# Quantum mechanics

*An overview*

John O'Neall

## Table of Contents



## 1. Vector and Hilbert spaces

In QM, the space of states of a physical system is a mathematical ***Hilbert space***, an abstract construction of a type of space called a ***vector space***. A Hilbert space is a complete vector space possessing the structure of an inner product. It may have any number of dimensions.

A vector space must obey a number of rules. The sum of any two vectors is a vector, and addition is commutative and associative. There exists a zero vector and, for every vector, an inverse vector. The product of a scalar and a vector is a vector and therefore so is a ***linear combination*** of vectors, a sum of such products. Scalar addition is associative and scalar multiplication is distributive and associative.

A vector is ***linearly independent*** of a set of vectors if it can not be represented as a linear combination of vectors in the set. Each vector in a set of linearly independent vectors is independent of all the other members of the set. If every vector in the space can be expressed as a linear combination of vectors in the set, the set Is said to ***span*** the state. Such a set of linearly independent vectors which span the space is called a ***basis***. (Think of $\hat{\imath}, \hat{j}, \hat{k}$ in 3d Euclidean space.) Since they are linearly independent their number is minimal and represents the dimension of the space.

In physics, the basis vectors of such a state may be discrete or continuous. In the latter case, we are interested in functions which are square-integrable over a specified interval, a to b, a space mathematicians call $L^2$(a,b).

# 2. Physical states, observables and operators

The ***state*** of a system is a represented by its state vector, a unit (normalized) vector in the vector space of states. A physical ***observable*** is described by a linear ***operator***.

Using Dirac's bra-ket notation, a state vector is a ***ket*** represented by $|A\rangle$. A bra $\langle B|$ is a member of the ***dual space*** of complex conjugates of the bras.

Vectors need not be intervals in the vector space. As soon as a set of functions obeys the above requirements for a vector space, it may be considered a set of vectors. This is true for the functions of physics.

Like good vectors in any Hilbert space, bras and kets can form an inner product denoted by

$$\langle A|B\rangle \text{ with } \langle B|A\rangle = \langle A|B\rangle^*.$$

The Dirac notation is conveniently the same whether the basis be discrete or continuous. In the discrete case, a ket vector may be represented as a sum of basis vectors, in which case

$$|A\rangle = \sum_i a_i|\lambda_i\rangle \text{ and } |B\rangle = \sum_i b_i|\lambda_i\rangle$$

for complex $a_i$ and $b_i$, assuming the $|\lambda_i\rangle$ are orthonormal basis vectors. Then the inner product is given by

$$\langle A|B\rangle = \sum_i {a_i}^* b_i$$

In the discrete case, it is often convenient to represent the bra and the ket as matrices.

When an observable is continuous, say x, the state is itself a function of continuous variables. The bra $\langle\psi|$ corresponding to a ket $|\psi\rangle$ represented by the function $\psi(x)$ is the complex conjugate $\psi^*(x)$. In these equations, $\psi(x)$is a complex-valued function of an independent real variable x. Then

$$\sum_i \rightarrow \int_i dx$$

and the inner product is defined by

$$\langle\Psi|\Phi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\phi(x)dx.$$

Normalization then requires that

$$\langle\Psi|\Psi\rangle = \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx \ = 1.$$

Although this integral may be infinite (and so not normalizable), it may nevertheless be useful over a limited range (a,b) of x, so the space is $L^2$(a,b). This means integrating from a to b rather than from $-\infty$ to $\infty$ in the above equation.

The important operators in QM are Hermitian operators. The ***Hermitian conjugat***e $T^\dagger$ of a linear operator (transformation) $T$ is defined by

$$\langle\phi|T\psi\rangle = \langle T^\dagger\phi|\psi\rangle \qquad (1)$$

which in discrete matrix form is the complex conjugate of the transposed (inverted) matrix

$$T^\dagger_{ij} = T^*_{ji}.$$

# 3. Principles

Several principles govern observables and basis vectors.[1]

Principle 1. A physical observable is represented by a linear Hermitian operator $L$.

$$L|A\rangle = |B\rangle,$$

where the Hermitian conjugate is defined above.

