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QUANTUM MECHANICS SURVIVAL KIT

In order to help the Mathematicians to follow the lecture, we collect basic definitions and results in quantum mechanics which we will need. We do not provide derivations, nor do we thoroughly motivate the definitions. It must suffice that the formalism of quantum mechanics has proven extremely useful in the sense that the theory has an enormous wealth of predictive power and an extremely high precision. The formalism is the result of an evolution process lasting several decades, where the theory nowadays called quantum mechanics was established which successfully resolved all the puzzles a classical physics description of many phenomena and observations in atomic physics, nuclear physics, optics and other areas posed.

**States.** The state of a quantum mechanical system is described by a vector in an abstract, infinite dimensional, space  $\mathcal{H}$ . It is helpful to use Dirac's bra-ket notation in which the state is denoted by the "ket"  $|\psi\rangle$ . The vector property is motivated by the well known superposition principle of waves. This, we demand that states can be added to yield a new state.

One subtlety is that a state is admissible in quantum mechanics only if it can be normalized. Thus, we demand that  $||\psi\rangle|^2 < \infty$ . Actually, only the direction of the vector contains quantum mechanical information, its length is irrelevant as long as it is finite. Thus, we identify states  $|\psi\rangle$  and  $|\phi\rangle$  if there exists a non-zero number  $c \in \mathbb{C}$  such that  $|\psi\rangle = c|\phi\rangle$ .

To compare whether two quantum mechanical systems are in similar states, we need to compare relative directions of states. We thus assume that the space of states can be equipped with a sesqui-linear form  $\langle\phi|\psi\rangle$ . The important properties are

$$\begin{aligned}\langle\phi|\psi\rangle &= \overline{\langle\psi|\phi\rangle}, \\ \langle\phi|c\psi\rangle &= c\langle\phi|\psi\rangle, \\ \langle c\phi|\psi\rangle &= \bar{c}\langle\phi|\psi\rangle.\end{aligned}$$

This makes  $\mathcal{H}$  a projective Hilbert space. One may think of the "bra"-state  $\langle\psi|$  as the Hermitean conjugate of  $|\psi\rangle$ , i.e.  $\langle\psi| = \overline{(|\psi\rangle)^t}$ . Of course, we greatly simplify matters here. An example of such a space of states is provided by the space  $L^2(\mathbb{R})$  of square-integrable functions  $\psi(x)$  equipped with the sesqui-linear form  $\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} dx \phi(x)\psi(x)$ .

The sesqui-linear form implies a norm as it is positive definite if it is taken on a vector with itself.

**Operators.** On this space of states may act operators. A measurement  $A$  of a physical quantity on a quantum mechanical system is described by the action of a Hermitean operator  $\hat{A}$ . To any possible measurement such an operator, called *observable*, can be assigned. Let  $A$  denote an arbitrary measurement device which may, for any individual measurement, yield one of its possible values  $a_1, a_2, \dots, a_i, \dots$ . The set of possible values may be finite, countable or even continuous.

Quantum mechanics is based on the assumption that to any such measurement value  $a_i$  of an (ideal) measurement device  $A$  one can prepare a state  $|\Lambda_i\rangle$  such that the measurement  $A$  on this state  $|\Lambda_i\rangle$  will yield this measurement value  $a_i$  with certainty.

However, experimental observation tells us that for a given, ideally prepared state  $|\psi\rangle$ , there always exist measurements  $A$  such that it cannot be predicted which of its measurement values  $a_1, a_2, \dots, a_n, \dots$  will actually be observed.

The experimental observation that repeated measurements  $A$  on identical states  $|\psi\rangle$  yield different values in random order and only with certain probabilities for each possible value is encoded in the following basic equation: If the state  $|\psi\rangle$  is measured with a device  $A$ , then

$$w(i, A, |\psi\rangle) = |\langle\Lambda_i|\psi\rangle|^2$$

is the probability that the  $i^{\text{th}}$  value  $a_i$  is observed. (For the sake of simplicity, we assume here that  $A$  distinguishes so fine that there belongs just one state  $|\Lambda_i\rangle$  to each possible value  $a_i$ . This state is called *Eigenstate* of  $A$  to the *Eigenvalue*  $a_i$ . If there is just one Eigenstate to a given measurement value, we say that this value is non-degenerate.) The scalar product  $\langle\Lambda_i|\psi\rangle$  is called the *probability amplitude*.

