

1 Summary of Quantum Mechanics

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3 Quantum mechanics is based on three fundamental theoretical entities:

- 4 • **States:** they are conventionally symbolized as $|\psi\rangle, |\phi\rangle, \dots$ and called *kets*.
5 The scalar product between $|\psi\rangle$ and $|\phi\rangle$ is indicated by

$$\langle\psi|\phi\rangle = \langle\phi|\psi\rangle^* . \quad (1)$$

6 The dual $\langle\psi| = |\psi\rangle^\dagger$ is its transposed complex conjugated vector called a *bra*.
7 Kets and bras constitute what is known as the Dirac's algebra. States are taken
8 as normal (their norm is =1). Any quantized state $|\psi\rangle$ can be expanded thanks
9 to an orthonormal basis $\{|b_j\rangle\}$ in a Hilbert space with a certain dimension n :

$$\begin{aligned} |\psi\rangle &= \sum_{j=1}^n c_j |b_j\rangle \\ &= \sum_{j=1}^n \langle b_j | \psi \rangle |b_j\rangle , \end{aligned} \quad (2)$$

10 where the c_j 's are (in general complex) coefficients called *probability ampli-*
11 *tudes*. A basis is orthonormal if

$$12 \quad \forall j, \langle b_j | b_j \rangle = 1 \text{ and } \forall j \neq k, \langle b_j | b_k \rangle = 0.$$

13 It is said that the state $|\psi\rangle$ above represents a *superposition* of kets $|b_j\rangle$. The
14 vectors constituting the basis can be written:

$$|b_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix}, \quad |b_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \dots \\ 0 \end{pmatrix}, \quad |b_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \dots \\ 0 \end{pmatrix}, \quad \dots, \quad |b_n\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \dots \\ 1 \end{pmatrix},$$

15 so that we can write

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \\ c_n \end{pmatrix} \quad (3)$$

16 The explicit vectorial forms of the bras are written in terms of row vectors
 17 instead of columnar ones. The square modulus of any of the coefficients, e.g.

$$|c_j|^2 = |\langle b_j | \psi \rangle|^2 = \langle b_j | \psi \rangle \langle \psi | b_j \rangle = \wp_j \quad (4)$$

18 gives the probability \wp_j to get the component $|b_j\rangle$ when a system in the state
 19 $|\psi\rangle$ is measured. I recall that probabilities are normalized.

20 In the case in which the expansion of the state is continuous (paramountly a
 21 free particle), we need to substitute the sum with an integral:

$$|\psi\rangle = \int c(j) |j\rangle dj. \quad (5)$$

22 In such a case we have to replace the notion of probability with that of prob-
 23 ability density.

24 States can be operationally understood as equivalence classes of *preparations*
 25 (representing the first stage of a measurement process). For instance, a photon
 26 can be prepared in a state of linear polarization by either (i) symmetrically
 27 superposing two photons, the one in a vertical polarization state and the other
 28 in a horizontal polarization state, or (ii) letting a photon in an arbitrary po-
 29 larization state pass a polarization filter at 45° (in such a case a part of the
 30 photons will be eliminated).

31 • **Observables:** The observables \hat{O} are the degrees of freedom of a system. They
 32 are represented by matrices and are therefore called q-numbers for differentiat-
 33 ing them from ordinary scalar numbers. Moreover, any observable needs to be
 34 represented by a Hermitian operator, i.e. $\hat{O} = \hat{O}^\dagger$, where \hat{O}^\dagger is the conjugate
 35 transposed matrix of \hat{O} (we take the complex conjugate of each element o_{jk}
 36 and interchange columns and rows). The reason is that the eigenvalues of a
 37 Hermitian operator are real and not complex numbers. In the n -dimensional
 38 space, an observable \hat{O} can be written as:

$$\hat{O} = \begin{bmatrix} o_1 & 0 & \dots & 0 \\ 0 & o_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & o_n \end{bmatrix}, \quad (6)$$

39 where the o_1, o_2, \dots, o_n are the *eigenvalues* of \hat{O} , so that they satisfy the eigen-
 40 values equation

$$\hat{O} |o_j\rangle = o_j |o_j\rangle. \quad (7)$$

41 The eigenvalue o_j is that (real or rational) number that we get on a graduate
 42 scale of an apparatus when measuring the observable \hat{O} and having $|o_j\rangle$ as

