Fundamental Concepts-Introduction to Quantum Mechanics

- The first quantum theory: Max Planck and black-body radiation
- Photons: the quantization of light
  - The photoelectric effect
  - Consequences of the light being quantized
- The quantization of matter: the Bohr model of the atom
- Wave-particle duality
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- Spin
- Development of modern quantum mechanics
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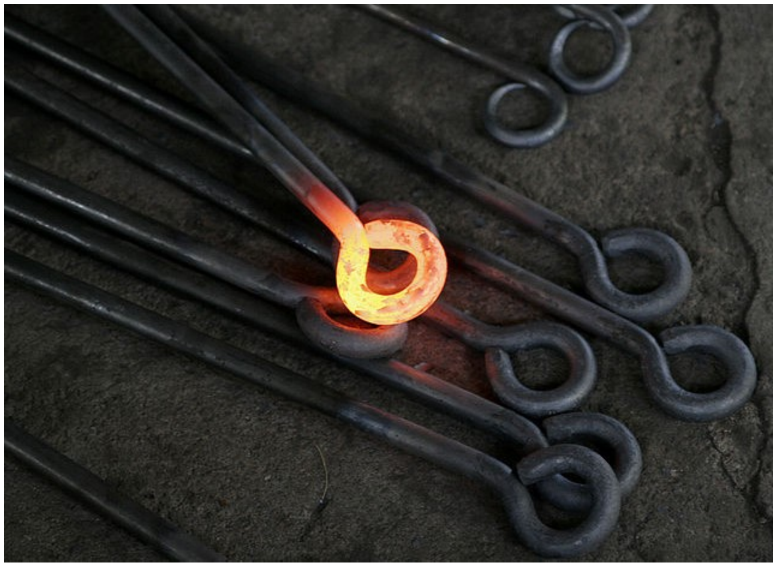
- Quantum field theory
- Quantum electrodynamics

Fundamental Concepts-Introduction to Quantum Mechanics

- The first quantum theory: Max Planck and black-body radiation

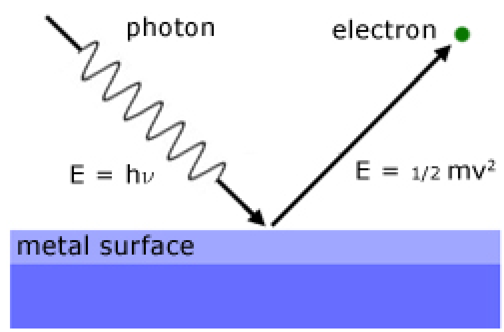


Hot metalwork. The yellow-orange glow is the visible part of the thermal radiation emitted due to the high temperature. Everything else in the picture is glowing with thermal radiation as well, but less brightly and at longer wavelengths than the human eye can detect. A far-infrared camera can observe this radiation.

Fundamental Concepts-Introduction to Quantum Mechanics

- Photons: the quantization of light
  - In 1905, Albert Einstein took an extra step. He suggested that quantization was not just a mathematical construct, but that the energy in a beam of light actually occurs in individual packets, which are now called photons.
  - The energy of a single photon is given by its frequency multiplied by Planck's constant:

$$E=hf$$



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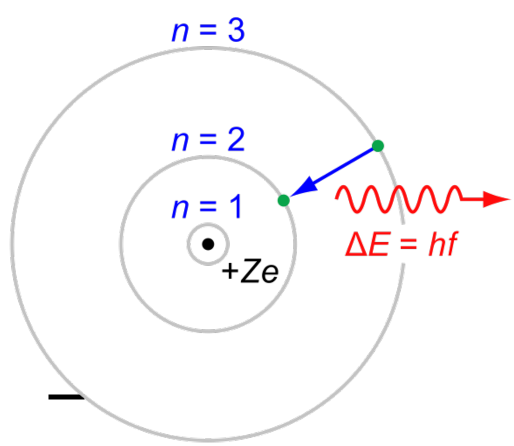
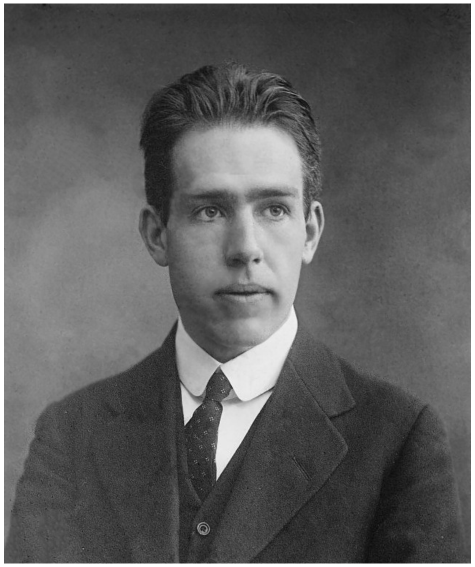
- The quantization of matter: the Bohr model of the atom
  – In 1913 Niels Bohr proposed a new model of the atom that included quantized electron orbits: electrons still orbit the nucleus much as planets orbit around the sun, but they are only permitted to inhabit certain orbits, not to orbit at any distance.



The Bohr model of the atom, showing an electron transitioning from one orbit to another by emitting a photon.