**Elementary consequences.** Our assumption on the Eigenstates imply that measurement with  $A$  on one of its Eigenstates  $|\Lambda_i\rangle$  yields the value  $a_i$  with certainty, i.e.  $w(i, A, |\Lambda_i\rangle) = |\langle\Lambda_i|\Lambda_i\rangle|^2 = 1$ . Thus, the Eigenstates are normalized,

$\langle \Lambda_i | \Lambda_i \rangle = 1$ . Moreover, if we measure with  $A$  on  $|\Lambda_j\rangle$  with  $j \neq i$ , the value  $a_i$  will be never observed, i.e.  $w(i, A, |\Lambda_j\rangle) = |\langle \Lambda_i | \Lambda_j \rangle|^2 = 0$ . Thus, Eigenstates to different Eigenvalues are orthogonal to each other, and we have

$$\langle \Lambda_i | \Lambda_j \rangle = \delta_{ij}.$$

More generally, an arbitrary normalized state  $|\psi\rangle$  is only fixed up to a complex phase, as for any observation  $A$  we have

$$w(i, A, |\psi\rangle) = w(i, A, e^{i\alpha}|\psi\rangle) \quad \forall \alpha \in \mathbb{R}.$$

More elegant is the formulation of states in terms of rays in Hilbert space. This means that we relax the condition that state be normalized vectors. Instead, states are equivalence classes. To any vector  $|\psi\rangle \neq 0$  in the Hilbert space we associate the complex one-dimensional subspace spanned by it as its ray. The fundamental equation is then modified to

$$w(i, A, |\psi\rangle) = \frac{|\langle \Lambda_i | \psi \rangle|^2}{\langle \Lambda_i | \Lambda_i \rangle \langle \psi | \psi \rangle}.$$

The drawback of this formulation is that rays cannot be simply added like vectors. Representatives  $|\psi\rangle$  and  $|\phi\rangle$  of two rays can, however, yield arbitrary superpositions in form of rays belonging to  $a|\psi\rangle + b|\phi\rangle \neq 0$ . The different superpositions of two states  $|\psi\rangle$  and  $|\phi\rangle$  form the space  $\mathbb{CP}^1 = S^2$ . Every superposition can be thought of as a point on a two-dimensional sphere. Superposition of two states is, in contrast to vector addition, neither associative nor commutative.

The rays in Hilbert space may be represented by corresponding projection operators

$$\Pi_{i,A} = \frac{|\Lambda_i\rangle\langle\Lambda_i|}{\langle\Lambda_i|\Lambda_i\rangle}$$

instead of representative vectors  $|\Lambda_i\rangle$ . For a generic state  $|\psi\rangle$ , we denote the corresponding projector by

$$\rho = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle},$$

which is called the *density matrix*. It is an Hermitean operator. The probability for observation of the  $i^{\text{th}}$  measurement value  $a_i$  of the observable  $A$  is the given by

$$w(i, A, \rho) = \text{tr}(\rho \Pi_{i,A}).$$

This form of the fundamental equation can easily be generalized to the case that Eigenvalues of  $A$  are degenerate, i.e. that the dimension of the Eigenspaces is larger than one. Let  $\{|\Lambda_{a,k}\rangle : k = 1, 2, \dots\}$  denote an orthonormal basis of the Eigenspace to Eigenvalue  $a$ . Then we further denote with  $\Pi_{a,A}$  the projector to the subspace spanned by all Eigenstates to Eigenvalue  $a$ ,

$$\Pi_{a,A} = \sum_k \frac{|\Lambda_{a,k}\rangle\langle\Lambda_{a,k}|}{\langle\Lambda_{a,k}|\Lambda_{a,k}\rangle}.$$