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an outcome. The $|o_j\rangle$ are called eigenvectors of \hat{O} and constitute another orthonormal basis, i.e. $\forall |\psi\rangle$ of dimension n we can write

$$\begin{aligned} |\psi\rangle &= \sum_{j=1}^n \eta_j |o_j\rangle \\ &= \sum_{j=1}^n \langle o_j | \psi \rangle |o_j\rangle , \end{aligned} \quad (8)$$

where the $\eta_j = \langle o_j | \psi \rangle$ are again probability amplitudes. We can pass to one basis to another thanks to the following transformations:

$$\langle o_1 | \psi \rangle = (\langle o_1 | b_1 \rangle \langle b_1 | + \langle o_1 | b_2 \rangle \langle b_2 | + \dots + \langle o_1 | b_n \rangle \langle b_n |) |\psi\rangle , \quad (9a)$$

$$\langle o_2 | \psi \rangle = (\langle o_2 | b_1 \rangle \langle b_1 | + \langle o_2 | b_2 \rangle \langle b_2 | + \dots + \langle o_2 | b_n \rangle \langle b_n |) |\psi\rangle , \quad (9b)$$

$$\dots = \dots$$

$$\langle o_n | \psi \rangle = (\langle o_n | b_1 \rangle \langle b_1 | + \langle o_n | b_2 \rangle \langle b_2 | + \dots + \langle o_n | b_n \rangle \langle b_n |) |\psi\rangle . \quad (9c)$$

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These transformations can be written in a compact form as:

$$\begin{pmatrix} \langle o_1 | \psi \rangle \\ \langle o_2 | \psi \rangle \\ \dots \\ \langle o_n | \psi \rangle \end{pmatrix} = \begin{bmatrix} \langle o_1 | b_1 \rangle & \langle o_1 | b_2 \rangle & \dots & \langle o_1 | b_n \rangle \\ \langle o_2 | b_1 \rangle & \langle o_2 | b_2 \rangle & \dots & \langle o_2 | b_n \rangle \\ \dots & \dots & \dots & \dots \\ \langle o_n | b_1 \rangle & \langle o_n | b_2 \rangle & \dots & \langle o_n | b_n \rangle \end{bmatrix} \begin{pmatrix} \langle b_1 | \psi \rangle \\ \langle b_2 | \psi \rangle \\ \dots \\ \langle b_n | \psi \rangle \end{pmatrix} \quad (10)$$

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where the matrix

$$\hat{U} = \begin{bmatrix} \langle o_1 | b_1 \rangle & \langle o_1 | b_2 \rangle & \dots & \langle o_1 | b_n \rangle \\ \langle o_2 | b_1 \rangle & \langle o_2 | b_2 \rangle & \dots & \langle o_2 | b_n \rangle \\ \dots & \dots & \dots & \dots \\ \langle o_n | b_1 \rangle & \langle o_n | b_2 \rangle & \dots & \langle o_n | b_n \rangle \end{bmatrix} \quad (11)$$

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represents a *unitary* operator. Unitary operators express in quantum mechanics the concept of reversible transformations. They owe their name to the property

$$\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I} , \quad (12)$$

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where \hat{U}^\dagger is the conjugate transposed matrix of \hat{U} and \hat{I} is the identity matrix, i.e. the matrix that induces no transformation of the vectors and is the diagonal sum of all 1s (all other elements are 0):

$$\hat{I} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{bmatrix} . \quad (13)$$

53 Operationally speaking, an observable can be defined as an equivalence class
 54 of premeasurements (the second step of the measurement process). In fact,
 55 we can perform the same kind of experiment and decide to measure the path
 56 followed by the particle by either (i) choosing an interferometer (a device for
 57 splitting e.g. light beams) or (ii) performing a so-called double-slit experiment
 58 (we let a beam of particles or photons go to both or one of two slits on a
 59 screen or wall). In this step we couple (through an unitary transformation) an
 60 apparatus with an object system and in such a way we select a specific degree
 61 of freedom. In fact, when choosing to measure \hat{O} , we have

$$\hat{U}(|\psi\rangle|A_0\rangle) = \sum_j \xi_j |o_j\rangle |a_j\rangle, \quad (14)$$

62 where the ξ_j 's are some coupling constants, the apparatus is assumed to be
 63 in an initial (ready) state $|A_0\rangle$ but after the coupling is expanded in the basis
 64 $\{|a_j\rangle\}$ that is correlated with the basis $\{|o_j\rangle\}$. In fact, the two systems, as the
 65 result of this unitary transformation, are said to be *entangled*, that is, they are
 66 in a state that is no longer factorable (it cannot be written as product of two
 67 separated expansions). A factorable state in the simple case of two dimensions
 68 is:

$$|o_1\rangle|a_1\rangle + |o_2\rangle|a_2\rangle + |o_1\rangle|a_2\rangle + |o_2\rangle|a_1\rangle = (|o_1\rangle + |o_2\rangle)(|a_1\rangle + |a_2\rangle). \quad (15)$$