Principle 2. The possible results of measurements of observables are eigenvalues of the Hermitian operator representing the observable:

$$L|\lambda\rangle = \lambda|\lambda\rangle \tag{2}$$

where λ is the ***eigenvalue*** of the eigenvector ket |λ>. The operator transforms the vector into a multiple of itself. A ***Hermitian operator*** is one which is equal to its Hermitian conjugate

$$L^\dagger = L,$$

which guarantees that its eigenvalues are positive and ***real***. The set of all eigenvalues of an operator is called its ***spectrum***.

Principle 3a. Unambiguously distinguishable states are represented by ***orthogonal*** vectors. i.e., for two eigenvalues, $\lambda_1 \neq \lambda_2$, the corresponding eigenvectors are orthogonal:

$$\langle\lambda_1\lambda_2\rangle = \langle\lambda_2|\lambda_1\rangle = 0 \tag{3}$$

Principle 3b. The eigenvectors of an operator are a ***complete*** set. This means that any vector can be expressed as a linear sum of eigenvectors.

$$|A\rangle = \sum_i \alpha_i|\lambda_i\rangle \tag{4}$$

where the complex coefficients are inner products

$$\alpha_i = \langle\lambda_i|A\rangle \tag{5}$$

In other words, the eigenvectors of a Hermitian operator may be chosen to form an ***orthonormal*** basis. The set of inner-product coefficients $\alpha_i$ is the ***wave function*** of the system in the basis defined by the observable $\mathbf{L}$. More on that in section 6. The number of eigenvectors in the basis is the dimension of the Hilbert space, or at least that part of it corresponding to this observable. So the dimension is greater than or equal to the number of eigenvalues. If the eigenvalues are continuous, the dimension is infinite and this may apply to many or all observables.

Principle 3c. Two orthogonal eigenvectors may have the same eigenvalue, in which case they are referred to as ***degenerate*** states. Even then, it is possible to construct a set of orthonormal basis vectors.

Principle 4. For a normalized state vector $|A\rangle$ and observable $\mathbf{L}$, the probability of observing value $\lambda_i$ by measurement is given by the ***Born rule***

$$P(\lambda_i) = \langle A|\lambda_i\rangle\langle\lambda_i|A\rangle = |\langle A|\lambda_i\rangle|^2 \tag{6}$$

where

$$L|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$$

and

1 Principles adapted from Susskind, 69-74.

$$\sum_i P(\lambda_i) = 1$$

for total probability (normalization).

With the Dirac notation, we can define the expectation value of a Hermitian operator $\mathbf{L}$ by

$$\langle L \rangle = \langle \psi | L | \psi \rangle = \langle \psi | L\psi \rangle = \langle \psi L | \psi \rangle \qquad (7)$$

since $L$ is Hermitian. More generally, if a basis of orthonormal state vectors is represented by $|a, b, c, ...\rangle$ for eigenvalues (a,b,c,...), then any state vector may be expanded as

$$|\Psi\rangle = \sum_{a,b,c,...} \psi(a, b, c, ...)|a, b, c, ...\rangle \qquad (8)$$

where the *set of coefficients* $\psi(a, b, c, ...)$ is called the ***wave function*** of the system in the basis defined by the observables, A, B, C, ….[2] We can expand $|\Psi\rangle$in terms of another set of basis vectors corresponding to different observables and the wave function set will be different even though they describe the same system state. The two sets of basis vectors correspond to different ***representations*** of the system, for the two different observables.

After measurement of an observable in such a superposition of states, the wave function is no longer a superposition (One says it has “collapsed” to a single state.) and a second measurement gives the same result as the first, which is logical.

