CHAPTER

4 Foundations of quantum mechanics

de Broglie's Ansatz, the basis of Schrödinger's equation, operators, complex numbers and functions, momentum, free particle wavefunctions, expectation values

We return to the starting points of quantum mechanics and how to motivate Schrödinger's equation. The advances in the quantum mechanics of radiation by Planck and Einstein guided pioneers applying quantum mechanics to matter. We follow that route below and find that the operators which emerge require complex numbers. We thus first review imaginary numbers. We shall see that quantum mechanics is an intrinsically complex subject; ψ has in general both real and imaginary parts. We wander off into the complex plane and appreciate that momentum, free particles and their currents, and dynamics (Chapter 5) all require a complex ψ. Important problems such as barrier penetration and tunnelling become accessible to us.

4.1 Mathematical preliminaries — Complex numbers

What number, when squared, gives -1? We define the number i (alluding to *i*maginary) to have this property:

$$\mathrm{i}^2 = -1 \quad \text{or equivalently} \quad \sqrt{-1} = \mathrm{i}. \tag{4.1}$$

Imaginary numbers are not confined to have size 1, but can take a continuum of values $\mathrm{i}I$ where I is a real number in the interval $-\infty$ to $+\infty$.

The imaginary axis is conventionally drawn vertically, the real horizontally. When we combine real and imaginary numbers, $z = R + \mathrm{i}I$, we get complex numbers, z, which sit in the complex plane and are sometimes written $z = x + \mathrm{i}y$ for obvious reasons[1]; see the picture Fig. 4.1 of this plane, known as an Argand diagram. One might reasonably ask — are there still further

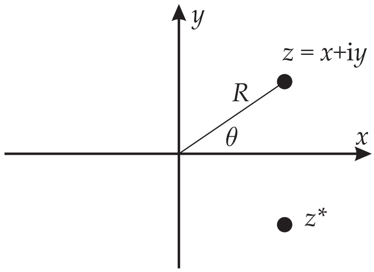

Figure 4.1: The complex plane of points $z = x + \mathrm{i}y$, with absolute value or modulus R, and with complex conjugate z^*. The angle θ is the phase or argument of z; see Eq. (4.8).

types of numbers? There are, for instance quaternions, octonions, Grassmanns, ..., but one can prove that extending reals to imaginary numbers is sufficient for our purposes here. A function can take complex values too, so for instance $\psi(x) = \psi_R(x) + \mathrm{i}\psi_I(x)$ is broken down into its real and imaginary parts ψ_R and ψ_I (both real functions of x, but ψ_I is accompanied by i when in ψ). As we shall soon see, functions can also take complex arguments.

The usual rules of algebra apply:

$$z^2 = (x + \mathrm{i}y)(x + \mathrm{i}y) = x^2 - y^2 + 2\mathrm{i}xy \tag{4.2}$$
$$zz' = (x + \mathrm{i}y)(x' + \mathrm{i}y') = xx' - yy' + \mathrm{i}(x'y + xy'). \tag{4.3}$$

The $-$ in front of y^2 and yy' is from $\mathrm{i}^2 = -1$. One gets a good feeling for complex numbers by placing them in the complex plane:

Exercise 4.1: Put the following numbers onto a complex plane diagram: i, $-1, -\mathrm{i}, 1 + \mathrm{i}, \frac{1}{\mathrm{i}}, \frac{1+\mathrm{i}}{\sqrt{2}}, \left(\frac{1+\mathrm{i}}{\sqrt{2}}\right)^2, \left(\frac{-1+\mathrm{i}}{\sqrt{2}}\right)^2$.
Hint: Some of these will require some evaluation before plotting. In particular get the imaginary numbers into the numerator by multiplying fractions

[1] It is sometimes conventional in engineering to use j rather than i.

top and bottom by the same suitable number. What does plotting the final two tell you about $\sqrt{}$ on the complex plane?

The size or magnitude of a complex number is its distance from the origin (much like the length of a radius vector, but in the complex plane). For $x + \mathrm{i}y$, the radius vector is $\sqrt{x^2 + y^2}$ (Pythagoras). It is called the modulus of (sometimes called the absolute value of) z, written $|z|$. Confirm that the square of this distance is $|z|^2 = x^2 + y^2$ which can be written $(x + \mathrm{i}y)(x - \mathrm{i}y)$. When every i in z is replaced by $-\mathrm{i}$, the result is called $z^* = x - \mathrm{i}y$, and is known as the *complex conjugate* of z. Thus the modulus squared is $|z|^2 = zz^*$ and, from the above, is guaranteed to be real. For instance:

$$\psi\psi^* = |\psi|^2 = (\psi_\mathrm{R} + \mathrm{i}\psi_\mathrm{I})(\psi_\mathrm{R} - \mathrm{i}\psi_\mathrm{I}) = \psi_\mathrm{R}^2 + \psi_\mathrm{I}^2. \tag{4.4}$$

Note that $(z^*)^* = z$.