69 • **Properties:** Properties are assigned to quantum systems when certain detec-
 70 tion event occur. Detections represent the third and final step of a measure-
 71 ment process, so that the whole process can be understood as a sequence of
 72 (i) preparing a system with a certain information variety, (ii) establish a mu-
 73 tual information between apparatus and a system, and finally (iii) selecting a
 74 specific output, where this output itself cannot be controlled. In other words,
 75 we get say the eigenvalue o_j when the object system is collapsed into the state
 76 $|o_j\rangle$. In fact, the latter is only one of the possible components of the state (8).
 77 We represent this component (and therefore the relative property) by means
 78 of another operator called projector that has the peculiarity of having only a
 79 single 1 on the diagonal correspond into that component, otherwise we have
 80 all 0s. Supposing that e.g. this component is $|o_1\rangle$, we have

$$\begin{aligned} \hat{P}_1 = |o_1\rangle\langle o_1| &= \begin{pmatrix} 1 \\ 0 \\ \dots \\ 0 \end{pmatrix} (1 \ 0 \ \dots \ 0) \\ &= \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \end{bmatrix}, \end{aligned} \quad (16)$$

81 and similarly for the other components. The algebraic form that a projector
82 takes is

$$\hat{P}_k = |o_k\rangle\langle o_k|, \quad (17)$$

83 which when applied to an arbitrary state $|\psi\rangle$ immediately shows its selective
84 effect:

$$\begin{aligned} \hat{P}_k |\psi\rangle &= |o_k\rangle\langle o_k| \left(\sum_j \eta_j |o_j\rangle \right) \\ &= \eta_k |o_k\rangle, \end{aligned} \quad (18)$$

85 thanks to the properties of the scalar product among vectors of any orthonormal
86 basis. In other words, the projector \hat{P}_k acts on a state $|\psi\rangle$ by selecting the
87 component $|o_k\rangle$ with a reduced output $|\eta_k|^2 \leq 1$: for instance, a polarization
88 filter prepares systems in a certain state by throwing away a part of them.

Projectors have the following properties:

$$\hat{P}_j \hat{P}_k = \delta_{jk} \hat{P}_k, \quad (19a)$$

$$\sum_j \hat{P}_j = \hat{I}, \quad (19b)$$

89 where the sum must be understood over the whole orthonormal basis (for
90 instance, $\{|o_j\rangle\}$ for the object system). The previous formalism allows us to
91 write the observable \hat{O} as a sum of projectors in conjunction with eigenvalues:

$$\begin{aligned} \hat{O} &= o_1 \hat{P}_1 + o_2 \hat{P}_2 + \dots + o_n \hat{P}_n \\ &= o_1 \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \end{bmatrix} + o_2 \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \end{bmatrix} + \dots + o_n \begin{bmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 1 \end{bmatrix} \\ &= \begin{bmatrix} o_1 & 0 & \dots & 0 \\ 0 & o_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & o_n \end{bmatrix}. \end{aligned} \quad (20)$$

92 We can use projectors for writing any state in the following form:

$$\begin{aligned} \hat{\rho}_\psi &= \hat{P}_\psi = |\psi\rangle\langle\psi| \\ &= \sum_j |c_j|^2 |b_j\rangle\langle b_j| + \sum_{k \neq j} c_j c_k^* |b_j\rangle\langle b_k| \\ &= \begin{bmatrix} \wp_1 & c_1 c_2^* & \dots & c_1 c_n^* \\ c_2 c_1^* & \wp_2 & \dots & c_2 c_n^* \\ \dots & \dots & \dots & \dots \\ c_n c_1^* & c_n c_2^* & \dots & \wp_n \end{bmatrix}. \end{aligned} \quad (21)$$

93 The symbol $\hat{\rho}_\psi$ is called a density matrix. Note that the density matrix presents
 94 off-diagonal terms that are also called *interference terms*. In such a case the
 95 system is said to be in a *pure state* (it is represented by a single projector).
 96 However, a density matrix can represent a (proper) mixture (for instance, a
 97 collection of particles in different states) and here it is expressed by a weighted
 98 sum of projectors:

$$\hat{\rho}'_\psi = \sum_j \wp_j \hat{P}_j = \begin{bmatrix} \wp_1 & 0 & \dots & 0 \\ 0 & \wp_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & \wp_n \end{bmatrix}. \quad (22)$$

99 Such a density matrix is deprived of interference terms. Those terms corre-
 100 spond to the interference among different components of a superposition. Both
 101 for pure states and mixtures the trace of a density matrix (i.e. the sums of
 102 diagonal elements) is =1:

$$\text{Tr}(\hat{\rho}_\psi) = 1. \quad (23)$$

103 Note that a projector expresses a property, and therefore a density matrix can
 104 be considered an observable. However, it is a peculiar case of observable, one
 105 whose measurement will give each time either 0 or 1 as a result (due to the
 106 dual nature of every projector).

