

Lecture 5

B. Zwiebach
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1 Equations for a wavefunction

We determined that the wavefunction or de Broglie wave for a particle with momentum p and energy E is given by

$$\Psi(x, t) = e^{i(kx - \omega t)}, \quad (1.1)$$

where ω and k are determined from

$$p = \hbar k, \quad E = \hbar\omega, \quad E = \frac{p^2}{2m} \quad (1.2)$$

The wavefunction (1.1) represents a state of definite momentum. It is then of interest to find an operator that extracts that information from the wavefunction. The operator must be, roughly, a derivative with respect to x , as this would bring down a factor of k . In fact more precisely, we take

$$\begin{aligned} \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi(x, t) &= \frac{\hbar}{i} (ik) \Psi(x, t) \\ &= \hbar k \Psi(x, t) \\ &= p \Psi(x, t) \end{aligned} \quad (1.3)$$

where the p factor in the last right-hand side is just the momentum. We thus identify the operator $\frac{\hbar}{i} \frac{\partial}{\partial x}$ as the *momentum operator* \hat{p}

$$\boxed{\hat{p} \equiv \frac{\hbar}{i} \frac{\partial}{\partial x}} \quad (1.4)$$

and we have verified that acting on the wavefunction $\Psi(x, t)$ for a particle of momentum p it gives p times the wavefunction:

$$\hat{p} \Psi = p \Psi. \quad (1.5)$$

The momentum operator it acts on wavefunctions, which are functions of space and time to give another function of x and t . Since \hat{p} on Ψ gives a number (p , in fact) times Ψ we say

that Ψ is an **eigenstate** of \hat{p} . The matrix algebra analogy is useful: matrices are the operators and column vectors are the states. Matrices act by multiplication on column vectors. An eigenvector of a matrix is a special vector. The matrix acting on an eigenvector gives a number times the eigenvector. After the action of the matrix the direction of the vector is unchanged but its magnitude can be scaled. The same for eigenstates of operators: an operator acting on an eigenstate gives the eigenstate up to a multiplicative constant. We also say that Ψ is a state of **definite momentum**.

Let us now consider extracting the energy information from the free particle wavefunction. This time we must avail ourselves of the time derivative:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = i\hbar(-i\omega)\Psi(x, t) = \hbar\omega \Psi(x, t) = E \Psi(x, t). \quad (1.6)$$

It would seem plausible to say that the time derivative $i\hbar \frac{\partial}{\partial t}$ is an energy operator but, for a free particle the energy is given in terms of the momentum, so we can construct the relevant energy operator by working on the above right-hand side

$$E\Psi = \frac{p^2}{2m}\Psi = \frac{p}{2m}p\Psi = \frac{p}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi, \quad (1.7)$$

where we used equation (1.5) to write $p\Psi$ as the momentum operator acting on Ψ . Since p is a constant we can move the p factor on the last right-hand side close to the wavefunction and then replace it by the momentum operator:

$$E\Psi = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} p\Psi = \frac{1}{2m} \frac{\hbar}{i} \frac{\partial}{\partial x} \frac{\hbar}{i} \frac{\partial}{\partial x} \Psi. \quad (1.8)$$

This can be written as

$$E\Psi = \frac{1}{2m} \hat{p} \hat{p} \Psi = \frac{\hat{p}^2}{2m} \Psi, \quad (1.9)$$

which suggests the following definition of the energy operator \hat{E} :

$$\hat{E} \equiv \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}. \quad (1.10)$$

Indeed, for our free particle wavefunction, (1.9) shows that $E\Psi = \hat{E}\Psi$.

