The Principles, Formulation and Mathematical Tools of Quantum Mechanics

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• http://www.cmi.ac.in/~govind These are brief notes for lectures at the above Workshop. Please let me know (govind@cmi.ac.in) of any comments or corrections. updated: 5 Jul, 2020.

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Lecture 4: Probability conservation, Ehrenfest theorem, Dispersion of a wave packet, Schrödinger and Heisenberg pictures.

• Here are some books on quantum mechanics.

1. E Wichmann, Quantum Physics, Berkeley Physics Course, Vol 4.
2. R P Feynman, R B Leighton and M Sands, Feynman Lectures on Physics, Vol 3.
3. H S Mani and G K Mehta, Introduction to Modern Physics.
4. B Dutta-Roy, Elements of Quantum Mechanics.
5. J J Sakurai and J J Napolitano, Modern Quantum Mechanics, 2nd Ed.
6. L I Schiff, Quantum Mechanics, 3rd Ed. McGraw-Hill (1968).
7. P J E Peebles, Quantum Mechanics, Princeton Univ Press (1992).

8. B H Bransden and C J Joachain, Quantum Mechanics, 2nd Ed., Pearson (2000).
9. D J Griffiths, Introduction to Quantum Mechancis.
10. R L Liboff, Introductory Quantum Mechancis.
11. R Shankar, Principles of Quantum Mechanics, 2nd Ed. Plenum Press (1994).
12. P M Mathews and K Venkatesan, A textbook of quantum mechanics, Tata McGraw-Hill (1977).
13. P A M Dirac, The principles of quantum mechanics, 4th Ed., Oxford (1958).
14. W Heitler, Elementary wave mechanics with applications to Quantum Chemistry.
15. L D Landau and E M Lifshitz, Quantum mechanics: Non-relativistic theory, 3rd Edition.
16. G Esposito, G Marmo and E C G Sudarshan, From Classical to Quantum Mechanics: An Introduction to the Formalism, Foundations and Applications, Cambridge Univ Press (2010).

2 Formulation of classical mechanics

• The set of possible instantaneous locations of a classical particle is called its configuration space. This is usually three dimensional Euclidean space $\mathbb{R}^3$. The number of coordinates needed to specify the instantaneous configuration of a system is the number of degrees of freedom. A system consisting of a pair of particles has 6 degrees of freedom $x_1, y_1, z_1, x_2, y_2, z_2$, its configuration space is $\mathbb{R}^3 \times \mathbb{R}^3 = \mathbb{R}^6$. A particle attached to a fixed support by a rod of fixed length has two degrees of freedom, its configuration space is a sphere. The configuration space and number of degrees of freedom are kinematical notions. They do not depend on the nature of forces between the particles.

• If the forces acting on/between the particles are known, then we may determine the dynamical time evolution of the system by solving Newton's equations for the trajectories. For one particle, $m\ddot{\mathbf{r}} = \mathbf{F}$. Newton's equations are second order in time, they require two sets of initial conditions, the initial positions $\mathbf{r}(0)$ and initial velocities $\dot{\mathbf{r}}(0)$. In other words, the initial coordinates $\mathbf{r}(0)$ and initial momenta $\mathbf{p}(0) = m\dot{\mathbf{r}}(0)$ determine the future trajectory. We say that the instantaneous **state** of the system is specified by giving the coordinates and momenta of all the particles. The set of possible instantaneous states of a system is its **phase space**. For a particle moving along a line, its phase space is the $x - p$ phase plane. Newton's equations may be formulated as Hamilton's 1st order equations for the time evolution of coordinates and momenta

$$\dot{x} = \frac{\partial H}{\partial p} \quad \text{and} \quad \dot{p} = -\frac{\partial H}{\partial x}. \tag{1}$$

For a particle in a potential $H(x,p) = \frac{p^2}{2m} + V(x)$ and Hamilton's equations are a pair of first order equations

$$\dot{x} = \frac{p}{m} \quad \text{and} \quad \dot{p} = -\frac{dV}{dx}, \tag{2}$$

which may be written as a single second order equation expressing Newton's second law $m\ddot{x} = -V'(x)$. The curve in phase space $(x(t), p(t))$ is called the phase trajectory. Draw the phase portrait for a free particle as well as for a simple harmonic oscillator, indicating the direction of trajectories. A dynamical variable that is constant along trajectories is called a constant of motion. Its value may differ from trajectory to trajectory. The hamiltonian $H = T + V$ is a conserved quantity for conservative systems (i.e. where the force is the negative gradient of a scalar potential).

• Dynamical variables like angular momentum and the hamiltonian are functions of the basic dynamical variables position and momentum. In general, any real function of position and momentum is called an observable. Observables are simply real-valued functions on phase space. They must be real since observables are physical quantities that may be measured.

3 States and observables in quantum mechanics

3.1 Hilbert space of states of a quantum system

• States of a quantum system are vectors in a linear space ("vector space") called a complex Hilbert space $\mathcal{H}$. For a particle moving on a line, its configuration space is $\mathbb{R}^1$, parametrized by one coordinate x. Its quantum state space $\mathcal{H} = L^2(\mathbb{R})$ is the space of square-integrable functions $\psi(x)$ on the classical configuration space. ψ is called the state function or state vector or wave function of the particle.

• By Born's probability postulate, $|\psi(x)|^2 dx$ is interpreted as the probability of finding the particle between x and $x + dx$. Since the total probability of the particle being somewhere should be one, we normalize the wave function $\int_0^\infty |\psi(x)|^2 dx = 1$. This is why we restrict to square-integrable wave functions. $\psi(x)$ itself is called a **probability amplitude**, its square is a probability density.

• Unlike the classical space of states (phase space) which can be a non-linear manifold (e.g. if a particle is constrained to move on a circle), the quantum Hilbert space is always a linear space. The sum of two states $\psi + \phi$ is a possible state and so is a complex multiple $c\psi$ of any state. This is the principle of linear superposition of states, used to explain the interference of matter waves in the double slit experiment.

• A complex Hilbert space $\mathcal{H}$ is a vector space over the complex numbers. It is a space of ket vectors $|\psi\rangle$ closed under linear superposition. If $|\psi\rangle$ and $|\chi\rangle$ are state vectors, then so is $\alpha|\psi\rangle + \beta|\chi\rangle$, for any $\alpha, \beta \in \mathbb{C}$. A simple example is the two dimensional complex vector space of spin states of a spin half particle which are usually denoted as column vectors $|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ in a suitable basis. Notably, the space of states of a quantum system is a complex, rather than a real vector space.

• The quantum state space is equipped with an inner or dot product. The inner product of a pair of vectors ψ, χ is denoted $\langle\psi|\chi\rangle$. For the spin-$\frac{1}{2}$ Hilbert space, the inner product is

$$\langle\psi|\chi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}^\dagger \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \begin{pmatrix} \psi_1^* & \psi_2^* \end{pmatrix} \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \psi^\dagger \chi = \psi_1^* \chi_1 + \psi_2^* \chi_2. \qquad (3)$$

$\psi^\dagger$ is called the hermitian adjoint, it is the complex conjugate transpose, it is a row vector. So associated with a vector space of colummn/ket vectors there is a 'dual' space of row/bra vectors, the adjoints of the kets $|\psi\rangle^\dagger = \langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* \end{pmatrix}$. The inner product may also be regarded as producing a complex number from a ket vector $|\chi\rangle$ and the bra vector dual/adjoint to $|\psi\rangle$: $\langle\psi|\chi\rangle$. However, the inner product of a non-zero vector with itself is always a positive real number $\langle\psi|\psi\rangle > 0$, it is called the square of the length of the vector.

• Another example is n-dimensional complex vector space $\mathbb{C}^n$ with the inner product $\langle u|v\rangle = \sum_i u_i^* v_i$. The Hilbert space of a particle moving on a line is $L^2(\mathbb{R})$ with $\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x) g(x)\, dx$.

- From these examples (keep $\langle u|v\rangle = u_i^* v_i$ in mind) we abstract the basic properties of the inner product (these are its defining properties in an axiomatic approach)

$$\langle \alpha u|v\rangle = \alpha^* \langle u|v\rangle, \quad \langle u|\beta v\rangle = \beta\langle u|v\rangle, \quad \langle u+v|w\rangle = \langle u|w\rangle + \langle v|w\rangle, \quad \langle u|v\rangle^* = \langle v|u\rangle. \qquad (4)$$

$\langle u|v\rangle$ is linear in the second vector v and anti-linear in the first vector u on account of complex conjugation of the components of the first vector.

- The norm/length of a vector is $||v|| = \sqrt{\langle v|v\rangle}$. The norm of a vector is unchanged upon multiplying by a phase $e^{i\alpha}$. If $\langle u|v\rangle = 0$ then the vectors are orthogonal.

- Two state vectors that differ by multiplication by a non-zero complex number $\psi_2(x) = c\psi_1(x)$ represent the **same physical state**. We often work with unit norm states.

