lie algebra commutation relation and a Lie group product relation. In this case the Lie algebra and Lie group are not just the Galilean translations and boosts, but a non-commutative extension that provides the constant term in the commutation relation and the extra phase in the group version.

The properties of Galilean transformations in quantum mechanics were studied beginning with Bargmann [2]. They have been subsequently analysed by various authors [H, Ma2, 10], who may be consulted for further information.

**Problems**

1. Show that the Heisenberg commutation relations cannot be satisfied by operators in a finite dimensional Hilbert space. (Hint: Take the trace of both sides.)

## 10.3 Uniqueness: Discrete translations

Consider the translation group $U_a = \exp(-iaP/\hbar)$ acting on $L^2$ of the line. Let $g$ be an increasing function. Then $U_a^* g(Q) U_a = g(Q + a)$, which is increasing as $a$ increases. It turns out that this property has deep implications for spectral theory: It is a diagonostic for absolutely continuous spectrum. (Indeed the operator $P$ has absolutely continuous spectrum.)

Take $g$ to be the indicator function of the right half-line. Let $M$ be the range of $g(Q)$ (the subspace where $Q \geq 0$). Note that $g(Q-a)U_a = U_a g(Q)$. We may think of the range of $g(Q-a)$ as the subspace where $Q \geq a$. This shows that $U_a$ takes the space $M$ where $Q \geq 0$ to the space $U_a M$ where $Q \geq a$. Thus the subspaces decrease as $a$ increases.

This setup has an interesting and useful discrete analog. Let $V$ be the translation to the right by one on the space $\ell^2$ of the integers. Let $M$ be the subspace of functions $f$ in $\ell^2$ such that $f(x) \neq 0$ only for $x \geq 0$. Then $V^n$ takes $M$ into the subspace of functions $f$ in $\ell^2$ such that $f(x) \neq 0$ only for $x \geq n$. Again the subspaces decrease as $n$ increases.

Notice that $V$ has a spectral representation given by Fourier series. The spectral measure is a measure on the circle that has a density, and so $V$ has absolutely continuous spectrum.

We would like to characterize this sort of situation in intrinsic Hilbert space terms, at least up to isomorphism and multiplicity. In this section we deal with the discrete case; the continuous case follows in the next section. The following definition makes no reference to the concrete form of the operators; it just gives a relation between a unitary operator and a closed subspace.

**Definition 19** *We say that $M$ is an outgoing subspace for the unitary operator $V$ if*

$$VM \subset M, \tag{10.15}$$

*and*

$$\cap_n V^n M = 0, \tag{10.16}$$

*and*

$$\text{closure} \cup_n V^n M = \mathcal{H}. \tag{10.17}$$

This definition is satisfied by the standard model we considered above. In this model the Hilbert space is $\ell^2(\mathbf{Z})$. The action of $V$ is the right shift

$Vf(x) = f(x-1)$. The subspace $M$ consists of all $f$ in $\ell^2(\mathbf{Z})$ such that $f(x) \neq 0$ implies $x \geq 0$. The definition is also satisfied by a direct sum of copies of the standard model.

**Proposition 31** *Let $V$ be a unitary operator and $M$ be an outgoing subspace of $\mathcal{H}$. Then the Hilbert space is a direct sum of Hilbert spaces in each of which $V$ and $M$ are isomorphic to the standard model.*

Proof: Since $V$ sends $M$ into $M$, the space $VM$ is a closed subspace of $M$. By the projection theorem, there is a closed subspace $N$ of $M$ such that the direct sum of $N$ with $VM$ is $M$.

It is not hard to check that the spaces $V^k N$ for $k \geq 0$ are orthogonal closed subspaces of $M$. If $\phi$ is a vector in $M$ that is orthogonal to all these closed subspaces, then it must be in $V^k M$ for all $k \geq 1$. From the definition of outgoing space it follows that it is the zero vector. The projection theorem then implies that $M$ is the direct sum of these closed subspaces.

Now consider the orthogonal closed subspaces $V^k N$ for all integer $k$. For arbitrarily negative $j$ we see from the first conclusion that that $V^j M$ is the direct sum of the $V^k N$ for $k \leq j$. From the definition of outgoing space it follows that the union of the $V^j M$ is dense in $\mathcal{H}$. It follows that the direct sum of the closed subspaces $V^k N$ is dense in $\mathcal{H}$. Since this direct sum is again a closed subspace, the projection theorem implies that it must be equal to $\mathcal{H}$.

Now let $\phi_j$ be a basis for $N$. For each $j$ the vectors $V^k \phi_j$ form a basis for a closed subspace $\mathcal{H}_j$ of $\mathcal{H}$. This basis defines an isomorphism of $\mathcal{H}_j$ with $\ell^2(\mathbf{Z})$. Q.E.D.

**Problems**

1. Find the spectral representation for $V$.

## 10.4 Uniqueness: Continuous translations

We wish to show that the Weyl relations have a unique solution up to multiplicity. For simplicity we give the complete proof only for the case of one dimension. The proof is taken from Lax and Phillips [LP].