Our work also allows us to find an differential equation for which our de Broglie wavefunction is a solution. Consider (1.6) and replace the right hand side $E\Psi$ by $\hat{E}\Psi$ giving us

$$\boxed{i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t).} \quad (1.11)$$

This is the free-particle Schrödinger equation. More schematically, using the energy operator, it can be written as

$$\boxed{i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{E} \Psi(x, t).} \quad (1.12)$$

It is worth re-checking that our de Broglie wavefunction satisfies the Schrödinger equation (1.11). Indeed for $\Psi = e^{i(kx-\omega t)}$ we find

$$i\hbar(-i\omega)\Psi = -\frac{\hbar^2}{2m}(ik)^2\Psi \quad (1.13)$$

which is a solution since the Ψ factors cancel and all that is needed is the equality

$$\hbar\omega = \frac{\hbar^2 k^2}{2m}, \quad (1.14)$$

which is recognized as the familiar relation $E = \frac{p^2}{2m}$.

Note that the Schrödinger equation admits more general solutions than the de Broglie wavefunction for a particle of definite momentum and definite energy. Since the equation is linear, any superposition of plane wave solutions with different values of k is a solution. Take for example

$$\Psi(x, t) = e^{i(k_1 x - \omega_1 t)} + e^{i(k_2 x - \omega_2 t)} \quad (1.15)$$

This is a solution, and note that while each summand corresponds to a state of definite momentum, the total solution is not a state of definite momentum. Indeed

$$\hat{p}\Psi(x, t) = \hbar k_1 e^{i(k_1 x - \omega_1 t)} + \hbar k_2 e^{i(k_2 x - \omega_2 t)}, \quad (1.16)$$

and the right hand side cannot be written as a number times Ψ . The full state is not a state of definite energy either. The general solution of the free Schrödinger equation is the most general superposition of plane waves:

$$\Psi(x, t) = \int_{-\infty}^{\infty} dk \Phi(k) e^{i(kx - \omega(k)t)}, \quad (1.17)$$

where $\Phi(k)$ is an *arbitrary* function of k that controls the superposition and we have written $\omega(k)$ to emphasize that ω is a function of the momentum, as in (1.14).

Exercise. Verify that Ψ in (1.17) solves the free Schrödinger equation.

We now have the tools to time-evolve any initial wavefunction. Namely, given the initial wavefunction $\Psi(x, 0)$ of any packet at time equal zero, we can obtain $\Psi(x, t)$. Indeed, using Fourier transformation one can write

$$\Psi(x, 0) = \int dk \Phi(k) e^{ikx}, \quad (1.18)$$

where $\Phi(k)$ is the Fourier transform of $\Psi(x, 0)$. But then, the time evolution simply consists in adding the exponential $e^{-i\omega(k)t}$ to the integral, so that the answer for the time evolution is indeed given by (1.17).

As we have discussed before, the velocity of a wave packet described by (1.17) is given by the group velocity evaluated for the dominant value of k . We confirm that this is indeed reasonable

$$v_g \equiv \frac{\partial\omega}{\partial k} = \frac{\partial\hbar\omega}{\partial\hbar k} = \frac{\partial E}{\partial p} = \frac{\partial}{\partial p} \left(\frac{p^2}{2m} \right) = \frac{p}{m}, \quad (1.19)$$

which is the expected velocity for a free non-relativistic particle with momentum p and mass m .

The Schrödinger equation has an explicit i on the left-hand side. This i shows that it is impossible to find a solution for real Ψ . If Ψ were real the right-hand side of the equation would be real but the left-hand side would be imaginary. Thus, the Schrödinger equation forces us to work with complex wavefunctions.

Note also that the Schrödinger equation does not take the form of a conventional wave equation. A conventional wave equation for a variable ϕ takes the form

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{1}{V^2} \frac{\partial^2 \phi}{\partial t^2} = 0. \quad (1.20)$$

The general solutions of this linear equation are $f_{\pm}(x \pm Vt)$. This would certainly allow for real solutions, which are not acceptable in quantum theory. The Schrödinger equation has no second-order time derivatives. It is first-order in time!