- A basis for the Hilbert space is a set of vectors $|e_i\rangle$ such that any vector $|v\rangle$ may be expressed as a linear combination of $|e_i\rangle$ in a unique way. The number of basis vectors is the dimension of the vector space. The standard basis vectors of the two dimensional spin Hilbert space $\mathbb{C}^2$ are

$$|e_1\rangle = \begin{pmatrix}1\\0\end{pmatrix}, \quad |e_2\rangle = \begin{pmatrix}0\\1\end{pmatrix}, \quad \text{so} \quad \begin{pmatrix}v_1\\v_2\end{pmatrix} = v_1|e_1\rangle + v_2|e_2\rangle. \qquad (5)$$

The coefficients v_i in the expansion $|v\rangle = \sum_i v_i|e_i\rangle$ are called the components of $|v\rangle$. The components of the adjoint are the complex conjugates: $\langle v| = \sum_i \langle e_i|v_i^*$. [We will often drop the summation symbol and assume repeated indices are summed.] E.g. the adjoints of the basis vectors are row bra-vectors

$$\langle e_1| = e_1^\dagger = \begin{pmatrix}1 & 0\end{pmatrix}, \quad \langle e_2| = e_2^\dagger = \begin{pmatrix}0 & 1\end{pmatrix}. \qquad (6)$$

$\mathbb{C}^n$ is an n-dimensional vector space. The state space of a particle moving on a line, $L^2(\mathbb{R})$ is infinite dimensional, it is called a function space. It is intuitively clear that this is an infinite dimensional space since the values of the function $\psi(x)$ at each $x \in \mathbb{R}$ can be freely specified (subject to normalizability). x here plays the role of the index $i = 1, 2$ in the two dimensional spin-half vector space $\mathbb{C}^2$. A possible basis for a function space is the set of monomials $\{1, x, x^2, x^3, x^4, \cdots\}$. Indeed, any function ψ that has a Taylor series around $x = 0$ admits a expression as a linear combination of these. The coefficients are the derivatives of ψ at $x = 0$:

$$\psi(x) = \psi(0) + \psi'(0)x + \frac{1}{2}\psi''(0)x^2 + \frac{1}{3!}\psi'''(0)x^3 + \cdots \qquad (7)$$

However this basis of monomials is a bit inconvenient. The basis vectors are not orthogonal, in fact they are not even normalizable with respect to the above L^2 inner product. A more convenient basis for $L^2(\mathbb{R})$ consists of the energy eigenstates of the harmonic oscillator $|n\rangle$.

- It is often convenient to work with an orthonormal (o.n.) basis, i.e., a basis of vectors $|e_i\rangle$ which are pairwise orthogonal and each normalized to have unit norm, $\langle e_i|e_j\rangle = \delta_{ij}$. The standard basis $|e_i\rangle$ for $\mathbb{C}^n$ with components $|e_i\rangle_j = \delta_{ij}$ is orthonormal with respect to the usual inner product $\langle u|v\rangle = \sum_i u_i^* v_j$.

- A set of orthonormal vectors is said to be a complete orthonormal set if it forms a basis for the vector space, i.e., if we may write any vector as a linear combination.

3.2 Linear operators, Adjoint, (anti-)Hermitian and Unitary operators

An observable A in quantum mechanics (e.g. hamiltonian, position, momentum, angular momentum, spin, magnetic moment) is a hermitian (self-adjoint) linear operator on the Hilbert space of states $\mathcal{H}$. Hermiticity is the quantum analogue of classical observables being real-valued functions. We will see that a hermitian operator has real eigenvalues, which are possible results when A is measured. To define a hermitian operator, we first note that a linear operator on a vector space takes vectors to vectors in a linear way: $A(a|\psi\rangle + b|\chi\rangle) = aA|\psi\rangle + bA|\chi\rangle$. When A acts on a vector $|v\rangle$ it produces a new ket vector $A|v\rangle$ which is also denoted $|Av\rangle$.

• A linear operator is an abstract concept, whose concrete realisation is a matrix. A linear operator on $\mathbb{C}^2$ is simply a 2×2 matrix, once we choose a basis to represent it. For example, the Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are linear operators represented as matrices in the standard basis for $\mathbb{C}^2$.

• If $|e_j\rangle$ are a basis for $\mathcal{H}$, then a linear operator A is determined by how it acts on the basis vectors. Since A takes vectors to vectors, $A|e_j\rangle$ must be a linear combination of the basis vectors themselves

$$A|e_j\rangle = \sum_k |e_k\rangle A_{kj}. \tag{8}$$

A_{kj} are the components of A in this basis, they may be written as entries in a matrix, with A_{kj} occupying the slot in the k^{th} row and j^{th} column. The vector that makes up the first column A_{k1} is the 'image' of e_1 (i.e. coefficients in the linear combination appearing in $A|e_1\rangle$), the second column A_{k2} is the image of e_2 and so on.

• If the basis e_i is orthonormal $\langle e_i|e_j\rangle = \delta_{ij}$, then we have

$$\langle e_i|A|e_j\rangle = \sum_k \langle e_i|e_k\rangle A_{kj} = \sum_k \delta_{ik} A_{kj} = A_{ij}. \tag{9}$$

We say that A_{ij} are the matrix elements of A between the o.n. basis states e_i and e_j.

• A matrix A is hermitian if it equals its own complex conjugate transpose. The latter is called its adjoint $A^\dagger = (A^*)^t$. So A is hermitian if $A = A^\dagger$, i.e., if it is self-adjoint. In terms of matrix entries, $A_{ij}^* = A_{ji}$. In particular, the diagonal entries of a hermitian matrix are real, while the off diagonal entries are complex conjugates of each other. The Pauli matrices are hermitian. Note that the adjoint of a product is the product of adjoints in the opposite order. $(AB)^\dagger = B^\dagger A^\dagger$ and that $(A|\psi\rangle)^\dagger = \langle\psi|A^\dagger$. We also denote $A|\psi\rangle = |A\psi\rangle$, so that $|A\psi\rangle^\dagger = \langle A\psi|$.

• The concept of hermiticity makes sense for a linear operator, even if we have not represented it explicitly as a matrix by choosing a basis. To explain the concept, we need the idea of matrix elements between states. If u, v are a pair of states, then $\langle u|A|v\rangle$ is called the **matrix element** of A between the states u and v. To know an operator is to know its matrix elements.

• The **adjoint** of A is the operator $A^\dagger$ defined via its matrix elements $\langle u|A^\dagger|v\rangle = \langle Au|v\rangle = \langle v|Au\rangle^*$. So if we know the matrix elements of A, then we may find the matrix elements of $A^\dagger$. A linear operator is **hermitian** if $\langle u|Av\rangle = \langle Au|v\rangle$ for all states $u, v \in \mathcal{H}$. A hermitian operator is also called symmetric by mathematicians since it does not matter whether A is written on the left or on the right.

• Now, let us see how this abstract definition of hermiticity reduces to the formula $A_{ij} = A_{ji}^*$

for hermitian matrices. We must equate the matrix elements of A and those of $A^\dagger$. Let e_i be an orthonormal basis, then the matrix element of A between the states e_i and e_j is just A_{ij}, as is seen by taking the inner product of the above equation with e_i

$$\langle e_i|A|e_j\rangle = \sum_k \langle e_i|e_k\rangle A_{kj} = \sum_k \delta_{ik} A_{kj} = A_{ij}. \tag{10}$$

On the other hand, what are the matrix elements of $A^\dagger$? By the definition of the adjoint,

$$\langle e_i|A^\dagger e_j\rangle = \langle Ae_i|e_j\rangle = \langle e_j|Ae_i\rangle^* = (A_{ji})^* \tag{11}$$

So a linear operator is self-adjoint if its matrix elements in an o.n. basis satisfy $A_{ij} = (A_{ji})^*$.

• An anti-hermitian operator is one that satisfies $A^\dagger = -A$. A unitary operator is one whose inverse is its adjoint, $UU^\dagger = U^\dagger U = I$. It is clear that the identity I is hermitian as well as unitary. If A is anti-hermitian, then iA is hermitian since $(iA)^\dagger = A^\dagger i^\dagger = -A(-i) = A$.

3.3 Outer products of vectors and completeness relation

• **Outer products of vectors:** Consider the vector space $\mathbb{C}^n$ with standard basis $|e_i\rangle$. Just as we may multiply row and column n-vectors to get a scalar inner product, we may also form their 'outer' product (column times a row), to get an $n\times n$ matrix. For $n=2$ show that

$$|e_1\rangle\langle e_1| = e_1 e_1^\dagger = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \quad |e_2\rangle\langle e_2| = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}, \quad |e_1\rangle\langle e_2| = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}, \quad |e_2\rangle\langle e_1| = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}. \tag{12}$$

More generally, check that $|e_i\rangle\langle e_j|$ is a matrix with a 1 in the ij-entry and 0's elsewhere. From this we see that a matrix whose entries are A_{ij} in the i^{th} row and j^{th} column, can be expressed as

$$A = \sum_{ij} A_{ij} |e_i\rangle\langle e_j| \tag{13}$$

Now let us use this expression to find how a matrix acts on a vector $v = v_k|e_k\rangle$. We get using the associativity of multiplication of operators (freedom to place brackets)

$$Av = \sum_{ij} A_{ij}\ |e_i\rangle\langle e_j|v_k|e_k\rangle = A_{ij} v_k |e_i\rangle\langle e_j|e_k\rangle = A_{ij} v_k \delta_{jk} |e_i\rangle = A_{ik} v_k |e_i\rangle. \tag{14}$$

So the i^{th} component of Av is $\sum_k A_{ik} v_k$.

• In particular, the identity operator I, may be expressed as

$$I = \sum_i |e_i\rangle\langle e_i| = \sum_{ij} \delta_{ij} |e_i\rangle\langle e_j| \tag{15}$$

The identity operator has the components δ_{ij} in any basis since it takes every vector to itself. This 'resolution' of the identity operator as a sum of outer products of a set of orthonormal basis vectors is called the **completeness relation**. It is quite useful in many physical problems and calculations. E.g. the energy eigenstates of the Harmonic oscillator form a complete orthonormal set and satisfy the above completeness relation. Coherent states for the harmonic oscillator also satisfy a completeness relation even though they are not orthogonal and are in fact an over-complete set.

• In the Hilbert space of a spin half particle $\mathbb{C}^2$, we have the basis vectors $|\uparrow\rangle$ and $|\downarrow\rangle$ which we will interpret as states where the z-component of spin S_z has the values $\pm\hbar/2$. Then $S_z = \hbar/2(|\uparrow\rangle\langle\uparrow| - |\uparrow\rangle\langle\uparrow|$. The raising and lowering operators are

$$S_+ = \hbar|\uparrow\rangle\langle\downarrow| \quad \text{and} \quad S_- = \hbar|\downarrow\rangle\langle\uparrow|. \tag{16}$$

Justify the names of $S_\pm$ by analysing how they act on $|\uparrow\rangle$ and $|\downarrow\rangle$.