**Theorem 23** *Let $P$ and $Q$ be self-adjoint operators acting in $\mathcal{H}$. Assume that for each real Borel function $g$ they satisfy the relations*

$$\exp(iaP/\hbar) g(Q) \exp(-iaP/\hbar) = g(Q + a) \tag{10.18}$$

*for all real $a$. Then the Hilbert space is a direct sum of Hilbert spaces in each of which $P$ and $Q$ are isomorphic to the standard momentum and position operators.*

We write $U_a = \exp(-iaP/\hbar)$ for the unitary group. Let $1_+$ denote the function that is one for $x \geq 0$ and zero for $x < 0$. The starting point is the commutation relation in the form

$$1_+(Q - a)U_a = U_a 1_+(Q). \tag{10.19}$$

We want to formulate this in terms of an outgoing subspace.

**Definition 20** *A closed subspace $M$ is an outgoing subspace for the unitary group $U_a$ if for all $a \geq 0$*

$$U_a M \subset M, \tag{10.20}$$

*and*

$$\cap_a U_a M = 0, \tag{10.21}$$

*and*

$$\text{closure}(\cup_a U_a M) = \mathcal{H}. \tag{10.22}$$

This definition says that the subspace $U_a M$ is contained in $M$ for $a \geq 0$, that it is decreasing to zero as $a \to \infty$, and that it is increasing to the whole space as $a \to -\infty$.

Let $M$ be the closed subspace that is the range of $1_+(Q)$. It is easy to check that $M$ is an outgoing subspace. The condition on the intersection follows by looking at large positive $a$, and the condition on the union follows by looking at large negative $a$.

Now we want to reduce the uniqueness problem for the continuous dynamics given by the unitary group to that for the discrete dynamics given by the powers of the unitary operator.

So consider a real constant $h > 0$ and the Cayley transform

$$V = (1 - iPh/2)(1 + iPh/2)^{-1} \tag{10.23}$$

**Lemma 9** *A subspace $M$ is invariant under the unitary group $U_a = \exp(-iaP/\hbar)$ for all $a \geq 0$ if and only if it is invariant under the unitary operator $V$.*

Proof: Assume that $M$ is invariant under the unitary group with $a \geq 0$. We know that from the unitary group with $a \geq 0$ we can recover the resolvent $(P - i\epsilon)^{-1}$ for $\epsilon > 0$. From the resolvent one can recover the Cayley transform. Thus $M$ is also invariant under the Cayley transform.

On the other hand, assume that $M$ is invariant inder the Cayley transform $V$ defined with some particular value of $h$. Then it is invariant under

$(P - i\epsilon)^{-1}$ for some $\epsilon > 0$. It is not difficult to show that it must be invariant under $(P - i\epsilon)^{-1}$ for all $\epsilon > 0$. Therefore it is invariant under $V$ for all values of $h > 0$. We may recover the unitary group $U_a$ from $V^n$ in the limit $n \to \infty$ with $nh \to a$. Therefore it is invariant under the unitary group for $a \geq 0$. Q.E.D.

**Lemma 10** *A subspace $M$ is an outgoing subspace for the unitary group $U_a$ if and only if $M$ is an outgoing subspace for the corresponding Cayley transform $V$.*

Proof: We give the proof for the case when the subspace $M$ is known to be an outgoing subspace for the unitary group and we want to conclude that it is an outgoing subspace for the Cayley transform.

Let $M_\infty = \cap_n V^n M$. It is easy to check that $V^n M_\infty \subset M_\infty$ for all $n$, positive or negative. It follows that $U_a M_\infty \subset M_\infty$ for all $a$, positive or negative. From the group property it is easy to check that $U_a M_\infty = M_\infty$ for all $a$. Since $M_\infty \subset M$, we have $M_\infty = \cup_a U_a M_\infty \subset \cup_a U_a M = \{0\}$.

Let $M_{-\infty} = \text{closure} \cup_n V^n M$. It is easy to check that $V^n M_{-\infty} \subset M_{-\infty}$ for all $n$, positive or negative. It follows that $U_a M_{-\infty} \subset M_{-\infty}$ for all $a$, positive or negative. From the group property it is easy to check that $U_a M_{-\infty} = M_{-\infty}$ for all $a$. Since $M \subset M_{-\infty}$, we have a dense subspace $\cup_a U_a M \subset \cup_a U_a M_{-\infty} = M_{-\infty}$, which implies that $M_\infty = \mathcal{H}$. Q.E.D.

Proof of theorem: Assume that we have a solution of the relation between the one-parameter group generated by $P$ and the operator $Q$. Then we have the one-parameter group and the outgoing subspace in the continuous case. It follows from the lemmas that we have the discrete group and outgoing subspace. We have seen in the previous section that all realizations of the discrete group and outgoing subspace are isomorphic, up to multiplicity. Since the continuous group may be recovered from the Cayley transform (by solving explicitly for the generator $P$), the same must be true for the continuous group and the outgoing subspace.

From the unitary group $U_a$ and from $M$ we can recover the subspaces $U_a$ where $Q \geq a$. This is enough to show that the original $P$ and $Q$ are uniquely determined, up to isomorphism and multiplicity. Q.E.D.

It does not follow from this theorem that the representation of $P$ and $Q$ is isomorphic to the standard representation; it may be isomorphic to a direct some of several copies. For an electron, which has spin, the representation is isomorphic to the direct sum of two copies.

**Problems**

1. Consider the standard Schrödinger representation of $P$ and $Q$. Use the explicit form for $V$ as an integral operator to verify that $V$ leaves $M$ invariant.