2 Schrödinger Equation for particle in a potential

Suppose now that our quantum particle is not free but rather is moving in some external potential $V(x, t)$. In this case, the total energy of the particle is no longer simply kinetic, it is the sum of kinetic and potential energies:

$$E = \frac{p^2}{2m} + V(x, t), \quad (2.1)$$

This naturally suggests that the energy operator should take the form

$$\hat{E} = \frac{\hat{p}^2}{2m} + V(x, t). \quad (2.2)$$

The first term, as we already know, involves second derivatives with respect to x . The second term acts multiplicatively: acting on any wavefunction $\Psi(x, t)$ it simply multiplies it by $V(x, t)$. We now postulate that the Schrödinger equation for a particle in a potential takes the form (1.12) with \hat{E} replaced by the above energy operator:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \Psi(x, t). \quad (2.3)$$

The energy operator \hat{E} is usually called the **Hamiltonian** operator \hat{H} , so one has

$$\hat{H} \equiv -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t), \quad (2.4)$$

and the Schrödinger equation takes the form

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \hat{H} \Psi(x, t). \quad (2.5)$$

Let us reconsider the way in which the potential $V(x, t)$ is an operator. We can do this by introducing a **position** operator \hat{x} that acting on functions of x gives another function of x as follows:

$$\hat{x}f(x) \equiv xf(x). \quad (2.6)$$

Note that it follows from this equation and successive applications of it that

$$\hat{x}^k f(x) \equiv x^k f(x). \quad (2.7)$$

If the potential $V(x, t)$ can be written as some series expansion in terms of x it then follows that

$$V(\hat{x}, t)\Psi(x, t) \equiv V(x, t)\Psi(x, t). \quad (2.8)$$

The operators we are dealing with (momentum, position, Hamiltonian) are all declared to be linear operators. A **linear operator** \hat{A} satisfies

$$\hat{A}(a\phi) = a\hat{A}\phi, \quad \hat{A}(\phi_1 + \phi_2) = \hat{A}\phi_1 + \hat{A}\phi_2, \quad (2.9)$$

where a is a constant. Two linear operators \hat{A} and \hat{B} that act on the same set of objects can always be added $(\hat{A} + \hat{B})\phi \equiv \hat{A}\phi + \hat{B}\phi$. They can also be multiplied, the product $\hat{A}\hat{B}$ is a linear operator defined by $\hat{A}\hat{B}\phi \equiv \hat{A}(\hat{B}\phi)$, meaning that you act first with \hat{B} , which is closest to ϕ and then act on the result with \hat{A} . The order of multiplication matters and thus $\hat{A}\hat{B}$ and $\hat{B}\hat{A}$ may not be the same operators. To quantify this possible difference one introduces the **commutator** $[A, B]$ of two operators, defined to be the linear operator

$$\boxed{[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.} \quad (2.10)$$

If the commutator vanishes, the two operators are said to commute. It is also clear that $[\hat{A}, \hat{A}] = 0$ for any operator \hat{A} .

We have operators \hat{x} and \hat{p} that are clearly somewhat related. We would like to know their commutator $[\hat{x}, \hat{p}]$. For this we let $[\hat{x}, \hat{p}]$ act on some arbitrary function $\phi(x)$ and then attempt simplification. Let's do it.

$$\begin{aligned} [\hat{x}, \hat{p}]\phi(x) &= (\hat{x}\hat{p} - \hat{p}\hat{x})\phi(x) = \hat{x}\hat{p}\phi(x) - \hat{p}\hat{x}\phi(x) \\ &= \hat{x}(\hat{p}\phi(x)) - \hat{p}(\hat{x}\phi(x)) \\ &= \hat{x}\left(\frac{\hbar}{i}\frac{\partial\phi(x)}{\partial x}\right) - \hat{p}(x\phi(x)) \\ &= x\frac{\hbar}{i}\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\phi(x)) \\ &= \frac{\hbar}{i}x\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}x\frac{\partial\phi(x)}{\partial x} - \frac{\hbar}{i}\phi(x) \\ &= -\frac{\hbar}{i}\phi(x) = i\hbar\phi(x), \end{aligned} \quad (2.11)$$