3.4 Hermiticity of position and momentum operators

• Physically interesting examples of hermitian operators for a particle with one degree of freedom moving on a line include the position operator $\hat{x}\psi(x) = x\psi(x)$, and momentum operator $\hat{p}\psi(x) = -i\hbar\psi'(x)$. Check that $\hat{x}^\dagger = \hat{x}$ and $\hat{d} = \frac{\partial}{\partial x}$ is anti-hermitian. We must show $\langle f|\hat{x}g\rangle = \langle \hat{x}f|g\rangle$ for any two states f, g. This is seen as follows:

$$\langle f|\hat{x}g\rangle = \int f^*(x)xg(x)\,dx = \int (xf(x))^*g(x)\,dx = \langle \hat{x}f|g\rangle. \tag{17}$$

Showing hermiticity of $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ requires integration by parts. Let us show that $\hat{d} = \frac{\partial}{\partial x}$ is anti-hermitian, from which it will follow that $\hat{p} = -i\hbar\hat{d}$ is hermitian. Let us denote complex conjugate of f by $\bar{f}$ here for convenience

$$\langle f|\hat{d}g\rangle = \int \bar{f}(x)g'(x)dx = -\int \bar{f}'(x)g(x)\,dx + \left[\bar{f}g\right]_{-\infty}^{\infty} = -\langle \hat{d}f|g\rangle. \tag{18}$$

Here we assumed f, g vanish at $\pm\infty$, which is the case for square-integrable functions. Boundary conditions play an important role in determining the hermiticity of momentum. If we have a particle moving on a finite interval $[a, b]$ (as in a square well), then

$$\langle f|\hat{d}g\rangle = \int_a^b \bar{f}(x)g'(x)dx = -\int_a^b \bar{f}'(x)g(x)\,dx + \left[\bar{f}g\right]_a^b = -\langle \hat{d}f|g\rangle + \left[\bar{f}g\right]_a^b. \tag{19}$$

For $\hat{d}$ to be anti-hermitian, the boundary term must vanish. This happens, for instance, if the functions vanish at the end points ($f(a) = f(b) = 0$, as in an infinite square well) or satisfy 'periodic boundary conditions' $f(a) = f(b)$.

3.5 Expectation values

• Of particular importance is the concept of **expectation value** of an observable A in a state ψ, which is defined as the normalized diagonal matrix element of A in the state ψ

$$\langle A\rangle_\psi = \frac{\langle\psi|A\psi\rangle}{\langle\psi|\psi\rangle} \tag{20}$$

The expectation value of a hermitian operator in any state is a real number. For, by hermiticity, and $\langle u|v\rangle = \langle v|u\rangle^*$, we have

$$\langle\psi|A\psi\rangle = \langle A\psi|\psi\rangle = \langle\psi|A\psi\rangle^* \tag{21}$$

In other words, the diagonal matrix element of A is equal to its own complex conjugate. We are familiar with this: the diagonal entries of a hermitian matrix in an orthonormal basis $\langle e_i|A|e_i\rangle = A_{ii}$ are real.

• It follows from the reality of expectation values of a hermitian operator that the eigenvalues (to be introduced shortly) of a hermitian operator are also real. In fact, the eigenvalues are simply the expectation values in the corresponding eigenstates.

3.6 Commutators of operators

• Multiplication of matrices/operators is in general not commutative $AB \neq BA$ (in general). The amount by which they fail to commute is called the commutator $[A,B] = AB - BA$. Any operator commutes with itself or any power of itself $[A, A^n] = A^{n+1} - A^{n+1} = 0$. On the other hand, check that $xp - px = [x,p] = i\hbar I$ by acting on a state $\psi(x)$:

$$xp\psi = -i\hbar x\psi'(x), \quad \text{while} \quad px\psi = -i\hbar\frac{\partial}{\partial x}(x\psi) = -i\hbar x\psi'(x) - i\hbar\psi(x) \quad \Rightarrow \quad [x,p]\psi = i\hbar\psi. \tag{22}$$

• x and p are said to be canonically conjugate observables. In QM, the commutator plays the role that the Poisson bracket plays in CM. Just as the Poisson bracket $\{f,g\}$ of two observables is another observable, $\frac{1}{i\hbar}[A,B]$ is again an observable (i.e., hermitian) if A, B are hermitian. To show this it suffices to check that $[A,B]$ is anti-hermitian if A and B are hermitian.

$$([A,B])^\dagger = (AB - BA)^\dagger = B^\dagger A^\dagger - A^\dagger B^\dagger = BA - AB = -[A,B]. \tag{23}$$

An important property of the commutator is the product or Leibnitz rule, check that

$$[A, BC] = [A,B]C + B[A,C]. \tag{24}$$

• In three dimensions, we have three coordinate and momentum operators x, y, z and $p_x = -i\hbar\frac{\partial}{\partial x}, p_y = -i\hbar\frac{\partial}{\partial y}, p_z = -i\hbar\frac{\partial}{\partial z}$. It is easily seen that the momenta commute with each other and the coordinates commute among themselves, more over $[x, p_x] = i\hbar$ while $[x, p_y] = 0$ etc. These so-called **Heisenberg canonical commutation relations** may be summarised as $[x_i, p_j] = i\hbar\,\delta_{ij}$.

3.7 Eigenvalue problem for hermitian operators

• The **eigenvalue problem** for a linear operator (hermitian or not) is the equation $A|\psi\rangle = \lambda|\psi\rangle$. A non-zero vector $|\psi\rangle \neq 0$ that satisfies this equation for some complex number λ is called an eigenvector of A with eigenvalue λ. Taking the adjoint of the eigenvalue equation we also have

$$(A|\psi\rangle)^\dagger = \langle\psi|A^\dagger = \lambda^*\langle\psi| \tag{25}$$

So if $|\psi\rangle$ is an eigen-ket of A with eigenvalue λ, then $\langle\psi|$ is an eigen-bra of $A^\dagger$ with eigenvalue λ^*. In particular, if $A = A^\dagger$ is hermitian, then $\langle\psi|A^\dagger = \langle\psi|A = \lambda^*\langle\psi|$. In other words, if $|\psi\rangle$ is an eigen-ket of A, then $\langle\psi|$ is an eigen-bra of A with eigenvalue λ^*. We will soon show that λ is real if A is hermitian (see also §3.5).

• The eigenstate of the position operator $\hat{x}$ with eigenvalue x' is denoted $|x'\rangle$, i.e., $\hat{x}|x'\rangle = x'|x'\rangle$. We will see that measurement of the position of a particle that is in state $|x'\rangle$ is guaranteed to give the value x'. The 'position-space' or 'coordinate-space' wave function of any state $|\psi\rangle$ is defined as the inner product $\langle x|\psi\rangle = \psi(x)$. It follows that $\psi^*(x) = \langle\psi|x\rangle$.

- Similarly, the eigenvalue problem for momentum is $\hat{p}|k\rangle = \hbar k|k\rangle$. It is conventional to write the momentum eigenvalue in terms of wave number as $\hbar k$. We will see that $|k\rangle$ is a state in which a measurement of the particle's momentum will give $\hbar k$. The momentum space wave function of a particle in state $|\psi\rangle$ is defined as $\tilde{\psi}(k) = \langle k|\psi\rangle$. $\tilde{\psi}$ is pronounced 'psi-tilde'.

- Here are some **useful facts about hermitian matrices/operators**:

1. The eigenvalues of a hermitian operator are real. This is because the eigenvalues of a hermitian operator are simply the (necessarily real) expectation values in the corresponding eigenstates

$$A|\psi\rangle = \lambda|\psi\rangle \quad \Rightarrow \quad \langle\psi|A|\psi\rangle = \langle\psi|\lambda\psi\rangle = \lambda\langle\psi|\psi\rangle \quad \Rightarrow \quad \lambda = \frac{\langle\psi|A|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{26}$$

2. Eigenvectors $|\chi\rangle, |\psi\rangle$ corresponding to distinct (necessarily real) eigenvalues $\mu \neq \lambda$ are orthogonal. To see this, we calculate $\langle\chi|A\psi\rangle$ in two ways using hermiticity and reality of eigenvalues and subtract.

$$\langle\chi|A\psi\rangle = \lambda\langle\chi|\psi\rangle \quad \text{and} \quad \langle\chi|A\psi\rangle = \langle A\chi|\psi\rangle = \langle\psi|A\chi\rangle^* = \mu^*\langle\psi|\chi\rangle^* = \mu\langle\chi|\psi\rangle. \tag{27}$$

   Thus $(\lambda - \mu)\langle\chi|\psi\rangle = 0$. Since $\lambda \neq \mu$ we must have $\langle\chi|\psi\rangle = 0$, i.e., eigenvectors corresponding to distinct eigenvalues are orthogonal.

3. It can be shown that a hermitian operator can be diagonalised by a unitary transformation $U^\dagger H U = \Lambda$ where Λ is a diagonal matrix with eigenvalues along the diagonal. Moreover, the eigenvectors of a hermitian operator can be chosen to form a complete orthonormal basis for $\mathcal{H}$

$$A|\psi_i\rangle = \lambda_i|\psi_i\rangle, \quad \langle\psi_i|\psi_j\rangle = \delta_{ij}, \quad \sum_i |\psi_i\rangle\langle\psi_i| = I, \quad . \tag{28}$$

   Furthermore, two hermitian operators which commute can be simultaneously diagonalised. In other words, there is a basis of common eigenvectors in which both are diagonal. And if they do not commute, as in the case of $[x,p] = i\hbar I$, they cannot be simultaneously diagonalised. Operators that commute are said to be compatible, we will see that they can be simultaneously measured.

4. The eigenvalue problem for the momentum operator is $\hat{p}|k\rangle = \hbar k|k\rangle$. The position space eigenfunction $\langle x|k\rangle$ of the momentum operator is a plane wave. $\hat{p}\psi(x) = \hbar k\psi(x)$ becomes $-i\hbar\psi' = \hbar k\psi$ or $\psi = Ae^{ikx}$. We will choose $A = 1$. In other words $\langle x|k\rangle = e^{ikx}$ and so $\langle k|x\rangle = e^{-ikx}$. Note that $\psi_k(x) = e^{ikx}$ has an infinite norm.