## 10.5 Multidimensional systems

Much the same story applies to the case of several dimensions. The standard Schrödinger realization is with the momentum operators

$$\mathbf{a} \cdot \mathbf{P} = -i\hbar \mathbf{a} \cdot \nabla_{\mathbf{x}} \tag{10.24}$$

and the position operators

$$\mathbf{b} \cdot \mathbf{Q} = \mathbf{b} \cdot \mathbf{x}. \tag{10.25}$$

As before we may take functions of each of these operators. In particular, they generate unitary groups. One is the translation group

$$\exp(-i\mathbf{a} \cdot \mathbf{P}/\hbar) f(\mathbf{x}) = f(\mathbf{x} - \mathbf{a}), \tag{10.26}$$

and the other consists of multiplication operators.

$$\exp(-i\mathbf{b} \cdot \mathbf{Q}/\hbar) f(\mathbf{x}) = \exp(-i\mathbf{b} \cdot \mathbf{x}/\hbar) f(\mathbf{x}). \tag{10.27}$$

Again the translation group acts on functions of position $\mathbf{Q}$ by

$$\exp(i\mathbf{a} \cdot \mathbf{P}/\hbar) g(\mathbf{Q}) \exp(-i\mathbf{a} \cdot \mathbf{P}/\hbar) = g(\mathbf{Q} + \mathbf{a}). \tag{10.28}$$

Similarly, the boost group acts on functions of momentum by

$$\exp(i\mathbf{b} \cdot \mathbf{Q}/\hbar) g(\mathbf{P}) \exp(-i\mathbf{b} \cdot \mathbf{Q}/\hbar) = g(\mathbf{P} + \mathbf{b}). \tag{10.29}$$

There are still other ways of writing this relation. We may differentiate

$$\exp(it\mathbf{a} \cdot \mathbf{P}/\hbar) \mathbf{b} \cdot \mathbf{Q} \exp(-it\mathbf{a} \cdot \mathbf{P}/\hbar) = \mathbf{b} \cdot \mathbf{Q} + t\mathbf{a} \cdot \mathbf{b} \tag{10.30}$$

to obtain the *Heisenberg commutation relation*

$$(\mathbf{a} \cdot \mathbf{P})(\mathbf{b} \cdot \mathbf{Q}) - (\mathbf{b} \cdot \mathbf{Q})(\mathbf{a} \cdot \mathbf{P}) = -i\hbar \mathbf{a} \cdot \mathbf{b}. \tag{10.31}$$

We may write this in a abbreviated tensorial form as

$$[\mathbf{P}, \mathbf{Q}] = \mathbf{PQ} - \mathbf{QP} = -i\hbar\delta. \tag{10.32}$$

Or we may relate the two groups by the *Weyl relations*

$$\exp(-i\mathbf{b}\cdot\mathbf{Q}/\hbar) \exp(-i\mathbf{a}\cdot\mathbf{P}/\hbar) = \exp(-i\mathbf{a}\cdot\mathbf{P}/\hbar) \exp(-i\mathbf{b}\cdot\mathbf{Q}/\hbar) \exp(-i\mathbf{a}\cdot\mathbf{b}/\hbar) \tag{10.33}$$

It is possible to prove a version of the uniqueness theorem theorem as long as $\nu < \infty$.

## 10.6 The Galilean group and quantum dynamics

The Galilean group consists of space translations, time translations, rotations, and boosts. We will neglect discussion of the rotations and concentrate on the relation between space translations, time translations, and boosts. In quantum mechanics the corresponding tranformations are generated by self-adjoint operators. The generators of space-translations, time translations, and boosts are the operators $\mathbf{P}$, $H$, and $m\mathbf{Q}$.

We shall always assume that the relation between space translations and boosts is given by the Heisenberg commutation relation

$$\frac{i}{\hbar}[\mathbf{P}, m\mathbf{Q}] = -i\hbar m\delta. \tag{10.34}$$

If the quantum system is Galilean invariant, a situation that corresponds to free motion, then the time translation generator is just $H = \mathbf{P}^2/(2m)$. In this case the relation between time translations and boosts is given by

$$\frac{i}{\hbar}[H, m\mathbf{Q}] = \mathbf{P}. \tag{10.35}$$

Finally, the relation between time translation and space translation is simply

$$[H, \mathbf{P}] = 0. \tag{10.36}$$

This last equation says that the time evolution is translation invariant: No part of space is preferred to any other.

Quantum systems are usually not Galilean invariant. There are electric and magnetic fields that affect the time translation. With electric fields the third Galilean commutation relation fails; the electric potential is different in different parts of space. With magnetic fields the second commtation relation relation also fails.

When magnetic fields are present it is necessary to distinguish between momentum $\mathbf{P}$ and velocity $\dot{\mathbf{Q}}$; they are no longer related by $\mathbf{P} = m\dot{\mathbf{Q}}$. However it is assumed that boosts act on velocities in the same way that they act on momenta. Thus we have the relation

$$\frac{i}{\hbar}[m\dot{\mathbf{Q}}, m\mathbf{Q}] = m\delta. \tag{10.37}$$

The second Galilean commutation relation is replaced by

$$\frac{i}{\hbar}[H, m\mathbf{Q}] = m\dot{\mathbf{Q}}. \tag{10.38}$$

From these relations we can find a suitable form for the time translation generator $H$. The fact that $\mathbf{P}$ and $m\dot{\mathbf{Q}}$ have the same commutator with $\mathbf{Q}$ suggests that they differ by a function of $\mathbf{Q}$, so that

$$m\dot{\mathbf{Q}} = \mathbf{P} - \mathbf{a}(\mathbf{Q}). \tag{10.39}$$

This extra term represents the magnetic vector potential.