Fundamental Concepts-Introduction to Quantum Mechanics

- Wave-particle duality
  - Matter behaving as a wave was first demonstrated experimentally for electrons: a beam of electrons can exhibit diffraction, just like a beam of light or a water wave.

Louis de Broglie in 1929. De Broglie won the Nobel Prize in Physics for his prediction that matter acts as a wave, made in his 1924 PhD thesis.

  –

Fundamental Concepts-Introduction to Quantum Mechanics

- Spin
  - In 1922, Otto Stern and Walther Gerlach shot silver atoms through an (inhomogeneous) magnetic field.
  - They demonstrated that the property of the atom which corresponds to the magnet's orientation must be quantized, taking one of two values (either up or down), as opposed to being chosen freely from any angle.

Fundamental Concepts-Introduction to Quantum Mechanics

- Development of modern quantum mechanics
  - In 1925, Werner Heisenberg attempted to solve one of the problems that the Bohr model left unanswered, explaining the intensities of the different lines in the hydrogen emission spectrum.
  - In the same year, building on de Broglie's hypothesis, Erwin Schrödinger developed the equation that describes the behavior of a quantum mechanical wave. The mathematical model, called the Schrödinger equation after its creator, is central to quantum mechanics, defines the permitted stationary states of a quantum system, and describes how the quantum state of a physical system changes in time.

Erwin Rudolf Josef Alexander Schrödinger (12 August 1887–4 January 1961), was a Nobel Prize-winning Austrian physicist who developed a number of fundamental results in the field of quantum theory.

Werner Karl Heisenberg (5 December 1901 – 1 February 1976) was a German theoretical physicist and one of the key pioneers of quantum mechanics.

Fundamental Concepts-Introduction to Quantum Mechanics

- Copenhagen interpretation
  - The main principles of the Copenhagen interpretation are:
    - A system is completely described by a wave function, usually represented by the Greek letter {φ} ("psi"). (Heisenberg)
    - How {φ} changes over time is given by the Schrödinger equation.
    - The description of nature is essentially probabilistic.
    - It is not possible to know the values of all of the properties of the system at the same time; those properties that are not known with precision must be described by probabilities. (Heisenberg's uncertainty principle)
    - Matter, like energy, exhibits a wave–particle duality. An experiment can demonstrate the particle-like properties of matter, or its wave-like properties; but not both at the same time. (Complementarity principle due to Bohr)
    - Measuring devices are essentially classical devices, and measure classical properties such as position and momentum
    - The quantum mechanical description of large systems should closely approximate the classical description. (Correspondence principle of Bohr and Heisenberg)

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Linear algebra is the study of vector spaces and of linear operations on those vector spaces
- the chief obstacle to assimilation of the postulates of quantum mechanics is not the postulates themselves, but rather the large body of linear algebraic notions required to understand them.

This book is written as much to disturb and annoy as to instruct.
– The first line of *About Vectors, by Banesh Hoffmann.*

Life is complex – it has both real and imaginary parts.
- – Anonymous

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- The basic objects of linear algebra are *vector spaces*
- The vector space of most interest to us is C^n*, the space of all n-tuples of complex numbers, (z1, . . . , zn)*
- The elements of a vector space are called *vectors, and we will sometimes use the column matrix notation*
-

$$\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- In C^n *the addition operation for vectors is defined by*

$$\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} + \begin{bmatrix} z_1' \\ \vdots \\ z_n' \end{bmatrix} \equiv \begin{bmatrix} z_1 + z_1' \\ \vdots \\ z_n + z_n' \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- In a vector space there is a *multiplication by a scalar operation. In* C^n this operation is defined by

$$z \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} \equiv \begin{bmatrix} z z_1 \\ \vdots \\ z z_n \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Quantum mechanics is our main motivation for studying linear algebra, so we will use the standard notation of quantum mechanics for linear algebraic concepts. The standard quantum mechanical notation for a vector in a vector space is the following:

$$|\psi\rangle$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

Summary of some standard quantum mechanical notation for notions from linear algebra. This style of notation is known as the *Dirac notation*

Notation	Description
z^*	Complex conjugate of the complex number z. $(1+i)^* = 1-i$
$\|\psi\rangle$	Vector. Also known as a *ket*.
$\langle\psi\|$	Vector dual to $\|\psi\rangle$. Also known as a *bra*.
$\langle\varphi\|\psi\rangle$	Inner product between the vectors $\|\varphi\rangle$ and $\|\psi\rangle$.
$\|\varphi\rangle \otimes \|\psi\rangle$	Tensor product of $\|\varphi\rangle$ and $\|\psi\rangle$.
$\|\varphi\rangle\|\psi\rangle$	Abbreviated notation for tensor product of $\|\varphi\rangle$ and $\|\psi\rangle$.
A^*	Complex conjugate of the A matrix.
A^T	Transpose of the A matrix.
$A^\dagger$	Hermitian conjugate or adjoint of the A matrix, $A^\dagger = (A^T)^*$. $\begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$.
$\langle\varphi\|A\|\psi\rangle$	Inner product between $\|\varphi\rangle$ and $A\|\psi\rangle$. Equivalently, inner product between $A^\dagger\|\varphi\rangle$ and $\|\psi\rangle$.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Bases and linear independence
  - A *spanning set for a vector space is a set of vectors*