A method for solving such an equation is to first rewrite it in matrix form (if possible) as

$$(L - \lambda \mathbf{I})|\lambda\rangle = 0$$

where $\mathbf{I}$ is the identity matrix. If $(\mathbf{L} - \lambda_i \mathbf{I})$ has an inverse, we can let It operate on both sides of the above equation and show that $|\lambda\rangle$ must be zero, which is not an interesting case. So it must not have an inverse and therefore is singular and has determinant zero.

$$det(L - \lambda \mathbf{I}) = \begin{vmatrix} (L_{11} - \lambda) & L_{12} & ... & L_{1n} \\ L_{21} & (L_{22} - \lambda) & ... & L_{2n} \\ ... & & & \\ L_{n1} & L_{n2} & ... & (L_{nn} - \lambda) \end{vmatrix} = 0$$

This gives an equation, the ***characteristic equation***, which (hopefully) may be solved for the eigenvalues. Then, putting the eigenvalues back into equation (2), one can solve for the eigenvectors.[3]

# 4. Unitarity and evolution in time

Susskind calls the minus-first law the statement that information is never lost, meaning that distinctions are conserved. The QM version of this is ***unitarity***, the fifth principle.

Principle 5. The evolution of state-vectors with time is ***unitary***.

This means that distinctions are conserved, which in turn means that eigenvectors remain orthogonal over time. If

$$\langle \Psi(0) | \Phi(0) \rangle = 0 \qquad (9)$$

and the ***time-development operator*** $\mathbf{U}$ is defined by

2 Susskind’s notation. Griffiths uses a different definition of the wave function, but this one keeps it separate from the state vector.

3 Griffiths, 476-7.

$$|\Psi(t)\rangle = \mathbf{U}(t)|\Psi(0)\rangle \tag{10}$$

then orthogonality leads to U being ***unitary***, meaning that

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{I} \tag{11}$$

the identity, i.e.

$$\langle i|\mathbf{U}^\dagger(t)\mathbf{U}(t)|j\rangle = \delta_{ij}. \tag{12}$$

Then time evolution is unitary. For small time $\epsilon$, we can write

$$\mathbf{U}(t) = \mathbf{I} - \epsilon\mathbf{H} \tag{13}$$

which leads to $\mathbf{H}$ being Hermitian

$$\mathbf{H}^\dagger = \mathbf{H} \tag{14}$$

and then (tossing in $\hbar$ to correct units)

$$\boxed{i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \mathbf{H}|\Psi\rangle} \tag{15}$$

which is the ***generalized*** (***time-dependent***) ***Schrödinger equation***. The presence of $\hbar$ gives $\mathbf{H}$ the units of energy: It is the ***quantum Hamiltonian***.

For another operator $\mathbf{L}$, one can show

$$\frac{d\langle L\rangle}{dt} = -\frac{i}{\hbar}\langle[L, H]\rangle \tag{16}$$

where the ***commutator***

$$[L, M] = LM - ML \tag{17}$$

Is in general not equal to zero. In classical mechanics, the time derivative can be expressed in terms of Poisson brackets as

$$\dot{F} = \{F, H\}$$

so that the correspondence between classical and quantum mechanics is

$$[F, G] \Leftrightarrow i\hbar\{F, G\} \tag{18}$$

where the smallness of $\hbar$ makes the term negligible in the classical limit. Then equation (16) expressed in classical mechanics becomes

$$\frac{dL}{dt} = \{L, H\} \tag{19}$$

So if the commutator of an observable with the Hamiltonian is zero, the quantity is conserved. The simplest case

$$[H, H] = 0$$

assures ***conservation of energy***. Possible energy states are represented by the eigenvalues of the Hamiltonian:

$$\mathbf{H}|E_j\rangle = E_j|E_j\rangle \tag{20}$$

Since the eigenvectors form a complete set of basis vectors,

$$|\Psi\rangle = \sum_i \alpha_i|E_i\rangle \tag{21}$$

and if the Hamiltonian does not depend explicitly on time, then

$$\alpha_j(t) = \alpha_j(0)e^{-\frac{i}{\hbar}E_j t}. \tag{22}$$

Since $\alpha_i(0) = \langle E_i|\Psi(0)\rangle$, then

$$|\Psi(t)\rangle = \sum_i |E_i\rangle\langle E_i|\Psi(0)\rangle e^{-\frac{i}{\hbar}E_j t} \tag{23}$$