5. The position-space or coordinate-space eigenfunctions of the position operator are delta-functions. Let's see why. The eigenvalue problem is

$$\hat{x}\,\psi(x) = x\psi(x) = \lambda\psi(x) \quad \text{where} \quad \lambda \quad \text{is a constant.} \tag{29}$$

   The only way this can be satisfied for all x is for $\psi(x)$ to vanish at all $x \neq \lambda$. Now if $\psi(x)$ were to vanish at $x = \lambda$ as well, then it would be the zero function and not qualify as a non-trivial eigenvector. The value of $\psi(x)$ at $x = \lambda$ can either be finite or $\psi(\lambda) = \pm\infty$. If $|\psi(\lambda)| < \infty$, then the state will have zero norm and cannot describe a particle that can be found somewhere. So ψ must be infinite at $x = \lambda$. In fact, $\psi(x)$ is proportional to the Dirac delta function. It is normalized so that $\psi(x) = \delta(x - \lambda)$. It is conventional to denote the position eigenvalue by x' rather than λ. So $\delta(x - x')$ is an eigenfunction of the position operator with eigenvalue x', it is a function of x that is zero every where except at x'. Think of it as a limit of functions that are sharply peaked at $x = x'$. Thus the coordinate space wave function of the eigenstate $|x'\rangle$ of $\hat{x}$ is $\langle x|x'\rangle = \delta(x - x')$. Now if we have two position eigenstates $|x'\rangle$ and $|x''\rangle$, then their coordinate space wave functions are $\langle x|x'\rangle = \delta(x - x')$ and $\langle x|x''\rangle = \delta(x - x'')$. Their inner product is

$$\langle x''|x'\rangle = \int \delta(x - x'')\delta(x - x')\, dx = \delta(x' - x''). \tag{30}$$

So position eigenstates are orthogonal and 'delta-normalized'. They form a complete set in the sense that they satisfy a completeness relation

$$\int dx\, |x\rangle\langle x| = I. \tag{31}$$

To see this, take the matrix elements of the LHS between coordinate basis states $|x'\rangle$ and $|x''\rangle$

$$\int dx\, \langle x'|x\rangle\langle x|x''\rangle = \int dx\, \delta(x - x')\delta(x - x'') = \delta(x' - x''). \tag{32}$$

On the other hand, the matrix elements of the identity are also the same $\langle x'|I|x''\rangle = \langle x'|x''\rangle = \delta(x' - x'')$. Since $\int dx\, |x\rangle\langle x|$ and I have the same matrix elements, they are equal.

• Similarly, momentum eigenstates form a complete set

$$\int \frac{dk}{2\pi} |k\rangle\langle k| = I. \tag{33}$$

Check this by evaluating the matrix elements between position basis states $|x'\rangle$ and $|x''\rangle$. On the rhs we get $\langle x'|I|x''\rangle = \delta(x' - x'')$. On the lhs we get the same using the Fourier representation of the delta function

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi}\, \langle x'|k\rangle\langle k|x''\rangle = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ikx'} e^{-ikx''} = \delta(x' - x''). \tag{34}$$

How do we get the last equality? If $x' = x''$ then we are integrating the function 1, and the answer should be infinite, and indeed $\delta(0) = \infty$. On the other hand, when $x' \neq x''$, then we have

$$\int \frac{dk}{2\pi}[\cos(k(x' - x'')) + i\sin(k(x' - x''))] = 0 \tag{35}$$

Since the average value of both the sine and cosine functions is zero.

• Momentum eigenstates with distinct wave numbers are orthogonal (as we expect for the eigenstates of a hermitian operator)

$$\langle k'|k''\rangle = \int dx\, \langle k'|x\rangle\langle x|k''\rangle = \int dx\, e^{-ik'x} e^{ik''x} = 2\pi\, \delta(k' - k''). \tag{36}$$

6. Among hermitian operators, the positive operators are particularly interesting physically. A hermitian operator is positive (or non-negative) if its diagonal matrix element (or expectation value) in *every* state is non-negative $\langle\psi|A|\psi\rangle \geq 0$, for all $\psi \in \mathcal{H}$. Since eigenvalues are simply the expectation values in eigenstates, we see that positive operators have non-negative eigenvalues. If A is any linear operator, then we check that $A^\dagger A$ and $AA^\dagger$ are both hermitian and positive operators.

$$\text{E.g.} \quad (AA^\dagger)^\dagger = A^{\dagger\dagger} A^\dagger = AA^\dagger. \tag{37}$$

To check positivity, we work out the expectation value in any (unit norm) state:

$$\langle\psi|A^\dagger A|\psi\rangle = \langle A\psi|A\psi\rangle = ||A\psi||^2 \geq 0 \quad \text{and} \quad \langle\psi|AA^\dagger|\psi\rangle = \langle A^\dagger\psi|A^\dagger\psi\rangle = ||A^\dagger\psi||^2 \geq 0. \tag{38}$$

An example is kinetic energy $T = \frac{1}{2m}p^2 = \frac{1}{2m}p^\dagger p = \frac{1}{2m}pp^\dagger$, since $p = p^\dagger$ is hermitian. So we may conclude that the energy eigenvalues of a free particle must all be non-negative.

3.8 Measured value of observables in states and interpretation of expectation values

• Measurement of an observable A in state ψ of unit norm produces a real number that is one of the eigenvalues of A. Born's probability postulate: Suppose we have several identically prepared systems in the same unit norm state ψ and we measure the value of A in each system and collect the values. Then the frequency of occurrence of the measured value λ is $p_\lambda = |\langle\psi_\lambda|\psi\rangle|^2$ where ψ_λ is the unit norm eigenstate corresponding to the eigenvalue λ. More generally,

$$p_\lambda = \frac{|\langle\psi_\lambda|\psi\rangle|^2}{||\psi_\lambda||^2||\psi||^2}. \tag{39}$$

• The expectation value of an observable A in a state ψ is the mean value obtained when A is measured on many copies of the system prepared in the same state ψ. How do we see this? Each measurement gives a (possibly different) eigenvalue λ with probability p_λ. So the mean measured value is a sum over the eigenvalues of A (counted with multiplicity)

$$\sum_\lambda p_\lambda \lambda = \sum_\lambda \lambda|\langle\psi|\psi_\lambda\rangle|^2 = \sum_\lambda \lambda\langle\psi|\psi_\lambda\rangle\langle\psi|\psi_\lambda\rangle^* = \sum_\lambda \lambda\langle\psi|\psi_\lambda\rangle\langle\psi_\lambda|\psi\rangle = \sum_\lambda \langle\psi A|\psi_\lambda\rangle\langle\psi_\lambda|\psi\rangle = \langle\psi|A|\psi\rangle. \tag{40}$$

We used the eigenvalue equation and completeness of the normalized eigenvectors $\sum_\lambda |\psi_\lambda\rangle\langle\psi_\lambda| = I$.

• **Physical interpretation** of $\langle x|k'\rangle = e^{ik'x}$ and $\langle x|x'\rangle = \delta(x-x')$ in the context of probability of results of measurements. Suppose a particle is in a position eigenstate $|x'\rangle$. Then its coordinate space wave function is $\langle x|x'\rangle = \delta(x-x')$. Now suppose we make a measurement of its position. Then the probability of getting the value x is $p_x \propto |\langle x|x'\rangle|^2$. Notice that $p_x = 0$ for $x \neq x'$. So if we measure the position of a particle known to be in the position eigenstate $|x'\rangle$, then the only value of position that can result is x' itself.

• Suppose a particle is in a position eigenstate $|x'\rangle$. Then its momentum space wave function is $\langle k|x'\rangle = e^{-ikx'}$. Suppose we make a measurement of its momentum. Then the probability of getting the value $\hbar k$ is $p_k \propto |\langle k|x'\rangle|^2 = |e^{ikx}|^2 = 1$. In other words, all momenta are equally probable. This makes physical sense in light of the Heisenberg uncertainty principle. If the particle is in a position eigenstate, then its position is known with perfect accuracy. So we would expect its momentum to be maximally uncertain. And indeed, what we find is that all possible momenta are equally likely, so we have no knowledge as to what the result of a momentum measurement may give.

• After measuring an observable A and getting the eigenvalue λ, the state of the system 'collapses' from state ψ to eigenstate ψ_λ corresponding to the eigenvalue λ ($A|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$).

• **Reproducibility of measurements:** If A is measured again, soon after a previous measurement of A, then the same value λ will be obtained and the system will remain in the same eigenstate of A. If a system is in an eigenstate $|\psi_0\rangle$ of energy, then we know in advance that measurement of energy will result only in the eigenvalue E_0 and that the state will not change after the measurement.

• If two observables (hermitian operators A, B) commute, they have common eigenvectors and are simultaneously diagonalisable. We say they are simultaneously measurable or compatible. What this means is that if A has been measured, and a value a obtained, then a measurement of B will not affect the eigenstate $|\psi_a\rangle$ of A to which the system had collapsed. This is because $|\psi_a\rangle$ is an eigenstate of B as well. An immediate measurement of B will certainly result in the eigenvalue of B corresponding to the eigenvector ψ_a. A subsequent measurement of A will again result in the value a. It is in this sense that A and B can be simultaneously measured.

• Let us indicate why commuting observables have common eigenfunctions. Suppose A is hermitian and has eigenvalues λ_i (assumed non-degenerate) with corresponding eigenfunctions ψ_i, so $A\psi_i = \lambda_i\psi_i$. Non-degeneracy means that each eigenspace is one dimensional. Now suppose B commutes with A. Then consider $B(A\psi)$, we evaluate it in two ways. On the one hand, $B(A\psi_i) = \lambda_i B\psi_i$. On the other, $BA\psi_i = AB\psi_i$. Thus $A(B\psi_i) = \lambda_i(B\psi_i)$. In other words, both ψ_i and $B\psi_i$ are eigenfunctions of A with the same eigenvalue. Since the eigenspaces of A are assumed one dimensional $B\psi_i$ and ψ_i must be linearly dependent, i.e. multiples of eachother: $B\psi_i = \mu_i\psi_i$. In other words we have shown that an eigenfunction of A is also an eigenfunction of B! What happens if A has a degenerate eigenvalue?