$$|v_1\rangle, \ldots, |v_n\rangle$$

  - *such that any vector |v> in the vector space can be written as a linear combination*

$$|v\rangle = \sum_i a_i|v_i\rangle$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- For example, a spanning set for the vector space C^2 is the set

$$|v_1\rangle \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix}; \quad |v_2\rangle \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- since any vector

$$|v\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

- in C^2 can be written as a linear combination
-

$$|v\rangle = a_1|v_1\rangle + a_2|v_2\rangle$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Generally, a vector space may have many different spanning sets. A second spanning set for the vector space C^2 is the set:

$$|v_1\rangle \equiv \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}; \quad |v_2\rangle \equiv \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

- Since any arbitrary vector can be written as follows:

$$|v\rangle = \frac{a_1 + a_2}{\sqrt{2}}|v_1\rangle + \frac{a_1 - a_2}{\sqrt{2}}|v_2\rangle$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A set of non-zero vectors *|v_1>, . . . , |v_n> are linearly dependent if there exists a set of* complex numbers *a_1, . . . , a_n with $a_i \neq 0$ for at least one value of i, such that*

$$a_1|v_1\rangle + a_2|v_2\rangle + \cdots + a_n|v_n\rangle = 0$$

- A set of vectors is *linearly independent if it is not linearly dependent.*
- It can be shown that any two sets of linearly independent vectors which span a vector space *V contain the* same number of elements. We call such a set a *basis for V .*
- (Linear dependence: example) Show that (1,−1), (1, 2) and (2, 1) are linearly dependent.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Linear operators and matrices
  - A *linear operator between vector spaces V and W is defined to be any function A : V → W which is linear in its inputs,*

$$A\left(\sum_i a_i|v_i\rangle\right) = \sum_i a_i A\left(|v_i\rangle\right)$$

- An important linear operator on any vector space *V is the identity operator,* I_V, *defined by* the equation

$$I_V|v\rangle \equiv |v\rangle$$

-

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Suppose *V,W, and X are vector spaces, and A : V → W and B : W → X are* linear operators. Then we use the notation *BA to denote the composition of B with A,* defined by

$$(BA)(|v\rangle) \equiv B(A(|v\rangle))$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- The most convenient way to understand linear operators is in terms of their *matrix representations.* In fact, the linear operator and matrix viewpoints turn out to be completely equivalent. The matrix viewpoint may be more familiar to you, however. To see the connection, it helps to first understand that an *m by n complex matrix A with entries A_{ij} is in fact a linear operator sending vectors in the vector space C^n to the vector space* C^m, *under matrix multiplication of the matrix A by a vector in C^n. More precisely, the* claim that the matrix *A is a linear operator just means that*
- $$A\left(\sum_i a_i|v_i\rangle\right) = \sum_i a_i A|v_i\rangle$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- The Pauli matrices
  - Four extremely useful matrices which we shall often have occasion to use are the *Pauli matrices.*
  - The Pauli matrices are so useful in the study of quantum computation and quantum information

$$\sigma_0 \equiv I \equiv \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \sigma_1 \equiv \sigma_x \equiv X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_2 \equiv \sigma_y \equiv Y \equiv \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma_3 \equiv \sigma_z \equiv Z \equiv \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Inner Products
  - An inner product is a function which takes as input two vectors |v> and |w> from a vector space and produces a complex number as output
  - The standard quantum mechanical notation for the inner product (|v>, |w>) is <v|w>

$$\langle v|(|w\rangle) \equiv \langle v|w\rangle \equiv (|v\rangle, |w\rangle)$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A function (·, ·) *from V × V to C is an inner product if it satisfies the requirements* that:
  - 1) (·, ·) is linear in the second argument,

$$\left(|v\rangle, \sum_i \lambda_i |w_i\rangle\right) = \sum_i \lambda_i \left(|v\rangle, |w_i\rangle\right)$$

  - 2) (|v>, |w>) = (|w>, |v>)*
  - 3) (|v>, |v>) ≥ 0 with equality if and only if |v> = 0.
  - For example, C^n has an inner product defined by
  - $$((y_1, \ldots, y_n), (z_1, \ldots, z_n)) \equiv \sum_i y_i^* z_i = \left[y_1^* \ldots y_n^*\right] \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: Show that any inner product $(\cdot, \cdot)$ is conjugate-linear in the first argument,

$$\left(\sum_i \lambda_i |w_i\rangle, |v\rangle\right) = \sum_i \lambda_i^* (|w_i\rangle, |v\rangle).$$

- Discussions of quantum mechanics often refer to *Hilbert space.*
- Vectors |w> and |v> are orthogonal if their inner product is zero.
- We define the norm of a vector |v> by
- $$\| |v\rangle \| \equiv \sqrt{\langle v|v\rangle}\,.$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A unit vector is a vector |v> such that, $\| |v\rangle \| = 1.$

- We also say that |v> is normalized if $\| |v\rangle \| = 1.$

- It is convenient to talk of normalizing a vector by dividing by its norm;

$$|v\rangle / \| |v\rangle \|$$

- A set |i> of vectors with index i is ortho-normal if each vector is a unit vector, and distinct vectors in the set are orthogonal, that is, <i|j> = δ_{ij}, where i and j are both chosen from the index set

- Exercise : Verify that |w ≡ (1, 1) and |v ≡ (1,−1) are orthogonal. What are the normalized forms of these vectors?