The fact that $H$ and $\dot{\mathbf{Q}}^2/(2m)$ have the same commutator with $m\mathbf{Q}$ (namely $m\dot{\mathbf{Q}}$) suggests that they differ by a function of $\mathbf{Q}$. Thus

$$\frac{1}{2m}\dot{\mathbf{Q}}^2 = H - v(\mathbf{Q}). \tag{10.40}$$

This last equation determines the form of the Schrödinger equation. From now on we shall mainly use it in the conventional form

$$H = \frac{1}{2m}(\mathbf{P} - \mathbf{a}(\mathbf{Q}))^2 + v(\mathbf{Q}). \tag{10.41}$$

The commutation relation between the various components of $m\dot{\mathbf{Q}}$ is non-trivial. We have

$$\frac{i}{\hbar}[m\dot{\mathbf{Q}}, m\dot{\mathbf{Q}}] = ((\nabla\mathbf{a}(\mathbf{Q}))^T - \nabla\mathbf{a}(\mathbf{Q})), \tag{10.42}$$

where $T$ denotes transpose. We may now compute the final commutator between $H = (1/2)m\dot{\mathbf{Q}}^2 + v(\mathbf{Q})$ and $m\dot{\mathbf{Q}}$. We obtain

$$\frac{i}{\hbar}[H, m\dot{\mathbf{Q}}] = \dot{\mathbf{Q}} \cdot (\nabla\mathbf{a}(\mathbf{Q}))^T - (\dot{\mathbf{Q}} \cdot \nabla)\mathbf{a}(\mathbf{Q}) - \nabla v(\mathbf{Q}). \tag{10.43}$$

This is the usual form of the force law with a magnetic and electric field.

**Problems**

1. Let $g$ be a smooth real function and define $U = \exp(-ig(\mathbf{Q})/\hbar)$. Let $\tilde{P} = U^*PQ$. Show that the pair $\tilde{P}, Q$ is isomorphic to the pair $P, Q$.

2. Let $\tilde{a} = a - \nabla g$. Show that $\dot{Q} = \tilde{P} - \tilde{a}(Q)$.

3. Show that if $\nu = 1$, then $g$ may be chosen so that $\tilde{a} = 0$. Thus there are no magnetic fields in one dimension.

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# Chapter 11

# Operator Sums

This chapter is the beginning of the analysis of quantum dynamics. This is determined by the sum of two self-adjoint operators, and one is interested in the question of when the sum is self-adjoint. The most elementary concept of sum is the operator sum, and we begin with that.

## 11.1 Quantum dynamics

We have seen that the Schrödinger equation may be written

$$i\hbar\frac{d\psi(t)}{dt} = H\psi(t). \tag{11.1}$$

If $H$ is self-adjoint, then this has the solution

$$\psi(t) = \exp(-itH/\hbar)\psi(0). \tag{11.2}$$

In practice $H$ is often the sum of a kinetic energy part $H_0$ and a potential energy part $V$. In the standard situation

$$H_0 = \frac{\mathbf{P}^2}{2m} \tag{11.3}$$

and

$$V = v(Q), \tag{11.4}$$

where $v$ is a real measurable function. Each of these operators is self-adjoint. However they certainly do not commute.

We would like to define

$$H = H_0 + V \tag{11.5}$$

as a self-adjoint operator in an unambiguous way. This is not possible in general. However we shall see that there are important cases when the situation is satisfactory. The most elementary is when $V$ is a bounded operator. This will establish that the Schrödinger equation has a uniquely determined solution whenever $v$ is a bounded measurable function.

Of course it is also desirable to allow $v$ to have singularities. This will require further analysis.

## 11.2 Operator Sums

The obvious definition of operator sum is to define $A+B$ on $D(A)\cap D(B)$ by $(A+B)\psi = A\psi+B\psi$. It is not at all clear that this has nice properties. For instance it is possible that $D(A)$ and $D(B)$ are both dense linear subspaces of the Hilbert space, but the intersection contains only the zero vector. In that case $A + B$ is rather degenerate. In particular, its adjoint is not even an operator.

If one is interested in adjoints, all that one can say in general about the adjoint of a sum is that $A^* + B^* \subset (A + B)^*$. The simplest case when one can say something more positive is when one of the operators is bounded.

**Theorem 24** *If $A$ is a densely defined operator and $B$ is a bounded operator, then*

$$(A + B)^* = A^* + B^*. \tag{11.6}$$

*In particular, if $A$ is a self-adjoint operator and $B$ is a bounded self-adjoint operator, then $A + B$ is self-adjoint.*

Proof: It is easy to check that for arbitrary densely defined operators whose sum is densely defined we have $A^* + B^* \subset (A + B)^*$.