• It is worth noting that measurement of an observable in a state ψ is a complicated process that is still not well-understood, and is certainly not the multiplication of the operator A with the state vector ψ (which would produce a vector rather than a real number).

3.9 Heisenberg uncertainty principle and inequality

• Given an observable A and a unit norm state $|\psi\rangle$, we have the variance of A in the state ψ (or the square of the standard deviation or simply the square of the uncertainty of A)

$$(\Delta A)^2 = \langle\psi|(A - \langle A\rangle)^2|\psi\rangle = \langle A^2\rangle - \langle A\rangle^2 \tag{41}$$

The uncertainty in A measures the spread/width of the distribution of possible measured values of A in the state $|\psi\rangle$. It depends *both* on A and $|\psi\rangle$. If ψ is an eigenstate of A with eigenvalue a, then the uncertainty of A is zero. We say that A takes a definite value a in an eigenstate. We say that A has quantum fluctuations in the state ψ if $\langle A^2\rangle \neq \langle A\rangle^2$.

• Suppose ψ is a unit norm state, then the Heisenberg uncertainty inequality is $\Delta x \Delta p \geq \frac{1}{2}\hbar$. It says that if you prepare a large number of copies of a system in the same state ψ, and make measurements of position on half of them and momentum on the other half, the product of standard deviations in the measurements of position and momentum is bounded below by $\hbar/2$.

• An extreme case: if ψ is a position eigenstate $|x_0\rangle$. In such a state, the uncertainty in x is zero, a measurement of position always results in the value x_0. However, the uncertainty in momentum is infinite in a position eigenstate, all values of momentum are equally likely.

• The ground state ψ_0 of the SHO is a minimum uncertainty state. $\Delta x\Delta p = \hbar/2$ in this state. Check this statement.

- To show this we define an uncertainty functional U in a unit norm state ψ for a pair of observables A, B with $[A,B] = iC$. Later we will specialize to $A = x, B = p, C = \hbar I$.

$$U(\psi) = (\Delta A)^2(\Delta B)^2 = \langle\psi|(A-\bar{A})^2|\psi\rangle\langle\psi|(B-\bar{B})^2|\psi\rangle = \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \tag{42}$$

where $|\alpha\rangle = (A-\bar{A})|\psi\rangle \equiv \delta A|\psi\rangle$ and $|\beta\rangle = (B-\bar{B})|\psi\rangle = \delta B|\psi\rangle$. By the Cauchy-Schwarz inequality,

$$U \geq |\langle\alpha|\beta\rangle|^2 = |\langle\psi|\ \delta A\ \delta B\ |\psi\rangle|^2 \tag{43}$$

We bring in the commutator and the anticommutator via

$$\delta A \delta B = \frac{1}{2}[\delta A, \delta B] + \frac{1}{2}\{\ \delta A, \delta B\ \} = \frac{1}{2}iC + \frac{1}{2}\{\ \delta A, \delta B\ \}. \tag{44}$$

Now C is hermitian as is $\{\ \delta A, \delta B\ \}$. It follows that $\frac{1}{2}\langle iC\rangle$ is purely imaginary and $\frac{1}{2}\langle\{\ \delta A, \delta B\ \}\rangle$ is real. So the absolute square of the sum is just the sum of the squares of the imaginary and real parts:

$$U \geq |\frac{i}{2}\langle C\rangle + \frac{1}{2}\langle\{\ \delta A, \delta B\ \}\rangle|^2 = \frac{1}{4}\langle C\rangle_\psi^2 + \frac{1}{4}\langle\psi|\{\delta A, \delta B\}|\psi\rangle^2. \tag{45}$$

The second term is ≥ 0. So we get

$$(\Delta A)^2(\Delta B)^2 = U \geq \frac{1}{4}\langle C\rangle_\psi^2. \tag{46}$$

Specializing to $A = x, B = p, C = \hbar I$ we get the Heisenberg uncertainty inequality $\Delta x \Delta p \geq \hbar/2$.

3.10 Relation between wave function in position and momentum space

- The wave function is a complete specification of the state of a quantum mechanical system, just as giving the position and momentum of a particle completely specifies its classical state. For a particle moving in 3-space, the coordinate space wave function is $\psi(x,y,z;t)$. For a system of n particles, the coordinate space wave function is a function of the three coordinates of each of the n particles $\psi(\vec{r}_1, \vec{r}_2, \cdots \vec{r}_n; t)$. In other words, the coordinate space wave function is a (time-dependent) function on the classical configuration space of the system.

- We have seen that the position space wave function of a state $|\psi\rangle$ is defined as $\psi(x) = \langle x|\psi\rangle$. Let us denote a momentum eigenstate with momentum eigenvalue $p = \hbar k$ by $|k\rangle$, where k is the wave number. Then the momentum space wave function of the same state $|\psi\rangle$ is $\tilde{\psi}(k) = \langle k|\psi\rangle$. The point is that $|\psi\rangle$ is an abstract state vector. We can study it ('represent it') via its components in any basis. In particular, we may look at its components $\langle x|\psi\rangle = \psi(x)$ in the basis of position eigenstates or its components $\langle k|\psi\rangle = \tilde{\psi}(k)$ in the basis of momentum eigenstates. Let us see how $\psi(x)$ is related to $\tilde{\psi}(k)$.

- Now inserting a complete set of momentum eigenstates and using $\langle x|k\rangle = e^{ikx}$,

$$\psi(x) = \langle x|\psi\rangle = \int \frac{dk}{2\pi}\langle x|k\rangle\langle k|\psi\rangle = \int \frac{dk}{2\pi} e^{ikx}\tilde{\psi}(k) \tag{47}$$

So the position space wave function is the inverse-Fourier transform of the momentum space wave function. Similarly, we have the Fourier transform

$$\tilde{\psi}(k) = \int dx e^{-ikx}\psi(x). \tag{48}$$

- $\psi(x)$ and $\tilde{\psi}(k)$ are to be compared with the state of a classical mechanical system, which is given by a *simultaneous* specification of coordinates **and** momenta. In the quantum theory, ψ cannot depend on both the coordinates and momenta (in an arbitrary manner). This is related to the uncertainty principle.

- The absolute square of the wave function $|\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$ gives the probability density for finding the particle at location x at time t. Similarly, $|\tilde{\psi}(k,t)|^2 \frac{dk}{2\pi}$ is the probability of finding the particle in momentum interval $[k, k+dk]$ at time t.

4 Time evolution in quantum mechanics

- When left to itself, the state of the system evolves according to the Schrödinger equation $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$. H is the hermitian hamiltonian. Given the initial state $|\psi(0)\rangle$, the SE determines the state at subsequent times, just as Hamilton's equations $\dot{x} = \frac{\partial H}{\partial p}, \dot{p} = -\frac{\partial H}{\partial x}$ do in classical mechanics.

- In the position basis, the SE is

$$i\hbar\frac{\partial}{\partial t}\langle x|\psi(t)\rangle = \langle x|H\psi(t)\rangle \quad \text{or} \quad i\hbar\frac{\partial \psi(x,t)}{\partial t} = (H\psi)(x,t) \tag{49}$$

For a particle in a potential $(H\psi)(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t)$, and we get

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x). \tag{50}$$

The SE is a linear PDE, first order in time and second order in space derivatives of the unknown ψ. Contrast this with Newton's equation which in general is a system of non-linear ODEs for $x_i(t)$.

- We often need to work with the adjoint of the Schrodinger equation, which is obtained using $H = H^\dagger$

$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|H. \tag{51}$$

In the coordinate basis, the adjoint of the SE reads

$$-i\hbar\frac{\partial}{\partial t}\langle\psi(t)|x\rangle = \langle\psi(t)|H|x\rangle = \langle H\psi|x\rangle = \langle x|H\psi\rangle^* \quad \Rightarrow \quad -i\hbar\frac{\partial}{\partial t}\psi^*(x,t) = ((H\psi)(x))^* \tag{52}$$

or $-i\hbar\frac{\partial}{\partial t}\psi^*(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi^*(x)}{\partial x^2} + V(x)\psi^*(x)$ for a particle in a real potential $V(x)$. So in the coordinate basis, the adjoint of the SE is just its complex conjugate.

4.1 Separation of variables, stationary states, time-independent Schrodinger equation

- The problem of time-evolution is to solve the Schrodinger equation $i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}|\Psi(t)\rangle$ given the initial state $\Psi(t=0)\rangle$. For a particle in a potential $V(x)$, the SE is a LINEAR partial differential equation for the unknown function $\Psi(x,t) = \langle x|\Psi(t)\rangle$.

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = (H\Psi)(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial t} + V(x)\Psi(x,t). \tag{53}$$

To solve it we use the method of separation of variables. We look for separable solutions in the form of a product $\Psi(x,t) = \psi(x)T(t)$. Now, not every solution of the SE is such a product. But due to the linearity of the equation linear combinations of solutions are again solutions. The idea is to find sufficiently many separable solutions so that every solution can be written as a linear combination of separable solutions. Putting the 'ansatz' (guess) $\Psi(x,t) = \psi(x)T(t)$ into the equation, we get

$$i\hbar\dot{T}(t)\psi(x) = T(t)(H\psi)(x). \tag{54}$$

Dividing by $T\psi$ we get

$$i\hbar\frac{\dot{T}(t)}{T(t)} = \frac{(H\psi)(x)}{\psi(x)} = E. \tag{55}$$

LHS depends only on time while the RHS depends only on position, provided H is not explicitly time-dependent. The only way these can be equal is for both to equal the same constant, say E, so-named, since it turns out to have the physical meaning of energy eigenvalue. Now we have two separate equations. The one for $T(t)$ has the solution $T(t) = c\exp(-iEt/\hbar)$. The other equation

$$(H\psi)(x) = E\psi(x) \quad \text{or} \quad \langle x|H|\psi\rangle = E\langle x|\psi\rangle \quad \text{or} \quad H|\psi\rangle = E|\psi\rangle \tag{56}$$

is simply the eigenvalue equation for the hamiltonian operator. It is also called the time-independent Schrodinger eigenvalue equation. It typically has lots of solutions, namely all the eigenstates $|\psi_n\rangle$ of the hamiltonian, with their corresponding energy eigenvalues E_n. As for any hermitian operator, we can take these $|\psi_n\rangle$ to be orthonormal. Thus the separable solutions of the Schrodinger equation are

$$\Psi_n(x,t) = c_n\psi_n(x)e^{-iE_nt/\hbar}. \tag{57}$$

where ψ_n are eigenstates of the hamiltonian. These separable solutions are called stationary states since the probability density in these states $P(x,t) = |\Psi(x,t)|^2 = |c_n|^2|\psi_n(x)|^2$ are independent of time. Stationary states have the simplest possible time dependence of all solutions of the Schrodinger equation, i.e., sinusoidal or harmonic time dependence.