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Suppose $|w_1\rangle, \ldots, |w_d\rangle$ is a basis set for some vector space V with an inner product. There is a useful method, the *Gram–Schmidt* procedure, which can be used to produce an ortho-normal basis set $|v_1\rangle, \ldots, |v_d\rangle$ for the vector space V . Define $|v_1\rangle \equiv |w_1\rangle / \| |w_1\rangle \|$, and for $1 \leq k \leq d - 1$ define $|v_{k+1}\rangle$ inductively by
- $$|v_{k+1}\rangle \equiv \frac{|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle}{\| |w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle \|}.$$
- Exercise : Prove that the *Gram–Schmidt* procedure produces an ortho-normal basis for *V* .

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- From now on, when we speak of a matrix representation for a linear operator, we mean a matrix representation with respect to ortho-normal input and output bases.
- We also use the convention that if the input and output spaces for a linear operator are the same, then the input and output bases are the same, unless noted otherwise.
- With these conventions, the inner product on a Hilbert space can be given a convenient matrix representation.

$$\langle v|w\rangle = \left(\sum_i v_i|i\rangle, \sum_j w_j|j\rangle\right) = \sum_{ij} v_i^* w_j \delta_{ij} = \sum_i v_i^* w_i$$

- $$= [v_1^* \ldots v_n^*] \begin{bmatrix} w_1 \\ \vdots \\ w_n \end{bmatrix}.$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- There is a useful way of representing linear operators which makes use of the inner product, known as the outer product representation. Suppose |v> is a vector in an inner product space V , and |w> is a vector in an inner product space W. Define |w><v| to be the linear operator from V to W whose action is defined by

$$\left(|w\rangle\langle v|\right)\left(|v'\rangle\right) \equiv |w\rangle\,\langle v|v'\rangle = \langle v|v'\rangle|w\rangle.$$

-

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- The usefulness of the outer product notation can be discerned from an important result known as the completeness relation for ortho-normal vectors. Let |i> be any ortho-normal basis for the vector space V , so an arbitrary vector |v> can be written

$$|v\rangle = \sum_i v_i |i\rangle$$

- Note that <i|v> = v_i and therefore

- $$\left(\sum_i |i\rangle\langle i|\right)|v\rangle = \sum_i |i\rangle\langle i|v\rangle = \sum_i v_i|i\rangle = |v\rangle. \Rightarrow \sum_i |i\rangle\langle i| = I.$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- This equation is known as the completeness relation. One application of the completeness relation is to give a means for representing any operator in the outer product notation. Suppose A : V → W is a linear operator, $|v_i>$ is an ortho-normal basis for V , and $|w_j>$ an ortho-normal basis for W. Using the completeness relation twice we obtain
-

$$A = I_W A I_V \quad = \sum_{ij} |w_j\rangle\langle w_j|A|v_i\rangle\langle v_i| = \sum_{ij} \langle w_j|A|v_i\rangle |w_j\rangle\langle v_i|,$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Eigenvectors and eigenvalues
  - An *eigenvector* of a linear operator A on a vector space is a non-zero vector $|v\rangle$ such that $A|v\rangle = v|v\rangle$, where v is a complex number known as the *eigenvalue* of A corresponding to $|v\rangle$.
  - The *characteristic function* is defined to be $c(\lambda) \equiv \det |A-\lambda I|$, where det is the *determinant* function for matrices
  - The solutions of the *characteristic equation* $c(\lambda) = 0$ are the eigenvalues of the operator A.
  - The *eigenspace* corresponding to an eigenvalue v is the set of vectors which have eigenvalue v.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A *diagonal representation* for an operator *A* on a vector space *V* is a representation $A = \sum_i \lambda_i |i\rangle\langle i|$.
- where the vectors $|i\rangle$ form an orthonormal set of eigenvectors for *A*, with corresponding eigenvalues λ_i.
- An operator is said to be *diagonalizable* if it has a diagonal representation.
- As an example of a diagonal representation, note that the Pauli *Z* matrix may be written
- $$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|,$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Diagonal representations are sometimes also known as *orthonormal decompositions*.
- When an eigenspace is more than one dimensional we say that it is *degenerate*. For example, the matrix A defined by

$$A \equiv \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- has a two-dimensional eigenspace corresponding to the eigenvalue 2. The eigenvectors (1, 0, 0) and (0, 1, 0) are said to be *degenerate* because they are linearly independent eigenvectors of A with the same eigenvalue.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: (Eigendecomposition of the Pauli matrices) Find the eigenvectors, eigenvalues, and diagonal representations of the Pauli matrices *X*, *Y* , and *Z*.
- Exercise: Prove that the matrix $\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$
- is not diagonalizable.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Adjoints and Hermitian operators
  - Suppose *A* is any linear operator on a Hilbert space, *V* . It turns out that there exists a unique linear operator $A^\dagger$ on *V* such that for all vectors $|v\rangle, |w\rangle \in V$,