so that, all in all, we have shown that for arbitrary $\phi(x)$ one has

$$[\hat{x}, \hat{p}]\phi(x) = i\hbar\phi(x). \quad (2.12)$$

Since this equation holds for any ϕ it really represents the equality of two operators. Whenever we have $\hat{A}\phi = \hat{B}\phi$ for arbitrary ϕ we simply say that $\hat{A} = \hat{B}$. The operators are the same because they give the same result acting on anything! We have therefore discovered the most fundamental commutation relation in quantum mechanics:

$$\boxed{[\hat{x}, \hat{p}] = i\hbar.} \quad (2.13)$$

The right hand side is a number, but should be viewed as an operator (acting on any function it multiplies by the number). This commutation relation can be used to prove Heisenberg's uncertainty principle, which states that the product of the position uncertainty and the momentum uncertainty must always exceed $\hbar/2$.

The idea that operators can fail to commute may remind you of matrix multiplication, which is also non-commutative. We thus have the following correspondences:

$$\begin{aligned} \text{operators} &\leftrightarrow \text{matrices} \\ \text{wavefunctions} &\leftrightarrow \text{vectors} \\ \text{eigenstates} &\leftrightarrow \text{eigenvectors} \end{aligned} \quad (2.14)$$

One can in fact formulate Quantum Mechanics using matrices, so these correspondences are actually concrete and workable.

As an example of useful matrices that do not commute, consider the Pauli matrices, three two-by-two matrices given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.15)$$

Actually these matrices are exactly what is needed to consider spin one-half particles. The spin operator \mathbf{S} has three components $S_i = \frac{\hbar}{2}\sigma_i$. Let us now see if σ_1 and σ_2 commute.

$$\begin{aligned} \sigma_1\sigma_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \\ \sigma_2\sigma_1 &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} \end{aligned} \quad (2.16)$$

We then see that

$$[\sigma_1, \sigma_2] = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2i\sigma_3 \quad (2.17)$$

In fact, one also has $[\sigma_2, \sigma_3] = 2i\sigma_1$ and $[\sigma_3, \sigma_1] = 2i\sigma_2$.

Matrix mechanics, was worked out in 1925 by Werner Heisenberg and clarified by Max Born and Pascual Jordan. Note that, if we were to write \hat{x} and \hat{p} operators in matrix form, they would require infinite dimensional matrices. One can show that there are no finite size matrices that commute to give a number times the identity matrix, as is required from (2.13). This shouldn't surprise us: on the real line there are an infinite number of linearly independent wavefunctions, and in view of the correspondences in (2.14) it would suggest an infinite number of basis vectors. The relevant matrices must therefore be infinite dimensional.

Two basic properties of the Schrödinger equation

1. The differential equation is first order in time. This means that for an initial condition it suffices to know the wavefunction completely at some initial time t_0 and the Schrödinger equation then determines the wave function for all times. This can be understood very explicitly. If we know $\Psi(x, t_0)$ for all x then the right-hand side of the Schrödinger equation, which just involves x derivatives and multiplication, can be evaluated at any point x . This means that at any point x we know the time-derivative of the wavefunction (left-hand side of the Schrödinger equation) and this allows us to calculate the wavefunction a little time later.
2. Linearity and superposition. The Schrödinger equation is a linear equation for complex wavefunctions. Therefore, given two solutions Ψ_1 and Ψ_2 , we can form new solutions as linear combinations $\alpha\Psi_1 + \beta\Psi_2$ with complex coefficients α and β .