- Now the general solution of the SE is got by taking a linear combination of stationary states

$$\Psi(x,t) = \sum_n c_n\psi_n(x)e^{-iE_nt/\hbar}. \tag{58}$$

To find the solution of the initial value problem, we must choose the c_n so that the initial state is $|\Psi(0)\rangle$. In other words, we must have

$$\sum_n c_n|\psi_n\rangle = |\Psi(0)\rangle \tag{59}$$

To find the c_n we take the inner product with $|\psi_m\rangle$, and use orthogonality of energy eigenstates

$$\sum_n c_n\langle\psi_m|\psi_n\rangle = \sum_n \delta_{mn}c_n = c_m = \langle\psi_m|\Psi(0)\rangle \quad \Rightarrow \quad c_m = \int \psi_m^*(x)\Psi(x,0)\,dx. \tag{60}$$

Thus we have solved the initial value problem for the Schrodinger equation.

4.2 Conserved probability density and current

• The absolute square of the wave function $|\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$ gives the probability density for finding the particle at location x at time t. Suppose n copies of a system are prepared in the same quantum mechanical state $\psi(x)$. (For example, we could have a hydrogen atom in its ground state in each of 100 different boxes) Then a measurement of the position of each particle (at the same time) gives a (possibly) different result (this is an experimental fact). Born's statistical interpretation of the wave function is that, as $n \to \infty$, the distribution of position measurements approaches the probability density $|\psi(x,t)^2|$.

• To qualify as a probability density, the total probability of finding the particle anywhere must be one. In other words, we need $||\psi||^2 = \int dx\, |\psi(x,t)|^2 = 1$. However, there could be a problem. For consistency, the total probability of finding the particle *somewhere* must remain equal to one at all times, total probability must be conserved. This is indeed the case, as is checked using the Schrödinger equation and its adjoint

$$i\hbar \frac{\partial}{\partial t} \langle \psi | \psi \rangle = \langle \psi | H \psi \rangle - \langle \psi H | \psi \rangle = 0. \tag{61}$$

In other words, if the wave function is normalized to one initially ($t = 0$), then it continues to have norm one in the future. This is called global conservation of probability. But it is not merely the total probability that is conserved. Probability cannot jump from one place to another, it flows continuously like a fluid. There is a local conservation of probability just like for mass in a fluid. The rate of increase of mass of fluid in a box is equal to the inward flux of fluid across the walls of the box (provided there isn't a source/sink of fluid inside the box). The probability density $|\psi(x,t)|^2$ satisfies a continuity equation with an associated probability current. Consider a particle in a potential

$$\begin{aligned} i\hbar\, \partial_t(\psi^*\psi) = i\hbar\, (\psi_t^*\psi + \psi^*\psi_t) &= \left(\frac{\hbar^2}{2m}\psi^{*\prime\prime} - V\psi^*\right)\psi + \psi^*\left(-\frac{\hbar^2}{2m}\psi'' + V\psi\right) \\ &= \frac{\hbar^2}{2m}\left[\psi^{*\prime\prime}\psi - \psi^*\psi''\right] = \frac{\hbar^2}{2m}\partial_x\left(\psi^{*\prime}\psi - \psi^*\psi'\right) \end{aligned} \tag{62}$$

Let $P(x,t) = |\psi(x,t)|^2$ and define the probability current density

$$j(x,t) = \frac{\hbar}{2mi}\left(\psi^*\psi' - \psi^{*\prime}\psi\right), \quad \text{then} \quad \partial_t P(x,t) + \partial_x j(x,t) = 0. \tag{63}$$

The last equation is called the law of local conservation of probability (in differential form) or a continuity equation. To interpret this formula we consider how the probability for the particle to be in an interval $[x_0, x_1]$ changes with time. So integrate $\partial_t P + \partial_x j = 0$ over this interval at a fixed time t to get the law of local conservation of probability in integral form:

$$\partial_t \int_{x_0}^{x_1} P(x)\, dx + \int_{x_0}^{x_1} \frac{\partial j(x)}{\partial x}\, dx = 0 \quad \Rightarrow \quad \partial_t \int_{x_0}^{x_1} P(x)\, dx = j(x_0) - j(x_1) \tag{64}$$

by the fundamental theorem of calculus. This equation says the rate of increase of probability in $[x_0, x_1]$ equals the probability current flowing in at x_0 minus that flowing out at x_1.

• All of this also works in three dimensions. The rate of increase of probability in a region (volume) Ω must equal the inward flux of probability across the surface $\partial\Omega$ that borders Ω.

$$P(\vec r, t) = \psi^*(\vec r, t)\psi(\vec r, t), \qquad \vec j = \frac{\hbar}{2mi}\left[\psi^*\left(\nabla\psi\right) - \left(\nabla\psi^*\right)\psi\right] = \frac{\hbar}{m}\Im\psi^*\nabla\psi$$

$$\begin{aligned}\partial_t P(\vec r,t) + \nabla\cdot\vec j(x,t) &= 0, \quad \text{i.e.} \quad \frac{\partial\rho}{\partial t} + \frac{\partial j_1}{\partial x} + \frac{\partial j_2}{\partial y} + \frac{\partial j_3}{\partial z} = 0.\\ \partial_t \int_\Omega P(\vec r,t) d^3r + \int_\Omega d^3r \nabla\cdot\vec j = 0 \quad &\text{or} \quad \partial_t \int P(\vec r,t) d^3r = -\int_{\partial\Omega} \vec j\cdot d\vec S. \end{aligned} \tag{65}$$

$d\vec S$ is the outward pointing area element on the bounding surface $\partial\Omega$. It says that the rate of increase of probability in a region must equal the inward flux of probability current across the surface of the region. We used the divergence theorem to write the volume integral of a divergence as a surface integral.

4.3 Ehrenfest's theorem

• The expectation values $\langle x\rangle, \langle p\rangle, \langle E\rangle$ etc are functions of time (space has been integrated over). The average position and momentum of an electron will depend on time in a way governed by the Schrödinger equation. According to Ehrenfest's theorem, these expectation values evolve as do the corresponding classical variables, whose evolution is given by Newton's/Hamilton's equations! E.g. $\frac{d\langle x\rangle}{dt} = \frac{\langle p\rangle}{m}$, so the average position evolves in the same way as given by the first of Hamilton's equations. To see this and related results, we first derive a general equation for the time evolution of the expectation value of an observable A in a unit-norm state that evolves via the SE

$$i\hbar\frac{\partial}{\partial t}\langle\psi|A|\psi\rangle = -\langle\psi|HA|\psi\rangle + \langle\psi|AH|\psi\rangle = \langle\psi|[A,H]|\psi\rangle. \tag{66}$$

• Putting $A = H$ and using $[H,H] = 0$ shows that the average energy (expectation value of hamiltonian) is constant $\frac{\partial\langle\hat H\rangle}{\partial t} = 0$. This is the analogue of the classical constancy of energy along a trajectory.

• Taking $A = p$ we find the time evolution of mean momentum for a particle subject to the hamiltonian $H = \frac{p^2}{2m} + V$. Show that

$$[p,H] = [p,V] = -i\hbar V' \tag{67}$$

Thus we have

$$\frac{\partial\langle p\rangle}{\partial t} = \langle -V'\rangle. \tag{68}$$

Thus Newton's second law (or the second of Hamilton's equations) $\dot p = -V'(x)$ continues to hold in quantum mechanics, but in the sense of expectation values. The average momentum evolves as though it is a classical variable subject to an 'average force'!

• If $A = x$, then $[x,H] = [x,\frac{p^2}{2m}] = \frac{i\hbar p}{m}$. So

$$\frac{\partial\langle x\rangle}{\partial t} = \left\langle\frac{p}{m}\right\rangle. \tag{69}$$

This is the first of Hamilton's equations $\dot x = \frac{\partial H}{\partial p} = \frac{p}{m}$, but now in the sense of expectation values.

• So if the electron is in the initial state $\psi(x,t=0)$, Schrödinger's equation tells us how the state evolves in time. We have used this to determine the motion of the average position of the electron and found that it is related to the average momentum in the same way as the actual position and momentum of a particle are related by Hamilton's equation of classical mechanics. To the extent that the expectation value of x provides an approximate position for a localized electron wave packet, we see that the quantum mechanical motion of the wave-packet mimics the classical motion of a particle. However, the wave packet typically spreads out in time, and ceases to be well-described by merely its mean position. This reduces the utility of the Ehrenfest result in determining where a quantum particle may be found at later times, based purely on its classical motion.