# 5. Simultaneous observables and uncertainty

It is clear from

$$\mathbf{LM}|\lambda,\mu\rangle = \lambda\mu|\lambda,\mu\rangle$$

that if $|\lambda,\mu\rangle$ is a simultaneous eigenvector basis for the two operators $\mathbf{L}$ and $\mathbf{M}$, then the result is independent of order and the two operators must commute:

$$[\mathbf{L},\mathbf{M}]|\lambda,\mu\rangle = 0.$$

In classical mechanics

$$\{x,p\} = 1$$

and in quantum mechanics

$$[\mathbf{X},\mathbf{P}] = i\hbar.$$

The case of non-commutation of two operators $A$ and $B$ plus some geometry leads to the ***generalized uncertainty principle***:

$$\Delta A\Delta B \geq \frac{1}{2}\langle\Psi|[A,B]|\Psi\rangle. \tag{24}$$

This result is not a separate postulate, but a consequence of the statistical interpretation of QM. It can also be shown to be

$$\sigma_a^2\sigma_b^2 \geq \left(\frac{1}{2i}\langle[A,B]\rangle\right)^2 \tag{25}$$

where the standard deviation of an observable is given by

$$\sigma^2 = \langle(A-\langle A\rangle)\Psi|(A-\langle A\rangle)\Psi\rangle. \tag{26}$$

This quickly leads to the usual version concerning position and momentum

$$\Delta x\Delta p \geq \frac{\hbar}{2}$$

and can be shown to be true also for energy and time

$$\Delta E\Delta t \geq \frac{\hbar}{2}.$$

This is a QM result and has nothing to do with SR four-vectors.

“No experiment can ever beat this limitation.”[4]

# 6. Bases and representations

Define two linear operators

4 Susskind, 270.

$$\mathbf{X}\psi(x) = x\psi(x) \tag{27}$$

and

$$-i\hbar\mathbf{D}\psi(x) = -i\hbar\frac{d\psi(x)}{dx} := \mathbf{P}\psi(x) \tag{28}$$

which is the definition of the ***momentum operator***, the factor $-i\hbar$ being necessary to ensure that **P** be Hermitian and the units correct. The momentum eigen-equation then is

$$-i\hbar\frac{d\psi(x)}{dx} = p\psi(x) \tag{29}$$

of which normalized solutions are of the form

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}} \tag{30}$$

which is the equation in the x basis of a wave of wavelength

$$\lambda = \frac{2\pi\hbar}{p} \tag{31}$$

known as the ***De Broglie formula***. Equations (27) and (30) are in the ***x basis*** or ***position representation***. We could also write

$$\psi_p(x) = \frac{1}{\sqrt{2\pi}}e^{\frac{ipx}{\hbar}} = \langle x|p\rangle. \tag{32}$$

In the position representation, the probability for a given value of x (although we should multiply by dx and say for a given increment of x) is

$$P(x) = \psi^*(x)\psi(x) \tag{33}$$

and for a given value of momentum

$$P(p) = {\psi_p}^*(x)\psi_p(x).$$

But we can also say that

$$P(p) = \widetilde{\psi}^*(p)\widetilde{\psi}(p) \tag{34}$$

where $\widetilde{\psi}(p)$ is the wave function in the ***momentum representation***.

Slipping back into Dirac notation, define the identity operator in both bases

$$\mathbf{I} = \int dx|x\rangle\langle x| \tag{35}$$

and

$$\mathbf{I} = \int dp|p\rangle\langle p|. \tag{36}$$

Supposing a state vector $|\Psi\rangle$, the wave function in the position-representation is

$$\psi(x) = \langle x|\Psi\rangle \tag{37}$$

and in the momentum representations

$$\tilde{\psi}(p) = \langle p|\Psi\rangle. \tag{38}$$

Note the order here:

*The **wave function** is the **projection** of the **state vector onto** the **eigenvectors** of the*

***representation.***

This should be clear in equations (37) and (38).