The work is to show that if $B$ is bounded, then $(A + B)^* \subset A^* + B^*$. The key is the fact that $B^*$ is also bounded. Let $\psi$ be in $D(A+B)^*$. Then for all $\phi$ is $D(A + B) = D(A)$ we have

$$\langle (A + B)^*\psi, \phi\rangle = \langle \psi, A\phi\rangle + \langle \psi, B\phi\rangle. \tag{11.7}$$

Hence

$$\langle \psi, A\phi\rangle = \langle (A + B)^*\psi, \phi\rangle - \langle B^*\psi, \phi\rangle. \tag{11.8}$$

Thus $\psi$ is in $D(A^*)$ with $A^*\psi = (A + B)^*\psi - B^*\psi$. This may be written $(A + B)^*\psi = A^*\psi + B^*\psi$, which is the desired conclusion. Q.E.D.

The application of this theorem to Schrödinger operators is immediate. Let $v$ be an arbitrary real Borel measurable function. Let $H_0 = \mathbf{P}^2/(2m)$

and $V = v(\mathbf{Q})$. Then $H = H_0 + V$ is self-adjoint. This result is remarkable, since there are no continuity conditions on $v$ and no conditions on the asymptotic behavior at infinity, other than being bounded. It is natural to ask: What are the boundary conditions at infinity needed for the Schrödinger equation to have a uniquely specified solution? The answer in this situation is: There are none. In particular, the result applies to extended media with irregular (non-periodic) potentials.

On the other hand, this result is lacking for some important applications. The Hydrogen atom problem involves a potential that is unbounded below; that case is not covered by the above theorem. The harmonic oscillator potential is unbounded above; that case certainly evades the present analysis. We will see below that there are more powerful results that take care of such cases.

In the rest of this section we survey other facts about the algebra of operators. We define the *operator sum* $A + B$ of $A$ and $B$ on $D(A + B) = D(A) \cap D(B)$ by $(A+B)\psi = A\psi + B\psi$. (The *operator difference* is of course $A - B = A + (-B)$.) We define the *operator product* $AB$ of $A$ and $B$ on $D(AB) = B^{-1}D(A) \cap D(B)$ by $(AB)\psi = AB\psi$.

The algebraic properties of these operations are not so nice. However there are a few useful identities. The proofs are mainly routine verifications [RN]. Whenever we are discussing adjoints we shall assume that the operator is densely defined, so that its adjoint is an operator.

For the operator sum we have the associative law $(A + B) + C = A + (B + C)$ and the commutative law $A + B = B + A$. There is an identity $A + 0 = 0 + A = A$. In general there is no inverse; all we have is $A - A = -A + A \subset 0$. For the adjoint all we have in general is $A^* + B^* \subset (A + B)^*$.

For the operator product we have the associative law $(AB)C = A(BC)$ and the law for the inverse of a product $(AB)^{-1} = B^{-1}A^{-1}$. Note the reversal of order in the last law. We have an identity $A1 = 1A = A$. In general there is no inverse; we get $AA^{-1} \subset 1$ and $A^{-1}A \subset 1$. For the adjoint all we have in general is $A^*B^* \subset (BA)^*$. Note again the reversal of order. We shall see in a later chapter that $(A^*A)^* = A^*A$.

For the combination of the sum and product we have the distributive law $BA + CA = (B + C)A$ on one side but not the other. All we have in general is $AB + AC \subset A(B + C)$.

We can do much better with the sum and product when one of the operators is bounded. When $B$ is bounded we have $A^* + B^* = (A + B)^*$ and $B^* + A^* = (B + A)^*$ in either order. When $B$ is bounded we also have $A^*B^* = (BA)^*$. In this case the order is important.

It is difficult to give a general definition of commuting operators. If one of the operators is bounded then there is a good definition. We say that a bounded operator $B$ *commutes* with an operator $A$ if $BA \subset AB$.

Some motivation for this definition comes from taking the case when $B = A^{-1}$ is bounded. Then $A^{-1}A \subset AA^{-1} = 1$.

If $B$ is bounded and $B$ commutes with $A$, then $B$ commutes with $A^{-1}$.

If $B$ is bounded and $B$ commutes with $A$, then $B^*$ commutes with $A^*$. (The proof is an easy computation. Since $BA \subset AB$, it follows that $(AB)^* \subset (BA)^*$. It follows that $B^*A^* \subset (AB)^* \subset (BA)^* = A^*B^*$.)

## 11.3 Hermitian operators

We want to give a more profound analysis of self-adjointness. For this we want to see how an operator can fail to be self-adjoint. This leads to the concept of Hermitian operator.

The *numerical range* of an operator is the set of all $\langle \psi, A\psi \rangle$ with $\psi$ in $D(A)$ and $\|\psi\| = 1$.

**Proposition 32** *Assume that $z$ is a distance $d > 0$ from the numerical range of $A$. Then and*

$$\|(A - z)^{-1}\psi\| \leq 1/d\|\psi\| \tag{11.9}$$

*for all $\psi$ in $R(A - z)$.*

Proof: For unit vectors $\psi$ in the domain of $A$ we have

$$d \leq |\langle \psi, A\psi \rangle - z| = |\langle \psi, (A - z)\psi \rangle| \leq \|(A - z)\psi\|. \tag{11.10}$$

The *spectrum* of an operator $A$ is the set of numbers $z$ such that it is false that $(A - z)^{-1}$ is a bounded operator defined on the entire Hilbert space.