$$(|v\rangle, A|w\rangle) = (A^\dagger|v\rangle, |w\rangle).$$

- This linear operator is known as the *adjoint or Hermitian conjugate of the operator A.*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: If *|w> and |v> are any two vectors, show that* $(|w\rangle\langle v|)^{\dagger} = |v\rangle\langle w|$.
- Exercise: Show that $(A^{\dagger})^{\dagger} = A$.
- In a matrix representation of an operator *A, the action of the Hermitian conjugation* operation is to take the matrix of *A to the conjugate-transpose matrix,* $A^{\dagger} \equiv (A^{*})^{T}$, where the $*$ *indicates complex conjugation, and T indicates the transpose operation. For* example, we have
-
$$\begin{bmatrix} 1+3i & 2i \\ 1+i & 1-4i \end{bmatrix}^{\dagger} = \begin{bmatrix} 1-3i & 1-i \\ -2i & 1+4i \end{bmatrix}$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- An operator *A whose adjoint is A is known as a Hermitian or self-adjoint operator.*
- An important class of Hermitian operators is the *projectors. Suppose W is a k-dimensional vector subspace of the d-dimensional vector space V . Using the Gram*–Schmidt procedure it is possible to construct an orthonormal basis *|1>, . . . , |d> for V* such that *|1>, . . . , |k> is an ortho-normal basis for W. By definition,*

$$P \equiv \sum_{i=1}^{k} |i\rangle\langle i|$$

- is the *projector onto the subspace W.*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- It is easy to check that this definition is independent of the ortho-normal basis *|1>, . . . , |k> used for W. From the definition it can be shown that |v><v| is Hermitian for any vector |v>, so P is Hermitian,* $P^\dagger = P$.
- The *orthogonal complement of P is the operator* $Q \equiv I - P$. *It is easy to see that Q is* a projector onto the vector space spanned by *|k + 1>, . . . , |d>*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: Show that any projector *P satisfies the equation* $P^2 = P$.
- An operator *A is said to be normal if* $AA^\dagger = A^\dagger A$.
- Clearly, an operator which is Hermitian is also normal.
- There is a remarkable representation theorem for normal operators known as the *spectral decomposition, which states that an operator is a normal* operator if and only if it is diagonalizable.
- Exercise: Show that a normal matrix is Hermitian if and only if it has real eigenvalues.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A matrix *U is said to be unitary if* $U^\dagger U = I$.
- It is easily checked that an operator is unitary if and only if each of its matrix representations is unitary.
- A unitary operator also satisfies $UU^\dagger = I$, *and therefore U is* normal
- Geometrically, unitary operators are important because they preserve inner products between vectors.
- the inner product of *U|v> and U|w> is the same as the inner product* of *|v> and |w>,*

$$(U|v\rangle, U|w\rangle) = \langle v|U^\dagger U|w\rangle = \langle v|I|w\rangle = \langle v|w\rangle.$$

-

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- This result suggests the following elegant outer product representation of any unitary *U.* Let $|v_i\rangle$ *be any ortho-normal basis set. Define* $|w_i\rangle \equiv U|v_i\rangle$, *so* $|w_i\rangle$ *is also an ortho-normal* basis set, since unitary operators preserve inner products.
- if $|v_i\rangle$ *and* $|w_i\rangle$ *are any two ortho-normal bases, then it is easily checked that* the operator *U defined by*

$$U \equiv \sum_i |w_i\rangle\langle v_i|$$

- is a unitary operator.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: Show that all eigenvalues of a unitary matrix have modulus 1, that is, can be written in the form $e^{i\vartheta}$ *for some real* ϑ.
- Exercise: (Pauli matrices: Hermitian and unitary) Show that the Pauli matrices are Hermitian and unitary.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- A special subclass of Hermitian operators is extremely important. This is the *positive operators.*
- A positive operator *A is defined to be an operator such that for any vector |v>, (|v>,A|v>) is a real, non-negative number.*
- If *(|v>,A|v>) is strictly greater than zero for* all *|v> ≠ 0 then we say that A is positive definite.*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Exercise: Prove that two eigenvectors of a Hermitian operator with different eigenvalues are necessarily orthogonal.
- Exercise: Show that the eigenvalues of a projector *P are all either 0 or 1.*
- Exercise: (Hermiticity of positive operators) Show that a positive operator is necessarily Hermitian. (*Hint: Show that an arbitrary operator A can be* written *$A = B + iC$ where B and C are Hermitian.)*
- Exercise: Show that for any operator *A*, *$A^\dagger A$ is positive.*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Tensor products
  - The *tensor product is a way of putting vector spaces together to form larger vector spaces.*
  - This construction is crucial to understanding the quantum mechanics of multi-particle systems.
  - Suppose *V and W are vector spaces of dimension m and n respectively. For convenience* we also suppose that *V and W are Hilbert spaces.*
  - Then V $\otimes$W *(read 'V tensor W') is an mn dimensional vector space.*