Exercise 4.2: What are the moduli of the numbers in Ex. 4.1? You may need to reconsider your drawing in that exercise!
Solution: 1, 1, 1, $\sqrt{2}$, 1, 1, 1, 1.

Two useful properties of z are

$$z + z^* = 2x \qquad z - z^* = 2\mathrm{i}y \tag{4.5}$$

$$x = \frac{1}{2}(z + z^*) \qquad y = \frac{1}{2\mathrm{i}}(z - z^*)\,, \tag{4.6}$$

which are good routes to the real and imaginary parts that are needed below.

Exercise 4.3: If z is a complex number, what is the modulus and phase of $Z = \frac{z}{z^*}$ in terms of those of z?

Complex exponentials

Let us revisit the differential equation of the SHM type

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi, \tag{4.7}$$

with the general solution $\psi = A\sin(kx) + B\cos(kx)$. We have repeatedly noticed the tantalising similarity between this equation and the exponential type of equation with $k^2 \to -k^2$, that is to $\frac{d^2\psi}{dx^2} = k^2\psi$ with $\psi = Ce^{kx} + De^{-kx}$ in general. We could try complex exponentials $e^{\pm ikx}$ in Eq. (4.7). Twice differentiating the exponential gives $(\pm ik)^2 e^{\pm ikx} = -k^2 e^{\pm ikx}$, and thus $e^{\pm ikx}$ are also solutions to the SHM equation. But since (4.7) is a second order differential equation, there are at most two independent solutions and hence the $e^{\pm ikx}$ must be combinations of $\sin(kx)$ and $\cos(kx)$.

Exercise 4.4: Prove that $\cos u = \frac{1}{2}\left(e^{iu} + e^{-iu}\right)$ and $\sin u = \frac{1}{2i}\left(e^{iu} - e^{-iu}\right)$.

Solution: In the first potential well problems, we fixed the constants weighting the two components to ψ by fitting to a boundary condition. Here we fix the weights of e^{iu} and e^{-iu} in $\cos u$ by checking that their combination is such that it reproduces $\cos 0 = 1$. This is trivially true since $e^0 = 1$ and thus at $u = 0$ we have $\frac{1}{2}(1+1) = 1$. The combination in $\sin u$ must also be correct since differentiating sin gives cos and differentiating $\left(e^{iu} - e^{-iu}\right)$ gives $i\left(e^{iu} + e^{-iu}\right)$ which on dividing by 2i yields the expression for cos.

Exercise 4.5: Show $e^{iu} = \cos u + i \sin u$ and $e^{-iu} = \cos u - i \sin u$.

Exercise 4.6: Draw on the complex plane the position of $z = Re^{i\theta}$ for $\theta = 0$, $\pi/4$, $\pi/2$, $3\pi/4$, π, 2π. Clearly R is the modulus (prove $|z|^2 = R^2$) while θ is known as the argument (or phase) of z, sometimes written $\arg(z)$. For a given θ draw in z^* (reflection is involved). What is the argument of z^*?

It is made explicit by Ex. 4.6 and by the expression $e^{iu} = \cos u + i \sin u$ that e^{iu} is function periodic in u, with period 2π, quite unlike e^u.

Exercise 4.7: Draw the trajectory of $z(t) = e^{i\omega t}$ on the complex plane. What is the motion of $x(t)$ and $y(t)$ on the real and imaginary axes? How long is one period, T.

Solution: The complex number $z = \cos(\omega t) + i \sin(\omega t)$ has unit modulus, so as t evolves, z moves around the unit circle uniformly. Since $e^{2\pi i} = 1$ (the argument 2π takes us back to where we started), then the period must be such that $\omega T = 2\pi$, that is, $T = 2\pi/\omega$.

The real and imaginary parts of $e^{i\omega t}$ are out of phase with each other, for instance when $\cos(\omega t) = 1$, then $\sin(\omega t) = 0$ and *vice versa*. In fact the two parts, which are the projections of the circular motion onto the x and

y axes, are like simple harmonic oscillations. The argument of z, that is ωt here, gives the phase of the motion.