**Corollary 9** *Assume that $z$ is a distance $d > 0$ from the numerical range of $A$. Assume also that $R(A-z) = \mathcal{H}$. Then $z$ is not in the spectrum of $A$.*

We write $A \subset B$ and say $A$ is a *restriction* of $B$ or $B$ is an *extension* of $A$ if the graphs satisfy $A \subset B$

Note that if $A \subset B$, then $B^* \subset A^*$.

A densely defined operator is said to be *Hermitian* if $A \subset A^*$. Notice that the closure $\bar{A}$ is also a Hermitian operator.

**Proposition 33** *Let $A$ be a Hermitian operator. Then the numerical range is real.*

We shall now see that for a Hermitian operator, if the spectrum is real, then the operator is self-adjoint. In fact, all that is needed is a pair of complex conjugate numbers $z$ and $z^*$ that are not in the spectrum.

**Theorem 25** *Let $A$ be a Hermitian operator such that $R(A-z) = \mathcal{H}$ and $R(A-z^*) = \mathcal{H}$. Then $A$ is self-adjoint.*

Proof: We have $A - z \subset A^* - z$. Since $R(A-z^*) = \mathcal{H}$, its adjoint $(A-z^*)^* = A^* - z$ is one-to-one. Since $R(A-z) = \mathcal{H}$, the only possibility is that $A - z = A^* - z$. But then $A = A^*$.

**Corollary 10** *Let $A$ be a Hermitian operator such that $R(A-z) = \mathcal{H}$ for some real $z$. Then $A$ is self-adjoint.*

Now we can give a perturbation theorem that is better than the one given before.

**Theorem 26** *Let $A$ be a self-adjoint operator with domain $D(A)$. Let $B$ be a self-adjoint operator such that $D(A) \subset D(B)$. Assume that for some pair of complex conjugate $z$ not in the spectrum of $A$ we have $\|B(A-z)^{-1}\| < 1$. Then $A + B$ is self-adjoint.*

Proof: It is clear that $A + B$ is Hermitian. In order to show that the range $R(A+B-z) = \mathcal{H}$ it is clearly sufficient to show that $(A+B-z)^{-1}$ is a bounded operator. However

$$(A+B-z)^{-1} = (A-z)^{-1}\left(1 + B(A-z)^{-1}\right)^{-1}. \tag{11.11}$$

The inverse on the right is given by a convergent geometric series in the operator $-B(A-z)^{-1}$. Q.E.D.

This series is often called a Neumann series or a Born series. In this particular context, when we are interested in the existence and uniqueness of dynamics, but not in a detailed description, we only need the series for $z$ far away from the spectrum.

The previous theorem on perturbations by bounded operators is a corollary.

**Corollary 11** *Let $A$ be a self-adjoint operator with domain $D(A)$. Let $B$ be a bounded self-adjoint operator. Then $A + B$ is self-adjoint.*

Proof: The norm of $(A-z)^{-1}$ may be made arbitrarily small by taking $z$ far enough away from the spectrum of $A$. Q.E.D.

## 11.4 Operator perturbation

We want to apply this to Schrödinger operators of the type arising in the Hydrogen problem [K]. Take $|v(\mathbf{x})| \leq c/r$, where $r = |\mathbf{x}|$ is the distance from the origin. Then it is not necessary that $v$ be bounded.

Let $H_0 = \mathbf{P}^2/(2m)$ and $V = v(\mathbf{Q})$. We wish to show that $H = H_0 + V$ is self-adjoint.

For this we use the local uncertainty principle bound

$$\langle\psi, \frac{1}{r^2}\psi\rangle \leq \frac{4}{(\nu-2)^2\hbar^2}\langle\psi, \mathbf{P}^2\psi\rangle \tag{11.12}$$

of the next section. This bound is valid whenever the dimension $\nu \geq 3$. It says that the expectation of $1/r^2$ is bounded by the expectation of the square of the momentum.

From this we immediately obtain the estimate

$$\langle\psi, \frac{1}{r^2}\psi\rangle \leq \frac{8m}{(\nu-2)^2\hbar^2}\langle\psi, H_0\psi\rangle \tag{11.13}$$

Finally we have the trivial estimate $(H_0 - b)^2 \geq 0$ which may be written $2bH_0 \leq (H_0 + b)^2$. This gives the second order estimate

$$\langle\psi, \frac{1}{r^2}\psi\rangle \leq \frac{1}{2b}\frac{8m}{(\nu-2)^2\hbar^2}\langle\psi, (H_0+b)^2\psi\rangle \tag{11.14}$$

which may be rewritten in terms of norms as

$$\|\frac{1}{r}\psi\|^2 \leq \frac{1}{2b}\frac{8m}{(\nu-2)^2\hbar^2}\|(H_0+b)\psi\|^2. \tag{11.15}$$

It follows easily that by taking $b > 0$ large enough we may arrange that the operator $(1/r)(H_0 + b)^{-1}$ has arbitrarily small norm. In particular we can arrange that $V(H_0 + b)^{-1}$ has norm less than one. This is enough to show that $D(H_0) \subset D(V)$ and that $H = H_0 + V$ is self-adjoint.

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# Chapter 12

# Uncertainty Principles

The self-adjoint operators representing quantum mechanical observables do not commute. This is the ultimate origin of all the uncertainty principles. Such principles say that the probability distributions of these observables cannot be simultaneously concentrated on a scale measured by Planck's constant $\hbar$.