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- We often use the abbreviated notations $|v\rangle|w\rangle$, $|v,w\rangle$ or even $|vw\rangle$ for the tensor product $|v\rangle\otimes|w\rangle$.
- By definition the tensor product satisfies the following basic properties:
  - (1) For an arbitrary scalar *z and elements* $|v\rangle$ *of V and* $|w\rangle$ *of W,*
  - $z(|v\rangle \otimes |w\rangle)=(z|v\rangle)\otimes |w\rangle = |v\rangle \otimes(z|w\rangle)$.
  - (2) For arbitrary $|v1\rangle$ and $|v2\rangle$ in V and $|w\rangle$ in W,
  - $(|v_1\rangle + |v_2\rangle)\otimes |w\rangle = |v_1\rangle \otimes |w\rangle + |v_2\rangle \otimes |w\rangle$.
  - (3) For arbitrary $|v\rangle$ in V and $|w_1\rangle$ and $|w_2\rangle$ in W,
  - $|v\rangle \otimes(|w1\rangle + |w2\rangle) = |v\rangle \otimes |w1\rangle + |v\rangle \otimes |w2\rangle$.

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- What sorts of linear operators act on the space V ⊗ W? Suppose |v> and |w> are vectors in V and W, and A and B are linear operators on V and W, respectively. Then we can define a linear operator A ⊗ B on V ⊗W by the equation

$$(A \otimes B)(|v\rangle \otimes |w\rangle) \equiv A|v\rangle \otimes B|w\rangle.$$

Fundamental Concepts-Introduction to Quantum Mechanics-Linear Algebra

- Suppose A is an m by n matrix, and B is a p by q matrix. Then we have the matrix representation:

$$A \otimes B \equiv \overbrace{\begin{bmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{bmatrix}}^{nq} \left.\vphantom{\begin{bmatrix} A \\ A \\ \vdots \\ A \end{bmatrix}}\right\} mp\,.$$

- In this representation terms like $A_{11}B$ denote p by q submatrices whose entries are proportional to B, with overall proportionality constant A_{11}. For example, the tensor product of the vectors (1, 2) and (2, 3) is the vector
-

$$\begin{bmatrix} 1 \\ 2 \end{bmatrix} \otimes \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 1 \times 2 \\ 1 \times 3 \\ 2 \times 2 \\ 2 \times 3 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 4 \\ 6 \end{bmatrix}$$

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- The tensor product of the Pauli matrices *X and Y is*

$$X \otimes Y = \begin{bmatrix} 0 \cdot Y & 1 \cdot Y \\ 1 \cdot Y & 0 \cdot Y \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{bmatrix}$$

- Finally, we mention the useful notation $|\psi\rangle^{\otimes k}$, which means $|\psi\rangle$ tensored with itself k times. For example $|\psi\rangle^{\otimes 2} = |\psi\rangle \otimes |\psi\rangle$.

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- Exercise: Let $|\psi\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Write out $|\psi\rangle^{\otimes 2}$ and $|\psi\rangle^{\otimes 3}$ explicitly, both in terms of tensor products like $|0\rangle|1\rangle$, and using the Kronecker product.
- Exercise: Calculate the matrix representation of the tensor products of the Pauli operators (a) X and Z; (b) I and X; (c) X and I.
- Exercise: Show that the tensor product of two unitary operators is unitary.
- Exercise: Show that the tensor product of two Hermitian operators is Hermitian.
- Exercise: Show that the tensor product of two positive operators is positive.

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- Exercise: Show that the tensor product of two projectors is a projector.
- Exercise: The Hadamard operator on one qubit may be written as

$$H = \frac{1}{\sqrt{2}}\left[(|0\rangle + |1\rangle)\langle 0| + (|0\rangle - |1\rangle)\langle 1|\right].$$

- Show explicitly that the Hadamard transform on *n qubits*, $H^{\otimes n}$, *may be written* as
- $$H^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x,y} (-1)^{x \cdot y} |x\rangle\langle y|.$$

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- Operator functions
  - It is possible to define a corresponding matrix function on normal matrices (or some subclass, such as the Hermitian matrices) by the following construction.

$$A = \sum_a a|a\rangle\langle a| \quad \Longrightarrow \quad f(A) \equiv \sum_a f(a)|a\rangle\langle a|$$

- As an example, $\exp(\theta Z) = \begin{bmatrix} e^{\theta} & 0 \\ 0 & e^{-\theta} \end{bmatrix}$

- since Z has eigenvectors |0> and |1>.

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- Another important matrix function is the *trace of a matrix. The trace of A is defined* to be the sum of its diagonal elements,

$$\mathrm{tr}(A) \equiv \sum_i A_{ii}.$$

- Exercise: Show that the Pauli matrices except for *I have trace zero.*
- Exercise: (Cyclic property of the trace) If A and B are two linear operators show that tr(AB) = tr(BA).
- Exercise: (Linearity of the trace) If A and B are two linear operators, show that tr(A + B) = tr(A) + tr(B)

- and if z is an arbitrary complex number show that
- tr(zA) = ztr(A).