Using the identity operator in the x basis

$$\tilde{\psi}(p) = \int dx \langle p|x\rangle\langle x|\Psi\rangle$$

so from the complex conjugate of the momentum eigenvector (32) and the wave function in the p basis (37),

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int dx e^{\frac{-ipx}{\hbar}} \psi(x). \tag{39}$$

Starting from the x-basis wave function (37) and using the identity operator (36) leads to

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int dp e^{\frac{ipx}{\hbar}} \widetilde{\psi}(p) \tag{40}$$

The two representations, position (40) and momentum (39), are ***Fourier transforms*** of each other. They are also the means for transforming a wave function from the position representation to the momentum representation and vice versa.

## 6.1. Useful example – the harmonic oscillator

This subject will help us ease into quantum field theory later on.

### 6.1.1. Simple harmonic oscillators (SHO)

A SHO is defined by a force proportional to the displacement of a mass and so a Schrödinger equation of the form

$$\Big( -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}Kx^2\Big)\psi = E\psi. \tag{41}$$

Solutions involve Hermite polynomials of degree n and the energy of each state is

$$E_n = \Big(n + \frac{1}{2}\Big)\hbar\omega, \tag{42}$$

where $\omega = \sqrt{K/m}$.

Skipping details such as the working out of the solutions to equation (41), define two *operators*

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} + \frac{i}{m\omega}\hat{p}\Big) \tag{43}$$

and its *complex (Hermitian) conjugate*

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\Big(\hat{x} - \frac{i}{m\omega}\hat{p}\Big) \tag{44}$$

in terms of operators $x_i$ and $\hat{p}$.[5] Note that

$$[\hat{a}, \hat{a}^\dagger] = 1.$$

The Hamiltonian then can be written

$$\hat{H} = \hbar\omega\Big(\hat{a}^\dagger\hat{a} + \frac{1}{2}\Big), \tag{45}$$

5 This section inspired mostly by Lancaster and Blundell, 19-23.

and the ***number operator***

$$\hat{n} = \hat{a}^\dagger \hat{a} \tag{46}$$

returns the number of units $\hbar\omega$ of energy in a given state:

$$\hat{n}|n\rangle = n|n\rangle. \tag{47}$$

Then $|n\rangle$ is also an ***eigenstate*** of the Hamiltonian, which may be written as

$$\hat{H} = \hbar\omega\left(\hat{n} + \frac{1}{2}\right) \tag{48}$$

so that

$$\hat{H}|n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|n\rangle \tag{49}$$

and the eigenvalues are equally spaced at intervals of $\hbar\omega$. Since

$$\hat{n}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger\hat{a}\hat{a}^\dagger|n\rangle = \hat{a}^\dagger(1 + \hat{a}^\dagger\hat{a})|n\rangle = (n+1)\hat{a}^\dagger|n\rangle, \tag{50}$$

it turns out that $\hat{a}^\dagger$ has the effect of increasing the energy of state $|n\rangle$; it is called a ***raising operator***.

Similarly,

$$\hat{n}\hat{a}|n\rangle = (n-1)|n\rangle, \tag{51}$$

so $\hat{a}$ is considered a ***lowering operator***. Since application of the raising operator to the ground state $|0\rangle$ can create any energy state, we can write the normalized state