The Heisenberg uncertainty principle $\Delta P \Delta Q \geq \hbar/2$ is the most famous but not the most useful uncertainty principle. In this chapter we also present local uncertainty principles that are much more powerful. Some of these are useful for deriving estimates. This subject is surveyed in more detail elsewhere [7].

## 12.1 Expectations and Variances

Let $A$ be a self-adjoint operator representing an observable. Let $\psi$ be a unit vector that determines a state. Then $A$ is isomorphic to multiplication by $\alpha$ on $L^2(X, \mu)$ and $\psi$ corresponds to some $W\psi$ in $L^2(X, \mu)$. We have

$$\Pr_{\psi}[A \in S] = \int_{\{x|\alpha(x)\in S\}} |W\psi(x)|^2 \, d\mu(x). \tag{12.1}$$

The *expectation* of $A$ in the state $\psi$ is the average of the values of $A$ weighted by the probability that $A$ has these values. Thus the expectation is

$$\langle A \rangle_{\psi} = \langle \psi, A\psi \rangle = \int \alpha(x) |W\psi(x)|^2 \, d\mu(x). \tag{12.2}$$

The integral defining the expectation converges absolutely whenever $|\alpha|^{1/2} W\psi$ is in $L^2$, that is $\psi$ is in $D(|A|^{1/2})$.

**Definition 21** *If $A$ is a self-adjoint operator, then its quadratic form domain $Q(A)$ is defined to be $D(|A|^{1/2})$. The quadratic form of $A$ is defined for $\psi$ in $Q(A)$ by the above integral and is denoted $\langle \psi, A\psi \rangle$ for all $\psi$ in $Q(A)$.*

Note that strictly speaking one should write the quadratic form as $\langle |A|^{1/2}\psi, \mathrm{sign}(A)|A|^{1/2}\psi \rangle$, but this is so clumsy to read that the form in the definition is preferred.

The *second moment* of $A$ in the state $\psi$ is the average of the values of $A^2$ weighted by the probability that $A$ has these values. Thus the second moment is

$$\langle A^2 \rangle_\psi = \|A\psi\|^2 = \int \alpha(x)^2 |W\psi(x)|^2 \, d\mu(x). \tag{12.3}$$

The integral defining the second moment converges absolutely whenever $\alpha W\psi$ is in $L^2$, that is $\psi$ is in $D(A)$.

Let $A$ be a self-adjoint operator and let $\psi$ be a state. Write $\langle A \rangle$ for the expectation of $A$ in this state. The *variance* $(\Delta A)^2$ in the state $\psi$ is defined for $\psi$ in $D(A)$ by

$$(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \|(A - \langle A \rangle)\psi\|^2 = \int (\alpha(x) - \langle A \rangle)^2 |W\psi(x)|^2 \, d\mu(x). \tag{12.4}$$

The *standard deviation* $(\Delta A)$ is the square root of the variance.

Note that $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$, so that $(\Delta A)^2 \leq \langle A^2 \rangle$.

## 12.2 The Heisenberg uncertainty principle

**Theorem 27** *The Heisenberg uncertainty principle*

$$\Delta P \Delta Q \geq \frac{\hbar}{2} \tag{12.5}$$

*is valid in every state.*

Proof: The Heisenberg commutation relation says that $PQ - QP = -i\hbar$. Let $P' = P - \langle P \rangle$ and $Q' = Q - \langle Q \rangle$. Then $P'$ and $Q'$ also satisfy the commutation relation. Thus

$$\langle P'\psi, Q'\psi \rangle - \langle Q'\psi, P'\psi \rangle = -i\hbar. \tag{12.6}$$

This may be rewritten

$$\Im \langle P'\psi, Q'\psi \rangle = \frac{\hbar}{2}. \tag{12.7}$$

Since $P$ and $Q$ are the closures of their restrictions to smooth functions with rapid decrease, this equation is valid for all $\psi$ in both $D(P)$ and $D(Q)$. The Schwarz inequality gives

$$\frac{\hbar}{2} = \Im\langle P'\psi, Q'\psi\rangle \leq |\langle P'\psi, Q'\psi\rangle| \leq \|P'\psi\|\|Q'\psi\| = \Delta P \Delta Q, \tag{12.8}$$

which is the theorem.

**Problems**

1. Find all states $\psi$ in which $\Delta P \Delta Q = \hbar/2$. Hint: Show that $Pf = zQf$ and then that $z = ic$ for some $c > 0$. Solve the resulting differential equation (in the Schrödinger representation).

## 12.3 The local uncertainty principle: dimension one

We now come to another uncertainty principle that is less symmetric but more powerful that the Heisenberg principle.