4.4 Free particle, Gaussian wave packet and its dispersive evolution

• Consider a particle free to move on the infinite real line, with hamiltonian $H = p^2/2m$. The time-independent SE is[1] (here $k' = \sqrt{2mE/\hbar^2} \geq 0$ is the positive square root)

$$\psi''(x) = -\frac{2mE}{\hbar^2}\psi(x) = -k'^2\psi(x) \tag{70}$$

There are two linearly independent solutions $e^{ik'x}$ and $e^{-ik'x}$ for any $k' > 0$. So we have two linearly independent energy eigenstates for each energy eigenvalue $E = \hbar^2 k'^2/2m > 0$. The ground state is the limiting case $E = 0$. The g.s. is non-degenerate, and corresponds to the constant eigenfunction $\psi(x) = 1$[2]

• However, the position space probability distribution in any of these eigenstates (e.g. $|Ae^{ik'x}|^2$) is spread out over all of x-space. None of these eigenfunctions (nor any linear combination of $e^{\pm ik'x}$) is square integrable. The energy eigenstates do not represent localized particles.

• Time dependence of any vector in the eigenspace corresponding to energy $E = \hbar^2 k'^2/2m = \hbar\omega$ is

$$(Ae^{ik'x} + Be^{-ik'x})e^{-iEt/\hbar} = Ae^{i(k'x-\omega t)} + Be^{-i(k'x+\omega t)} = e^{i(kx - \frac{\hbar k^2}{2m}t)}(A_{k>0} + B_{k<0}) \tag{71}$$

This is a linear combination of two traveling waves, a right-moving one and a left-moving one. In the last equality, we introduced a new wave vector variable $k = k'$ for right-moving waves and $k = -k'$ for left-moving waves (for $k > 0$).

• To summarize, the energy eigenstates $|k\rangle$ are the plane waves e^{ikx} for all $k \in \mathbb{R}$. The eigenstates labeled by k and $-k$ are degenerate in energy. The energy eigenstates are also eigenstates of momentum $-i\hbar\partial_x e^{ikx} = \hbar k e^{ikx}$, with eigenvalue $\hbar k$. States with momentum $k > 0$ move to the right and those with $k < 0$ move to the left.

• Energy eigenstates $|k\rangle$ are not localized in position. They do not represent wave packets. They do not have finite norm, though they are delta-normalized $\langle k'|k\rangle = 2\pi\delta(k-k')$, so energy eigenfunctions e^{ikx} do not have a probability interpretation. But we can draw an analogy with a fluid by computing the 'probability' current density $j(x,t) = \frac{\hbar}{2mi}(\psi^*\psi' - \psi^{*\prime}\psi)$ for the stationary state $\psi(x,t) = Ae^{i(kx-\omega(k)t)}$. We get $j(x,t) = |A|^2\frac{\hbar k}{m} = |A|^2 v$ where $v = p/m$ is the corresponding classical velocity and $P(x,t) = |\psi(x,t)|^2 = |A|^2$ is the 'probability' density. This is akin to ρv for the mass density current in a fluid flow. So energy eigenstates can be interpreted

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[1] Here we assume that the energy eigenvalue $E > 0$ since otherwise, the particle will have an ever growing amplitude of being found at larger and larger values of $|x|$, which is physically inappropriate to describe one or even a stream of particles.

[2] The linear solution $\psi(x) = Ax + B, A \neq 0$ for $E = 0$ is disallowed as the probability density grows without bound as $x \to \pm\infty$.

as an always-present constant stream of free particles ($|A|^2 dx$ particles in the interval dx). For $k > 0$, they enter from $x = -\infty$ and exit at $x = \infty$.

- Such non-normalizable wave functions with oscillatory $e^{\pm ikx}$ behavior as $|x| \to \infty$ are called *scattering states.* They correspond to particle trajectories that escape to infinity in classical mechanics. Though not normalizable, $\int_a^b |\psi(x)|^2$ is finite on any finite interval $[a,b]$. Though the total probability to be between $\pm\infty$ is infinite, we can still speak of relative probabilities. For example, in the state Ae^{ikx} with $k > 0$, the relative probability that a particle coming in from $-\infty$ scatters out to $+\infty$ is $\frac{|A|^2}{|A|^2} = 1$ while the relative probability for it to go back to $-\infty$ is $\frac{0}{|A|^2} = 0$.

- On the other hand, *bound states* are represented by normalizable wave functions that decay as $|x| \to \pm\infty$. Bound states correspond to classical particle trajectories that do not escape to infinity. All the eigenstates of the free particle hamiltonian are scattering states.

- Now we'd like to describe the evolution of an initial state that represents a particle, i.e., a localized wave packet $\psi(x)$ with finite norm. It cannot be an energy eigenstate, but may be expressed as a linear combination of energy eigenstates (same as momentum eigenstates) which evolve via $e^{-i\omega t}$

$$\psi(x,t) = \int_{-\infty}^{\infty} [dk]\tilde{\psi}(k) e^{i(kx - \frac{\hbar k^2}{2m} t)}. \tag{72}$$

- A particularly useful wave packet is the gaussian one corresponding to the initial state

$$\psi(x) = A e^{-\frac{x^2}{4a^2}}, \qquad A = \frac{1}{\sqrt{a}(2\pi)^{1/4}}, \quad ||\psi|| = 1, \quad |\psi(x)|^2 = \frac{1}{a\sqrt{2\pi}} e^{-x^2/2a^2} \tag{73}$$

$\langle x \rangle_\psi = 0$, so this packet is localized near $x = 0$. So $\psi(x) = Ae^{-(x-x_0)^2/4a^2}$ is located near $\langle x \rangle = x_0$. The width of the packet is $\Delta x = \sqrt{\langle x^2 \rangle} = a$. This is a state of zero mean momentum $\langle p \rangle_\psi$ as the integrand $\psi^*(x)(-i\hbar\partial_x)\psi(x)$ is odd.

- To find the time evolution of this Gaussian wave packet, we write it in the energy basis

$$\tilde{\psi}(k) = \int dx\, \psi(x) e^{-ikx} = \int A\, e^{-\left(\frac{x^2}{4a^2} + ikx\right)} dx = 2aA\sqrt{\pi} e^{-a^2k^2} = 2\sqrt{a}\left(\frac{\pi}{2}\right)^{1/4} e^{-a^2k^2}. \tag{74}$$

The integral is done by *completing the square*, the change of variable $y = \frac{x}{2a} + ika$ and using $\int_{-\infty}^{\infty} e^{-y^2} dy = \sqrt{\pi}$. The Fourier transform of the gaussian is again a gaussian.

- The width in momentum space is $\Delta p = \sqrt{\langle p^2 \rangle} = \frac{\hbar}{2a}$. We see that the Gaussian wave function minimizes the uncertainty product $\Delta x \Delta p = a\frac{\hbar}{2a} = \frac{\hbar}{2}$.

- Time evolution is simple in the energy basis

$$\psi(x,t) = \int [dk]\tilde{\psi}(k) e^{-iEt/\hbar} e^{ikx} = 2aA\sqrt{\pi} \int [dk] e^{-\left[k^2\left(a^2 + \frac{i\hbar t}{2m}\right) - ikx\right]} \tag{75}$$

This is again a Gaussian integral done by completing the square $l = k\sqrt{a^2 + \frac{i\hbar t}{2m}} - \frac{1}{2}\frac{ikx}{k\sqrt{a^2 + \frac{i\hbar t}{2m}}}$. We get

$$\psi(x,t) = \frac{1}{(2\pi)^{1/4}\sqrt{a + \frac{i\hbar t}{2ma}}} \exp\left\{-\frac{x^2}{4\left(a^2 + \frac{i\hbar t}{2m}\right)}\right\} \tag{76}$$

The probability density at time t is

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{a^2 + \frac{\hbar^2 t^2}{4m^2 a^2}}} \exp\left\{ \frac{-x^2}{2\left(a^2 + \frac{\hbar^2 t^2}{4m^2 a^2}\right)} \right\} = \frac{1}{a(t)\sqrt{2\pi}} e^{-x^2/2a(t)^2} \tag{77}$$

Here $a(t) \equiv \sqrt{a^2 + \frac{\hbar^2 t^2}{4m^2 a^2}}$. Width of the Gaussian $\sqrt{\langle x^2 \rangle} = a(t)$ grows with time. It remains centered at $\langle x \rangle = 0$. This is an indication of the dispersive behavior of de Broglie matter waves, the wave packet spreads out as its component plane waves travel at different phase speeds $c(k) = \omega/k = \hbar k/2m$.

- How fast does the wave packet disperse? We can write the width as

$$a(t) = a\sqrt{1 + \frac{\hbar^2 t^2}{4m^2 a^4}} = a\sqrt{1 + \frac{t^2}{\tau^2}}, \quad \tau = \frac{2ma^2}{\hbar}. \tag{78}$$

τ has dimensions of time and gives the rate of broadening. For $t << \tau$ there is not much broadening. For example, if we make a measurement of position with accuracy a, the wave function 'collapses' roughly to a packet of width a. A subsequent measurement (after time t) of position will yield roughly the same position as long as long as $t \ll \tau$. If we wait too long $t \gg \tau$ to make the next measurement, the wave packet broadens significantly (by a factor of $\sqrt{1 + t^2/\tau^2}$), and we are no longer guaranteed to get roughly the same position.

- For example, suppose we know the position of the center of a tennis ball of mass 60g to within an accuracy of $a \sim 1mm$. If we model the tennis ball as a wave packet with a width equal to the above accuracy, then $\tau = 1.8 \times 10^{26} s$. So it takes a very long time for the quantum mechanical broadening of the tennis ball wave packet to become significant. In other words, we will get the same position even if we wait several centuries between successive measurements of the position of a tennis ball (that was initially at rest and was acted upon by no forces).

- The uncertainty product $\Delta x \Delta p$ remains equal to $\hbar/2$ at all times, since all that changes is the width $a(t)$, and $\Delta x \Delta p = \hbar/2$ was independent of the width a.