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle.$$

### 6.1.2. Occupation number representation

We want a simple way to describe, in classical mechanics, a number of particles occupying momentum states. Rather than listing each particle and its momentum, we will consider how many particles there are in each momentum state. So we could have N particles and write their momentum states by

$$|n_1, n_2, n_3 ...\rangle \tag{52}$$

where $n_i$ is the number of particles in the i[th] momentum state.[6] This is called the ***occupation number representation***, since it says how many particles occupy each state. Acting on this state with the Hamiltonian and ignoring the ½ factor in equation (28) gives

$$\hat{H}|n_1, n_2, n_3 ...\rangle = (\sum_m \hat{H}_m)|n_1, n_2, n_3 ...\rangle = \Big[\sum_m n_{p_m} E_{p_m}\Big]|n_1, n_2, n_3 ...\rangle. \tag{53}$$

In this manner, the results of the preceding paragraphs on SHOs can be generalized to a state of N uncoupled SHOs. A creation or annihilation operator then exists for each member or the state, so that, for instance,

$$\hat{a}_2^\dagger|n_1, n_2, n_3 ...\rangle \propto |n_1, n_2 + 1, n_3 ...\rangle \tag{54}$$

and the operators obey the commutation relations

$$[\hat{a}_k, \hat{a}_q] = 0$$
$$[\hat{a}_k^\dagger, \hat{a}_q^\dagger] = 0$$

6 Lancaster and Blundell, 24, 30.

$$[\hat{a}_k, \hat{a}_q^\dagger] = \delta_{kq}. \tag{55}$$

Then the occupation number representation is

$$|n_1, n_2, ..., n_N\rangle = \frac{1}{\sqrt{n_1! n_2! ... n_N!}} (\hat{a}_1^\dagger)^{n_1} (\hat{a}_2^\dagger)^{n_2} ... (\hat{a}_N^\dagger)^{n_N} |0, 0, ...0\rangle \tag{56}$$

or

$$|\{n_k\}\rangle = \prod_k \frac{1}{\sqrt{n_k!}} (\hat{a}_k^\dagger)^{n_k} |0\rangle. \tag{57}$$

Since $\hat{a}^\dagger$ and $\hat{a}$ change the number of units in a state, we can call $\hat{a}^\dagger$ a ***creation operator*** and $\hat{a}$ an ***annihilation operator***.

### 6.1.3. Phonons

Now consider a linear chain of N coupled objects each of mass m and connected by springs. The normal positions of particle j is ja and it can be displaced by a small distance $x_j$. The Hamiltonian for the system is

$$\hat{H} = \sum_j \frac{\hat{p}_j^2}{2m} + \frac{1}{2} K (\hat{x}_{j+1} - \hat{x}_j)^2.$$

Since the structure is a sum of oscillators, its overall behavior is likely represented by a sum of waves of varying periodicity. So it is reasonable to look at its ***reciprocal space***, i.e., its decomposition in terms of frequencies of vibration.[7] The quantities which measure the wave distribution are simply the Fourier transforms from $\hat{x}$ and $\hat{p}$ representations to the $(\omega, \vec{k})$ representation. Enforcing periodic boundary conditions, one can define raising and lowering operators in the reciprocal space and derive a Hamiltonian of the same form as equation (24) summed over the different modes of the particles.[8]

$$\hat{H} = \sum_{k=1}^{N} \hbar\omega_k \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right). \tag{58}$$

The real-space coupled, oscillating masses behave in reciprocal space, the $(\omega, \vec{k})$ representation, as if they were independent oscillators, – as if uncoupled! These ***modes*** of the particles are called ***phonons***. Each such phonon mode can possess energy in an integral number of quanta – like particles.

This is comparable to N independent oscillators, each one possessing $n_{p_m}$ quanta of energy $\hbar\omega$. So we see an *analogy* between completely different systems, one of harmonic oscillators and one of identical particles.[9]

| Identical particles | SHO |
|---|---|
| Particles in momentum states | Quanta in oscillators |
| m$^{th}$ momentum mode $p_m$ | k$^{th}$ oscillator |
| $E = \sum_{m=1}^{N} n_{p_m} E_{p_m}$ | $E = \sum_{k=1}^{N} n_k \hbar\omega_k$ |