**Theorem 28** *Let $S$ be a set of measure $b$. Then in every state*

$$\Pr[Q \in S] \leq \frac{b\Delta P}{\hbar}. \tag{12.9}$$

Proof: We work in the Schrödinger representation for the pair $P - \langle P\rangle, Q$, so that $P - \langle P\rangle = -i\hbar d/dx$ and $Q$ is multipication by $x$. We have

$$\Pr[Q \in S] = \int_S |f(x)|^2\, dx. \tag{12.10}$$

Thus we must estimate $g(x) = f(x)^2$. We may write

$$2g(x) = \int_{-\infty}^{x} g'(t)\, dt - \int_{x}^{\infty} g'(t)\, dt. \tag{12.11}$$

Hence for each $x$ we have the estimate

$$2|g(x)| \leq \int_{-\infty}^{\infty} |g'(t)|\, dt. \tag{12.12}$$

It follows that for every $x$ we have

$$2|f(x)|^2 \leq \int_{-\infty}^{\infty} 2|f'(t)||f(t)|\, dt \leq 2\|f'\|\|f\| = 2\|(P - \langle P\rangle)f\| = \frac{2\Delta P}{\hbar}. \tag{12.13}$$

Thus

$$\Pr[Q \in S] = \int_S |f(x)|^2 \, dx \leq \frac{\Delta P}{\hbar} \int_S dx = \frac{\Delta P}{\hbar} b. \tag{12.14}$$

The local uncertainty principle is more powerful than the Heisenberg uncertainty principle. The latter says that if $\Delta P$ is small, then $\Delta Q$ is large, that is, it is probable that $Q$ has a wide range of values. The local uncertainty principle says something more: It is improbable that $Q$ is concentrated near some point. The fact that this is stronger follows form an elementary inequality from probability theory: Chebyshev's inequality.

**Proposition 34** *Let $c > 0$. Let $g$ be an increasing function. Then*

$$\Pr[A \geq c] \leq \frac{\langle g(A) \rangle}{g(c)}. \tag{12.15}$$

The following corollary is obtained by taking replacing $A$ by $|A - \langle A \rangle|$ and taking $g(u) = u^2$ for $u \geq 0$.

**Corollary 12** *Let $c > 0$. Then*

$$\Pr[|A - \langle A \rangle| \geq c] \leq \frac{(\Delta A)^2}{c^2}. \tag{12.16}$$

Now assume that we have operators $P$ and $Q$ for which the local uncertainty principle

$$\Pr[|Q - \langle Q \rangle| \leq b/2] \leq \frac{b \Delta P}{\hbar}. \tag{12.17}$$

is satisfied. If combine this with Chebyshev's inequality

$$\Pr[|Q - \langle Q \rangle| \geq b/2] \leq \frac{4(\Delta Q)^2}{b^2} \tag{12.18}$$

we obtain

$$1 - \frac{b \Delta P}{\hbar} \leq \frac{4(\Delta Q)^2}{b^2}. \tag{12.19}$$

Choose $b = \hbar/(2\Delta P)$. Then we obtain

$$\frac{\hbar}{4\sqrt{2}} \leq \Delta P \Delta Q. \tag{12.20}$$

This is not quite the Heisenberg uncertainty principle, because the constant is wrong. But it is qualitatively an inequality of the same kind. The point is that it is difficult to imagine that one could reverse the derivation and derive something like the local uncertainty principle from the Heisenberg uncertainty principle.

## 12.4 The local uncertainty principle: dimension three

There is a particularly useful form of the local uncertainty principle in dimension three or greater.

**Theorem 29** *Let $\nu \geq 3$. Let $r = |\mathbf{x}|$ be the distance form the origin. Then in every state $\psi$ we have the inequality*

$$\frac{(\nu-2)^2\hbar^2}{4}\langle\psi, \frac{1}{r^2}\psi\rangle \leq \langle\psi, \mathbf{P}^2\psi\rangle. \tag{12.21}$$

This looks more like an uncertainty principle when one writes it in the form

$$\frac{(\nu-2)\hbar}{2} \leq \langle\psi, \mathbf{P}^2\psi\rangle^{\frac{1}{2}}\langle\psi, r^{-2}\psi\rangle^{-\frac{1}{2}}. \tag{12.22}$$

Notice the corollary

$$\Pr[r \leq a] \leq a^2\frac{4}{(\nu-2)^2\hbar^2}\langle\psi, \mathbf{P}^2\psi\rangle. \tag{12.23}$$

which follows immediately using Chebyshev's inequality. The important thing to note is that in every dimension $\nu \geq 3$ the probability of being near a given point goes to zero quadratically as one approaches the point.

Proof: It is sufficient to prove the result

$$\frac{(\nu-2)^2}{4}\langle\psi, \frac{1}{r^2}\psi\rangle \leq \langle\frac{\partial}{\partial r}\psi, \frac{\partial}{\partial r}\psi\rangle. \tag{12.24}$$

For every real $\beta$ compute

$$\|(\frac{\partial}{\partial r} + \beta\frac{1}{r})\psi\|^2 = \|\frac{\partial}{\partial r}\psi\|^2 + \frac{\beta^2 - (\nu-2)\beta}{r^2}. \tag{12.25}$$

Take $\beta = (\nu-2)/2$. Q.E.D.

This local uncertainty principle shows that when $v(\mathbf{x}) \geq -c/r^2$ for some sufficiently small constant $c$, then Hamiltonian $H = \mathbf{P}^2/(2m) + v(\mathbf{Q})$ is bounded below. Thus rather severe negative local singularities are allowed.

There are more general criteria in which the condition is that $v$ be in some $L^p$ space (that $|v|^p$ be integrable) for suitable $p$. These are usually called *Sobolev inequalities*. It is remarkable that these Sobolev inequalities may be deduced from the local uncertainty principle given here [6].

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