- The (expectation value of) energy of the gaussian wave packet at $t = 0$ is

$$\langle H \rangle_{t=0} = \frac{\langle p^2 \rangle}{2m} = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{8ma^2}. \tag{79}$$

As we would expect from Ehrenfest's theorem on the evolution of expectation values, $\langle H \rangle$ is constant in time. This can be explicitly checked most easily in momentum space, where $\tilde{\psi}(k,t) = 2aA\sqrt{\pi} e^{-k^2(a^2 + \frac{i\hbar t}{2m})}$

$$\langle H \rangle_t = \int [dk] \, |\tilde{\psi}(k,t)|^2 \, \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 a^2 A^2}{m} \int dk \, k^2 e^{-2a^2 k^2} = \frac{\hbar^2}{8ma^2}. \tag{80}$$

- This is a general feature, the expectation value of energy in any state is constant under Schrödinger evolution, provided the hamiltonian is hermitian and does not depend explicitly on time. To see this we note that $i\hbar\dot{\psi} = H\psi$ and $-i\hbar\dot{\psi}^* = (H\psi)^*$, so that

$$\begin{aligned} i\hbar\partial_t \int \psi^* H\psi &= i\hbar \int \left(\dot{\psi}^* H\psi + \psi^* H\dot{\psi} \right) dx = \int \left(-(H\psi)^* H\psi + \psi^* HH\psi \right) dx \\ &= -\langle H\psi | H\psi \rangle + \langle \psi | HH\psi \rangle = 0. \end{aligned} \tag{81}$$

• So far, our wave packet represented a particle that was on average at rest. To get a gaussian wave packet with non-zero mean momentum $\langle p \rangle = \hbar k_0$, we merely have to center the gaussian at k_0 in momentum space $\tilde{\psi}(k) = 2aA\sqrt{\pi}e^{-a^2(k-k_0)^2}$ so that $\langle \hbar \hat{k} \rangle = \hbar k_0$. This corresponds to the wave packet

$$\psi(x) = \int [dk] e^{ikx} 2Aa\sqrt{\pi} e^{-a^2(k-k_0)^2} = e^{ik_0 x} \int [dl] e^{ilx} 2aA\sqrt{\pi} e^{-a^2 l^2} = A e^{ik_0 x} e^{-x^2/4a^2}. \tag{82}$$

Check directly that $\langle p \rangle = \hbar k_0$ by observing that $\psi^* \psi' = i\psi^* k_0 \psi_0 e^{ik_0 x} + \psi^* e^{ik_0 x} \psi_0'$, where $\psi = \psi_0 e^{ik_0 x}$. The second term does not contribute to $\langle \hat{p} \rangle$ as it is odd and the first gives $\langle p \rangle = \hbar k_0$.

• The gaussian wave packet with non-zero mean momentum also has minimal uncertainty product $\Delta x \Delta p = \hbar/2$. $\Delta x = a$ is unaffected by the phase $e^{ik_0 x}$. $\langle p \rangle = \hbar k_0$. $\langle p^2 \rangle = \hbar^2 k_0^2 + \frac{\hbar^2}{4a^2}$ is most easily evaluated in k-space. Thus $\langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2}{4a^2}$ is independent of k_0. So $\Delta p = \hbar/2a$ and $\Delta x \Delta p = \hbar/2$.

4.5 Schrödinger vs Heisenberg pictures and equations of motion

• So far our formulation of QM has been based on the idea that the state of the system ψ evolves in time via the Schrödinger equation. However, the wave function itself is not measured. Rather, when we measure an observable A in a normalized state ψ, we get one of its eigenvalues a with a probability given by the square of the inner product (projection) $|\langle \phi_a | \psi \rangle|^2$. The system collapses to a (normalized) eigenstate ϕ_a where $A\phi_a = a\phi_a$. And if we make several copies of the system in the same state $\psi(t)$, and measure A in each of the copies, the average value obtained is $\langle \psi(t) | A | \psi(t) \rangle$

• We can express this expectation value at time t in terms of the expectation value (of a different operator) at a reference time (say $t = 0$) using the unitary time-evolution operator $U = e^{-iHt}$:

$$\langle \psi(t) | A | \psi(t) \rangle = \langle \psi(0) | e^{iHt/\hbar} A e^{-iHt/\hbar} | \psi(0) \rangle \tag{83}$$

The operator $A_h(t) = e^{iHt/\hbar} A e^{-iHt/\hbar}$ is called the operator A in the Heisenberg picture. The original operator A (sometimes called A_s) is said to be in the Schrodinger picture. Operators in the Heisenberg picture are related to those in the Schrodinger picture via a unitary transformation $A_h(t) = U^\dagger A U$.

• Thus, to calculate the expected value of an observable A at time t in the Heisenberg picture, we must evaluate $\langle \psi(0) | A_h(t) | \psi(0) \rangle$. Since we only need $\psi(0)$, we will say that the state of the system in the Heisenberg picture is $\psi_h = \psi(0)$. We can of course also write $\psi_h = U^\dagger \psi(t)$.

• In the Heisenberg formulation, states don't change in time, but the operators do.

• In the Schrödinger formulation, the state of the system evolves in time, while operators do not change with time (except if they are explicitly time-dependent).

• The hamiltonian operator is the same in both pictures $H_h = U^\dagger H U = H$ since the time evolution operator U commutes with H.

• Irrespective of whether we work in the Schrödinger or Heisenberg pictures, physically measurable quantities are the same.

• E.g. the (measurable) eigenvalues of operators are the same in both pictures. This is because $A_s = A$ and $A_h = U^\dagger A U$ being related by a unitary transformation, share the same spectrum.

• We have already seen that expectation values are the same in both pictures $\langle \psi(t)|A|\psi(t)\rangle = \langle \psi_h|A_h|\psi_h\rangle$. In addition, inner products (projections, whose squares give probabilities of measurements) $\langle \phi(t)|\psi(t)\rangle = \langle \phi_h|\psi_h\rangle$ are also the same in both pictures. Here the system is in the Schrödinger state $\psi(t)$; we measure an observable, and get an eigenvalue corresponding to the eigenfunction $\phi(t)$.

• States do not evolve in time, so what replaces the Schrödinger equation in the Heisenberg picture? It is replaced by the Heisenberg equation of motion, which tells us how operators in the Heisenberg picture evolve. Suppose $A_h(t) = U^\dagger A U$ where A is a Schrödinger picture operator (that may have some explicit time dependence), then

$$i\hbar \frac{dA_h}{dt} = i\hbar \dot{U}^\dagger A U + i\hbar U^\dagger \frac{\partial A}{\partial t} U + i\hbar U^\dagger A \dot{U} \tag{84}$$

From $U = e^{-iHt/\hbar}$ and $U^\dagger = e^{-Ht/\hbar}$ we first observe that $H, U, U^\dagger$ all commute with each other (after all, each is a function of H and $[H,H]=0$). We also find

$$i\hbar \dot{U} = HU, \quad \text{and} \quad i\hbar \dot{U}^\dagger = -HU. \tag{85}$$

Thus the time evolution of A_h is given by the Heisenberg equation of motion

$$i\hbar \frac{dA_h}{dt} = i\hbar \frac{\partial A_h}{\partial t} + [A_h, H]. \tag{86}$$

In particular, if A does not have any explicit time dependence, then $i\hbar \dot{A}_h = [A_h, H]$. Moreover, if $[A,H]=0$ (which is equivalent to $[A_h,H]=0$), the Heisenberg operator $A_h(t)$ is a constant of motion. In other words, each of its matrix elements is time-independent.

• For a free particle, the Heisenberg picture momentum is a constant of motion $\dot{p}_h = 0$, since $[p, p^2/2m] = 0$.

5 Brief comparison of classical and quantum mechanical formalisms

• This is a good opportunity to compare certain features of classical and quantum mechanics.

1. In CM, the space of (pure) states is the phase space. In QM it is the quantum mechanical Hilbert space (vector space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$).
2. In CM, observables are smooth real-valued functions on phase space. In QM, observables (A, B etc) are self-adjoint (hermitian) operators on Hilbert space. Self-adjointness is the analogue of reality, both of which ensure that results of measurements are real numbers.
3. The Poisson bracket of observables in CM is replaced by the commutator of operators (upto a factor of $i\hbar$) in QM, e.g. $\{x,p\} = 1 \longrightarrow \frac{1}{i\hbar}[x,p] = 1$. Both operations map a pair of observables to a new observable.
4. In CM, time evolution is a 1-parameter family of canonical transformations. In QM, time evolution is a 1-parameter family of unitary transformations $U(t) = e^{-iHt/\hbar}$.

5. Unitary transformations ($|\psi\rangle \to |\psi'\rangle = U|\psi\rangle$ and $A \to A' = UAU^\dagger$ with $U^\dagger U = I$) are quantum analogs of canonical transformations. Both preserve the structure of the formalism. CTs preserve the fundamental p.b. while unitary transformations preserve the Heisenberg canonical commutation relations, since $[A', B'] = U[A, B]U^\dagger$ and in particular $[q', p'] = U[q, p]U^\dagger = U(i\hbar)U^\dagger = i\hbar$. Unitary transformations also preserve inner products $\langle U\phi|U\psi\rangle = \langle\phi|U^\dagger U\psi\rangle = \langle\phi|\psi\rangle$.

- The various formalisms of classical dynamics have their quantum counterparts:

1. Time-dependent Hamilton-Jacobi equation for Hamilton's principal function $\partial_t S + H(q, \frac{\partial S}{\partial q}) = 0$ or time-independent Hamilton-Jacobi equation for Hamilton's characteristic function $H(q, \frac{\partial W}{\partial q}) = E$ were $S = W - Et$ ↔ Time-dependent $i\hbar\partial_t\psi = H\psi$ and time-independent $H\psi = E\psi$ Schrödinger equations for wave function with $\psi \sim e^{iS/\hbar}$.
2. Hamilton's 1st order equations of motion expressed in terms of Poisson brackets $\dot{f} = \{f, H\}$ ↔ Heisenberg equations of motion $i\hbar\dot{\hat{f}} = [\hat{f}, \hat{H}]$.
3. Euler-Lagrange equations for trajectory joining two configurations as extrema of action ↔ Path integral representation of quantum mechanical amplitude.
4. Newtonian's second law, generally non-linear 2nd order ODE ↔ Stochastic ODE with quantum fluctuations entering through stochastic term in ODE.

It is noteworthy that the later formulations of classical mechanics were generalized to the quantum theory somewhat earlier than the original Newtonian approach.