Evaluating the phase (argument) of complex numbers

We have seen that the modulus $|z|$ of the complex number $z = Re^{i\theta}$ is R. Writing $z = R(\cos\theta + i\sin\theta)$ we have $\mathrm{Re}(z) = R\cos(\theta)$ and $\mathrm{Im}(z) = R\sin(\theta)$ where $\mathrm{Re}(z)$ is the real part of z and $\mathrm{Im}(z)$ is the imaginary part. Taking their ratio eliminates R and gives $\tan\theta = \mathrm{Im}(z)/\mathrm{Re}(z)$, a result we shall later find useful (and which is useful in any part of physics where phases arise). Note that if the imaginary part of z is zero, $\mathrm{Im}(z) = 0$, that is we have a real number, then the argument is zero. An equivalent expression for the argument is:

$$\arg(z) = \tan^{-1}\left(\frac{\mathrm{Im}(z)}{\mathrm{Re}(z)}\right). \tag{4.8}$$

Use for instance Eqs. (4.5–4.6) to get the real and imaginary parts to put in the expression (4.8). See Fig. 4.1 for $\theta = \arg(z)$. Clearly, $\arg(z^*) = -\theta$.

Hyperbolic functions

We have seen that $\sin x$ and $\cos x$ can be expressed in terms of complex exponentials. Indeed, they can be seen as the definitions of the trigonometric functions. Because the combination of the sum and difference of real exponentials also appears very often, they are given a special name — the hyperbolic functions. So, we define the functions

$$\sinh x = \frac{1}{2}\left(e^x - e^{-x}\right) \tag{4.9}$$

$$\cosh x = \frac{1}{2}\left(e^x + e^{-x}\right) \tag{4.10}$$

$$\tanh x = \frac{\sinh x}{\cosh x} = \frac{e^x - e^{-x}}{e^x + e^{-x}} \tag{4.11}$$

with $\mathrm{sech}(x)$ and $\mathrm{cosech}(x)$ being the reciprocals of $\cosh(x)$ and $\sinh(x)$ respectively. The complex exponentials for the trigonometrical functions[2] are replaced by real exponentials. These functions are plotted in Fig. 4.2. Accordingly, many trigonometrical identities carry over but with possible sign changes.

[2]Trigonometrical functions are also referred to as *circular* functions because they describe parametrically a circle. Similiarly, hyperbolic functions describe hyperbolae.

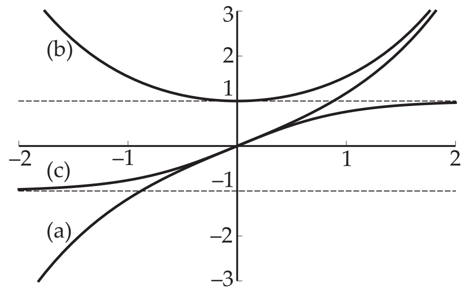

Figure 4.2: The hyperbolic functions (a) $\sinh(x)$, (b) $\cosh(x)$ and (c) $\tanh(x)$. Note which are even and which are odd functions, and that the asymptotes of $\tanh(x)$ are ± 1.

Exercise 4.8: Show that the hyperbolic functions are related to the trigonometrical ones by

$$\begin{aligned}
\sinh x &= -\mathrm{i}\sin(\mathrm{i}x), \\
\cosh x &= \cos(\mathrm{i}x), \\
\tanh x &= -\mathrm{i}\tan(\mathrm{i}x),
\end{aligned}$$

and the equivalent of the Pythagorean identity is

$$\cosh^2 x - \sinh^2 x = 1.$$

Show also that

$$\mathrm{sech}^2 x = 1 - \tanh^2 x.$$

Exercise 4.9: Find the derivatives of $\sinh x$, $\cosh x$ and $\tanh x$. What is the asymptotic (large argument, positive and negative) behaviour of $\sinh(x)$ and $\cosh(x)$?

Exercise 4.10: Show that $\int \frac{dx}{\sqrt{x^2-1}} = \cosh^{-1} x$, and $\int \frac{dx}{\sqrt{1+x^2}} = \sinh^{-1} x$. In particular compare the latter result with the last part of Ex. 1.19, and see the dynamics problem Ex. 4.32.

Exercise 4.32: Another classical problem: Consider a particle with energy E incident from $x < 0$ on a potential $V(x) = 0$ for $x < 0$ and $V(x) =$

$-\frac{1}{2}V_0(x/d)^2$ for $x > 0$. Show the time taken to reach a position $x_0 > 0$ from $x = 0$ is $t_0 \propto \sinh^{-1}\left(\sqrt{\frac{V_0}{2E}}\frac{x_0}{d}\right)$. Give the constant of proportionality. Examine the small time variation of position and how x_0 increases for large times.