107 It is quite obvious that we can operationally conceive a property as an equiv-
 108 alence class of detection events as far as different detection events and even
 109 with different detectors allows us to assign the same property to the system.

110 Since quantum observables are expressed by operators, they may not commute. This
 111 is in particular true for the (one-dimensional) position operator \hat{x} and its conjugate
 112 momentum \hat{p}_x , i.e. $\hat{x}\hat{p}_x \neq \hat{p}_x\hat{x}$:

$$[\hat{x}, \hat{p}_x] = i\hbar\hat{I}, \quad (24)$$

113 which is valid for any state and where the expression

$$[\hat{x}, \hat{p}_x] = \hat{x}\hat{p}_x - \hat{p}_x\hat{x} \quad (25)$$

114 is called the commutator of these two observables. The constant $\hbar = h/2\pi$ is read
 115 *h-bar* and h is the Planck constant (which has the dimension of action), given by:

$$h = 6.626069 \times 10^{-34} \text{J} \cdot \text{s}. \quad (26)$$

116 The commutation relation tells us that inverting the sequence of the measurements
 117 of the two conjugate observables on any state will in general affect the final result.

118 A consequence of the above commutation relation is the uncertainty relation,
 119 where the uncertainty $\Delta\hat{O}$ of the observable \hat{O} in the state $|\psi\rangle$ is defined by the
 120 square root of its variance in that state:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}. \quad (27)$$

121 This fundamental relation tells us that any increase in the determination of any of
 122 the two observables is paid in terms of an increase in uncertainty of the other.

123 A crucial observable is the energy that governs the time evolution (and therefore
 124 the dynamics) of quantum systems. The (three-dimensional) quantum-mechanical
 125 Hamiltonian, as the classical one, is the sums of a kinetic and potential component:

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\hat{\mathbf{r}}). \quad (28)$$

126 This allows us to write the fundamental Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle. \quad (29)$$

127 The Schrödinger equation expresses a reversible dynamics and therefore can be writ-
 128 ten using an unitary operator:

$$|\psi(t)\rangle = \hat{U}_t(t-t_0) |\psi(t_0)\rangle, \quad (30)$$

129 where t_0 is some initial time. We can take advantage of the Stone's theorem and
 130 write the unitary operator in the form:

$$\hat{U}(t-t_0) = e^{-\frac{i}{\hbar} \hat{H}(t-t_0)}, \quad (31)$$

131 in accordance with the Schrödinger equation. Its conjugate transpose for $\tau = t - t_0$
 132 is

$$\hat{U}_t^\dagger(\tau) = \left(e^{-\frac{i}{\hbar} \hat{H}\tau} \right)^\dagger = e^{+\frac{i}{\hbar} \hat{H}\tau}. \quad (32)$$

133 Multiplying both sides of Eq. (30) by

$$\hat{U}_t^\dagger(\tau) = \hat{U}_{-t}(\tau) = \hat{U}_t(-\tau), \quad (33)$$

134 and using the unitarity property of $\hat{U}_t(\tau)$, we obtain

$$|\psi(t_0)\rangle = \hat{U}_t(-\tau) |\psi(t)\rangle, \quad (34)$$

135 showing, as anticipated, that time evolution in quantum mechanics is indeed re-
 136 versible. The eigenvalue equation of the energy can be written as

$$\hat{H} |\psi_n\rangle = E_n |\psi_n\rangle. \quad (35)$$

137 The eigenstates of the energy are called *stationary states* since do not evolve with
138 time.

139 An arbitrary initial state vector $|\psi(0)\rangle$ (where $0 = t_0$) can be expanded as a
140 superposition of the energy eigenstates $|\psi_n\rangle$ as

$$|\psi(0)\rangle = \sum_n c_n(0) |\psi_n\rangle , \quad (36)$$

where $c_n(0) = \langle \psi_n | \psi(0) \rangle$ are the coefficients of the expansion at the initial time. An arbitrary state vector $|\psi(t)\rangle$ at a later time $t > 0$ can be found by utilizing the time evolution operator $\hat{U}_t(t)$ (since, having set $t_0 = 0$, we have $\tau = t$). From Eq. (30) we obtain

$$\begin{aligned} |\psi(t)\rangle &= \hat{U}_t(t) |\psi(0)\rangle \\ &= \sum_n c_n(0) \hat{U}_t(t) |\psi_n\rangle \\ &= \sum_n c_n(0) e^{-\frac{i}{\hbar} E_n t} |\psi_n\rangle , \end{aligned} \quad (37)$$

141 where used has been made of the fact that $|\psi_n\rangle$ are stationary states with energy
142 E_n .