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- If an operator is written down as an outer product, we take the trace by summing over inner products with the basis vectors. If we label a basis $|u_i>$, then

$$Tr(A) = \sum_{i=1}^{n} \langle u_i | A | u_i \rangle$$

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- Example:
- An operator expressed in the {|0>, |1>} basis is given by

$$A = 2i|0\rangle\langle 0| + 3|0\rangle\langle 1| - 2|1\rangle\langle 0| + 4|1\rangle\langle 1|$$

- Find the trace

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- Solution
- We find the trace by computing

$$Tr(A) = \sum_{i=1}^{n} \langle \phi_i | A | \phi_i \rangle = \langle 0 | A | 0 \rangle + \langle 1 | A | 1 \rangle$$

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- Then we compute each term individually and add the results. We have

$$\langle 0|A|0\rangle = \langle 0|(2i\,|0\rangle\langle 0| + 3|0\rangle\langle 1| - 2|1\rangle\langle 0| + 4|1\rangle\langle 1|)|0\rangle$$

$$= 2i\,\langle 0|0\rangle\langle 0|0\rangle + 3\langle 0|0\rangle\langle 1|0\rangle - 2\langle 0|1\rangle\langle 0|0\rangle + 4\langle 0|1\rangle\langle 1|0\rangle$$

- Recall that $\langle 0|1\rangle = \langle 1|0\rangle = 0$

- → $\langle 0|A|0\rangle = 2i\,\langle 0|0\rangle\,\langle 0|0\rangle$

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- Also recall that $\langle 0|0\rangle = \langle 1|1\rangle = 1$
- → $\langle 0|A|0\rangle = 2i\,\langle 0|0\rangle\langle 0|0\rangle = 2i$
- →

$$\begin{aligned}\langle 1|A|1\rangle &= \langle 1|(2i\,|0\rangle\langle 0| + 3|0\rangle\langle 1| - 2|1\rangle\langle 0| + 4|1\rangle\langle 1|)|1\rangle \\ &= 2i\,\langle 1|0\rangle\langle 0|1\rangle + 3\langle 1|0\rangle\langle 1|1\rangle - 2\langle 1|1\rangle\langle 0|1\rangle + 4\langle 1|1\rangle\langle 1|1\rangle \\ &= 4\langle 1|1\rangle\langle 1|1\rangle = 4\end{aligned}$$

- → $Tr(A) = \langle 0|A|0\rangle + \langle 1|A|1\rangle = 2i + 4$

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- **Important Properties of the Trace**
  - The trace is *cyclic*, meaning that $Tr(ABC)=Tr(CAB)=Tr(BCA)$.
  - The trace of an outer product is the inner product $Tr(|\varphi\rangle\langle\psi|)=\langle\varphi|\varphi\rangle$.
  - By extension of the above it follows that $Tr(A|\psi\rangle\langle\varphi|)=\langle\varphi|A|\psi\rangle$.
  - The trace is *basis independent*. Let $|u_i\rangle$ and $|v_i\rangle$ be two bases for some Hilbert space. Then $Tr(A)=\Sigma\langle u_i|A|u_i\rangle = \Sigma\langle v_i|A|v_i\rangle$.
  - The trace of an operator is equal to the sum of its eigenvalues. If the eigenvalues of A are labeled by λ_i, then

$$Tr(A) = \sum_{i=1}^{n} \lambda_i .$$

  - The trace is linear, meaning that $Tr(\alpha A)=\alpha Tr(A)$, $Tr(A+B)=Tr(A)+Tr(B)$.

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- **THE EXPECTATION VALUE OF AN OPERATOR**
  - The *expectation value* of an operator is the *mean* or *average value* of that operator with respect to a given quantum state.

$$\langle A \rangle = \langle \psi | A | \psi \rangle$$

  - Example:
  - A quantum system is in the state $|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$
  - What is the average or expectation value of *X* in this state?

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- Solution:
- We wish to calculate $\langle X \rangle = \langle \psi | X | \psi \rangle$. First let's write down the action of X on the state, recalling that $X|0\rangle = |1\rangle$, $X|1\rangle = |0\rangle$. We obtain

$$X|\psi\rangle = X\left(\frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle\right) = \frac{1}{\sqrt{3}}X|0\rangle + \sqrt{\frac{2}{3}}X|1\rangle = \frac{1}{\sqrt{3}}|1\rangle + \sqrt{\frac{2}{3}}|0\rangle$$

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- Using <0|1>=<1|0>=0, we find that

$$\begin{aligned}
\langle \psi | X | \psi \rangle &= \left(\frac{1}{\sqrt{3}} \langle 0| + \sqrt{\frac{2}{3}} \langle 1| \right) \left(\frac{1}{\sqrt{3}} |1\rangle + \sqrt{\frac{2}{3}} |0\rangle \right) \\
&= \frac{1}{3} \langle 0|1\rangle + \frac{\sqrt{2}}{3} \langle 0|0\rangle + \frac{\sqrt{2}}{3} \langle 1|1\rangle + \frac{2}{3} \langle 1|0\rangle \\
&= \frac{\sqrt{2}}{3} \langle 0|0\rangle + \frac{\sqrt{2}}{3} \langle 1|1\rangle \\
&= \frac{\sqrt{2}}{3} + \frac{\sqrt{2}}{3} = \frac{2\sqrt{2}}{3}
\end{aligned}$$

- It is important to recognize that the expectation value does not have to be a value that is ever actually measured. Remember, the eigenvalues of *X* are +1 and−1. No other value is ever measured for *X*, and the value we have found here for the average is never actually measured.