7 Reciprocal space, http://goodwin.chem.ox.ac.uk/goodwin/TEACHING_files/l1_handout.pdf.

8 Lancaster and Blundell, 25-26.

9 Lancaster and Blundell, 30.

Using creation and annihilation operators like those of equations (27) and (28) but with subscripts to denote the different particles, one can show that the reciprocal coordinate is given by[10]

$$\hat{x}_j = \frac{1}{\sqrt{N}}\Big(\frac{\hbar}{N}\Big)^{1/2}\sum_k \frac{1}{(2\omega_k)^{1/2}}[\hat{a}_k e^{ikja} + \hat{a}_k^\dagger e^{-ikja}]. \qquad (59)$$

This represents a time-independent position operator and is called the ***mode expansion*** of the scalar field.

# 7. Composite systems and entanglement

A state vector for two different, independent measurements or subsystems can be represented as a product of the two. But this is only one example of a state vector for a composite system, In general, they are not product states. For a product state, there exist two sets of normalization equations. For a spectrum of two states each with two eigenvalues, each is represented by two complex components and so four variables, but normalization reduces each by one and a negligible phase factor eliminates another, leaving only four independent components (degrees of freedom) for the product state. For a state vector for the same subsystems which is not a product state, there is only one normalization requirement and one phase factor, so there remain six independent parameters, making this a more complicated state. Such a state Is said to be ***entangled***.

The state of a system is a sum over basis vectors labeled by a collection of eigenvalues of mutually commuting operators. For instance, a may represent the eigenvalues of operator A, b of operator B and so on, so that the state vector for the composite system is

$$|\Psi\rangle = \sum_{a,b,\ldots}\langle a,b,\ldots|\Psi\rangle|a,b,\ldots\rangle = \sum_{a,b,\ldots}\psi(a,b,\ldots)|a,b,\ldots\rangle$$

where the set of components or projections

$$\psi(a,b,\ldots) = \langle a,b,\ldots|\Psi\rangle$$

is called the set of ***wave functions*** for the system in Susskind's terminology.[11] Griffiths calls $|\Psi\rangle$ the wave function. So watch out.

For a single state described by a state vector $|\Psi\rangle$, the basic formula for the ***expectation value*** of an observable whose operator is L is

$$\langle L\rangle = \langle\Psi|L|\Psi\rangle = \sum_{a\prime,a}\langle a\prime|\psi^*(a\prime)L\psi(a)|a\rangle = \sum_{a\prime,a}\psi^*(a\prime)\psi(a)L_{a\prime a}$$

where

$$L_{a\prime a} = \langle a\prime|L|a\rangle$$

is the matrix element of the operator L and a represents a complete set of observables for the system.

A composite system of two or more subsystems uses basis vectors labeled by eigenvalues of commuting operators for both subsystems. Such a system may or may not be described as a product system. Consider the case of two systems, Alice and Bob, with respective observables a and b, The composite state is formed by the tensor product of the subsystem state vectors and the composite wave functions are

$$\psi(a,b) = \langle ab|\psi\rangle.$$

Suppose Alice's and Bob's subsystems have observables represented by the operators L or M, each of

10 Lancaster and Blundell, 27, problem (2.3).

11 Susskind, 134.

which operates only on its own subsystem and leaves the other unchanged. Then

$$L_{a\prime a,b\prime b} = \langle a\prime b\prime|L|ab\rangle = \delta_{b\prime b}L_{a\prime a} \tag{60}$$

and similarly for Bob's subsystem.

if the two systems are completely independent (pure), the composite wave function may be given by a product of two wave functions. In this case.

$$\psi(ab) = \psi_A(a)\phi_B(b).$$

For such a product state,

$$\langle LM\rangle = \langle L\rangle\langle M\rangle$$

but for an entangled state, the ***correlation***

$$C(L,M) = \langle LM\rangle - \langle L\rangle\langle M\rangle \neq 0,$$

making this one way to test for an entangled system.