We have written the Schrödinger equation for a particle on a one-dimensional potential. How about for the case of a particle in a three-dimensional potential? As we will see now, this is easily done once we realize that in three dimensions the position and momentum operators have several components! Recall that the de Broglie wavefunction

$$\Psi(\mathbf{x}, t) = e^{i(\mathbf{k}\cdot\mathbf{x}-\omega t)} = e^{i(k_x x + k_y y + k_z z - \omega t)} \quad (2.18)$$

corresponds to a particle carrying momentum $\mathbf{p} = \hbar\mathbf{k}$, with $\mathbf{k} = (k_x, k_y, k_z)$. Just as we did in (1.3) we can try to extract the vector momentum by using a differential operator. The relevant operator is the gradient:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \quad (2.19)$$

with which we try

$$\frac{\hbar}{i} \nabla \Psi(x, t) = \frac{\hbar}{i} (ik_x, ik_y, ik_z) \Psi(x, t) = \hbar \mathbf{k} \Psi(x, t) = \mathbf{p} \Psi(x, t). \quad (2.20)$$

We therefore define the momentum operator $\hat{\mathbf{p}}$ as follows:

$$\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla. \quad (2.21)$$

If we call the momentum components $(p_1, p_2, p_3) = (p_x, p_y, p_z)$ and the coordinates as $(x_1, x_2, x_3) = (x, y, z)$ then we have that the components of the above equation are

$$\hat{p}_k = \frac{\hbar}{i} \frac{\partial}{\partial x_k}, \quad k = 1, 2, 3. \quad (2.22)$$

Just like we defined a position operator \hat{x} , we now have three position operators $(\hat{x}_1, \hat{x}_2, \hat{x}_3)$ making up $\hat{\mathbf{x}}$. With three position and three momentum operators, we now should state the nine possible commutation relations. If you recall our derivation of $[\hat{x}, \hat{p}] = i\hbar$ you will note that the commutator vanishes unless the superscripts on \hat{x} and \hat{p} are the same. This means that we have

$$[\hat{x}_i, \hat{p}_j] = i\hbar \delta_{ij}, \quad (2.23)$$

where the Kronecker delta is defined by

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases} \quad (2.24)$$

In order to write now the general Schrödinger equation we need to consider the kinetic energy operator, or the Hamiltonian:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{x}, t), \quad (2.25)$$

This time

$$\hat{\mathbf{p}}^2 = \hat{\mathbf{p}} \cdot \hat{\mathbf{p}} = \frac{\hbar}{i} \nabla \cdot \frac{\hbar}{i} \nabla = -\hbar^2 \nabla^2 \quad (2.26)$$

where ∇^2 is the Laplacian operator

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}. \quad (2.27)$$

The Schrödinger equation finally takes the form

$$i\hbar \frac{\partial}{\partial t} \Psi(\mathbf{x}, t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{x}, t) \right) \Psi(\mathbf{x}, t). \quad (2.28)$$

3 Interpreting the Wavefunction

Schrödinger thought that the wavefunction Ψ represents a particle that could spread out and disintegrate. The *fraction* of the particle to be found at x would be proportional to the magnitude of $|\Psi|^2$. This was problematic, as noted by Max Born (1882-1970). Born solved the Schrödinger equation for scattering of a particle in a potential, finding a wavefunction that fell like $1/r$, with r the distance to the scattering center. But Born also noticed that in the experiment one does not find fractions of particles going in many directions but rather particles remain whole. Born suggested a probabilistic interpretation. In his proposal,

The wavefunction $\Psi(x, t)$ doesn't tell us how much of the particle is at position x at time t but rather the probability that upon measurement taken at time t we would find the particle at position x .

To make this precise we use an infinitesimal volume element with volume $d^3\mathbf{x}$ centered around some arbitrary point \mathbf{x} . The probability dP to find the particle within the volume element $d^3\mathbf{x}$ at time t is

$$dP = |\Psi(\mathbf{x}, t)|^2 d^3\mathbf{x}. \quad (3.1)$$

Consistency requires that the total probability to find the particle *somewhere* in the whole space is unity. Thus the integral of dP over all of space must give one:

$$\int_{\text{all space}} d^3\mathbf{x} |\Psi(\mathbf{x}, t)|^2 = 1 \quad (3.2)$$

Next time we will explore the consistency of this equation with time evolution.

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

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