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- We can compute the expectation value of higher moments of an operator. It is common to compute

$$\langle A^2 \rangle$$

- This allows us to calculate the standard deviation or *uncertainty* for an operator, which is defined as

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

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- **UNITARY TRANSFORMATIONS**
  - A method known as a *unitary transformation* can be used to transform the matrix representation of an operator in one basis to a representation of that operator in another basis.
  - For simplicity, we consider the two dimensional vector space C^2. The *change of basis* matrix from a basis $|u_i>$ to a basis $|v_i>$ is given by

$$U = \begin{pmatrix} \langle v_1|u_1\rangle & \langle v_1|u_2\rangle \\ \langle v_2|u_1\rangle & \langle v_2|u_2\rangle \end{pmatrix}$$

$$|\psi'\rangle = U|\psi\rangle$$

$$A' = UAU^\dagger$$

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- Example:
- Find the change of basis matrix to go from the computational basis {|0>, |1>} to the {|±>} basis. Then use it to write

$$|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle$$

- And the operator $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$
- in the {|±>} basis

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- Solution:
  - Change of Basis → $U = \begin{pmatrix} \langle +|0\rangle & \langle +|1\rangle \\ \langle -|0\rangle & \langle -|1\rangle \end{pmatrix}$
  - and

$$\langle +|0\rangle = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$\langle +|1\rangle = (1/\sqrt{2})\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$\langle -|0\rangle = (1/\sqrt{2})\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$\langle -|1\rangle = (1/\sqrt{2})\begin{pmatrix} 1 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{1}{\sqrt{2}}$$

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- → $U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $U = U^\dagger$

$$|\psi\rangle = \frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}|1\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix}$$

$$|\psi'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ \sqrt{2} \end{pmatrix} = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+\sqrt{2} \\ 1-\sqrt{2} \end{pmatrix}$$

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$$TU^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ e^{i\pi/4} & -e^{i\pi/4} \end{pmatrix}$$

$$UTU^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ e^{i\pi/4} & -e^{i\pi/4} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 + e^{i\pi/4} & 1 - e^{i\pi/4} \\ 1 - e^{i\pi/4} & 1 + e^{i\pi/4} \end{pmatrix}$$

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- The commutator and anti-commutator
  - The commutator between two operators A and B is defined to be $[A,B] \equiv AB - BA$.
  - If $[A,B] = 0$, that is, $AB = BA$, then we say A commutes with B. Similarly, the anti-commutator of two operators A and B is defined by $\{A,B\} \equiv AB + BA$;
  - We say A anti-commutes with B if $\{A,B\} = 0$.

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- Exercise: (Commutation relations for the Pauli matrices) Verify the commutation relations

$$[X, Y] = 2iZ; \quad [Y, Z] = 2iX; \quad [Z, X] = 2iY.$$

- Exercise 2.41: (Anti-commutation relations for the Pauli matrices) Verify the anti-commutation relations

$$\{\sigma_i, \sigma_j\} = 0$$

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- **THE HEISENBERG UNCERTAINTY PRINCIPLE**
  - We can compute higher operator moments such as the mean value of A^2, which is given by

$$\langle A^2 \rangle = \langle \psi | A^2 | \psi \rangle$$

  - The *uncertainty A*, which is a statistical measure of the spread of measurements about the mean, is given by

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

  - Then, for two operators *A* and *B*, it can be shown that the product of their uncertainties satisfies

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

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- This is a generalization of the famous *Heisenberg uncertainty principle*. What this tells us is that there is a limit to the precision with which we can know the values of two incompatible observables simultaneously. The most famous uncertainty relation is that between position and momentum

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

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- The polar and singular value decompositions
  - The *polar and singular value decompositions are useful ways of breaking linear operators* up into simpler parts.
  - In particular, these decompositions allow us to break general linear operators up into products of unitary operators and positive operators.
  - While we don't understand the structure of general linear operators terribly well, we do understand unitary operators and positive operators in quite some detail.

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- *Theorem: (Polar decomposition) Let A be a linear operator on a vector space V .* Then there exists unitary *U and positive operators J and K such that*
- $A = UJ = KU,$
- where the unique positive operators *J and K satisfying these equations are* defined by $J \equiv \sqrt{A^\dagger A}$ *and* $K \equiv \sqrt{AA^\dagger}$. *Moreover, if A is invertible then U is* unique.
- We call the expression *$A = UJ$ the left polar decomposition of A, and $A = KU$ the right polar decomposition of A. Most often, we'll omit the 'right' or 'left' nomenclature,* and use the term 'polar decomposition' for both expressions, with context indicating which is meant.

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- *Corollary: (Singular value decomposition) Let A be a square matrix. Then* there exist unitary matrices *U and V , and a diagonal matrix D with* non-negative entries such that
- *$A = UDV$.*
- The diagonal elements of *D are called the singular values of A*
- *Proof: Book → Page 79*
- Exercise: Find the left and right polar decompositions of the matrix

$$\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$$