As an example, suppose that Alice and Bob each measure a two-valued observable (a spin, up or down) represented by an operator ($\sigma_A$ or $\sigma_B$). For the singlet state,

$$|sing\rangle = \frac{1}{\sqrt{2}}(|ud\rangle - |du\rangle),$$

$$\langle\sigma_{Az}\rangle = \langle\sigma_{Bz}\rangle = 0$$

but

$$\langle\sigma_{Az}\sigma_{Bz}\rangle = -1.$$

This means nothing is known about what a measurement of $\sigma_{Az}$ or $\sigma_{Bz}$ will give, each being equally likely to return +1 or -1. But once one is measured, the other is known. This state is ***maximally entangled***. The singlet state is an eigenstate of the operator

$$\vec{\sigma}_A \cdot \vec{\sigma}_B = \sigma_{Ax}\sigma_{Bx} + \sigma_{Ay}\sigma_{By} + \sigma_{Az}\sigma_{Bz}$$

with eigenvalue -3, although this observer is totally unknown to the separate subsystems. The full state is maximally characterized but *nothing* is known about the individual subsystems.[12]

It is not possible to isolate the wave functions of one subsystem of an entangled system. If we want to find the values of observables for one subsystem, the best we can do is use the density matrix, which describes the expected values. Since the observable L has no effect on the subsystem b part of the state, as in equation (60), the expected value of L is

$$\langle L\rangle = \sum_{a\prime,a,b\prime,b} \psi^*_{a\prime.b\prime}L_{a\prime a}\delta_{b\prime b}\psi_{ab} = \sum_{a\prime,a} \rho_{aa\prime}L_{a\prime a} \tag{61}$$

where the ***density matrix***

$$\rho_{aa\prime} = \sum_b \psi^*_{a\prime b}\psi_{ab} \quad ` \tag{62}$$

represents all A needs to know to calculate her system. Although subsystem A is a mixed state, not a pure one, the density matrix represents *everything* Alice can know about her subsystem, the expectation values of her variables being not at all affected by Bob's subsystem.

Equation (61) can be written as

12 Susskind, 174, 178; notes on on-line lectures 6 and 7.

$$\langle L \rangle = \sum_{a\prime,a} \rho_{aa\prime} L_{a\prime a} = \sum_{a} (\sum_{a\prime} \rho_{aa\prime} L_{a\prime a}) = Tr(\rho L),$$

so the expectation value is the trace of the density matrix time the matrix elements of the observable. This shows the usefulness of knowing the density matrix, but it fails to explain how that is easier than knowing the wave function since that still is necessary in order to construct the density matrix..

Even if his subsystem changes, but conserving distinctions, therefore by a unitary transformation U such that

$$\mathbf{U}^{\dagger}\mathbf{U} = \mathbf{I}$$

Alice's density matrix is unchanged.

$$\rho^{A}_{aa\prime} = \sum_{bb\prime\prime b\prime} \psi^{*}(a\prime b\prime\prime)(U^{\dagger}_{b\prime\prime b} U_{bb\prime})\psi(ab\prime) = \sum_{b\prime} \psi^{*}(a\prime b\prime)\psi(ab\prime) = \rho^{A}_{aa\prime}$$

This is what Susskind calls ***locality***: Bob's system, even if it is entangled with Alice's, has no influence on Alice's statistical predictions. This is all about expectation values, in the spirit of quantum mechanics. Adding the least little bit of non-unitary evolution to Bob's subsystem would mean that he could influence Alice's subsystem *faster than the speed of light*.

# 8. Bibliography


Griffiths, David J. and Schroeter, Darrell F. Introduction to quantum mechanis, 3rd edition. Cambridge: Cambridge University Press, 2018. Print.

Susskind, Leonard and Friedman, Art. *Quantum mechanics, the theoretical minimum*. New York: Basic Books, 2014. Print.

Susskind, Leonard. *The theoretical minimum: Quantum mechanics*. (Especially lectures 6 and 7 on entanglement.) http://theoreticalminimum.com/courses/quantum-mechanics/2012/winter. On-line lectures.