If we measure  $A$  on a state  $\rho$ , then the probability to observe the degenerate measurement value  $a$  is

$$w(a, A, \rho) = \text{tr}(\rho \Pi_{a,A}).$$

An interesting case is that the state  $|\psi\rangle$  is not pure, i.e. is not given as a sequence of identical objects in identical states on which repeated measurements can be performed. The typical case in physics is that the state  $|\psi\rangle$  is a mixture. The ensemble on which a measurement is performed thus consists out of a set of states  $|\psi_i\rangle$  which each appear with a certain (classical) probability  $p_i$ . The density matrix then reads

$$\rho = \sum_n p_n |\psi_n\rangle\langle\psi_n|, \quad \sum_n p_n = 1,$$

and obeys  $\text{tr}(\rho) = 1$ . The probability for a certain measurement value, however, is still given by  $w(i, A, \rho) = \langle \Lambda_i | \rho | \Lambda_i \rangle$ . It is easy to see that all Eigenvalues  $\rho_i$  of  $\rho$  are non-negative. A main diagonal element  $\langle \Lambda | \rho | \Lambda \rangle$  vanishes if and only if all products  $p_n \langle \psi_n | \Lambda \rangle$  vanish, i.e. if and only if  $\rho | \Lambda \rangle = 0$ .

**Completeness.** In quantum mechanics, we make one further assumption, namely that the Eigenstates  $|\Lambda_i\rangle$  form a basis. This means that any state  $|\psi\rangle$  may be written as a complex linear combination

$$|\psi\rangle = \sum_j |\Lambda_j\rangle \psi_j = \sum_j |\Lambda_j\rangle \langle \Lambda_j | \psi \rangle, \quad \psi_j \in \mathbb{C}.$$

Obviously, the components  $\psi_i$  are simply given by  $\psi_i = \langle \Lambda_i | \psi \rangle$ . The completeness of the set of Eigenstates of an observable  $A$  is often written in form of the equation

$$\sum_j |\Lambda_j\rangle \langle \Lambda_j| = \mathbb{I}.$$

The individual terms in this sum,  $\Pi_i = |\Lambda_i\rangle \langle \Lambda_i|$  are projectors to mutually orthogonal subspaces, i.e.  $\Pi_i^2 = \Pi_i$  and  $\Pi_i \Pi_j = 0$  for  $j \neq i$ .

**Matrix algebra.** The operator  $\hat{A}$  assigned to an observable is typically a Hermitean operator. The reason is that physically observable measurement values must be real numbers, i.e. the Eigenvalues of  $\hat{A}$  must be real. The quantities  $A_{ij} \equiv \langle \Lambda_i | \hat{A} | \Lambda_j \rangle$  are called the matrix elements of the operator  $\hat{A}$ .

The expectation value  $\langle \hat{A} \rangle$  of an operator  $A$  is the averaged sum of its possible measurement values (i.e. Eigenvalues), weighted with their respective probabilities,

$$\langle \hat{A} \rangle = \sum_i a_i w(i, A, \rho) = \text{tr}(\rho \hat{A}).$$

Here, the operator  $\hat{A}$  associated to the measurement  $A$  is given by

$$A = \sum_i a_i |\Lambda_i\rangle \langle \Lambda_i|.$$

The next important characterizing quantity of an ensemble  $\rho$  is the mean deviation. More precisely, one is interested in the expectation value of the squared deviation from the average value,

$$(\Delta_\rho A)^2 \langle (A - \langle A \rangle)^2 \rangle = \sum_n p_n \langle \psi_n | (A - \langle A \rangle)^2 | \psi_n \rangle = \langle A^2 \rangle - \langle A \rangle^2.$$

The quantity  $(\Delta_\rho A)$  is called the uncertainty of  $A$  in the ensemble  $\rho$ , and is non-negative. Obviously, it vanishes if and only if the ensemble consists entirely out of Eigenstates  $|\Lambda_n\rangle$  of  $A$ .

**Uncertainty relation.** Let us consider the sum

$$\sum_n p_n \left| \left( c_A (A - \langle A \rangle) + i c_B (B - \langle B \rangle) \right) \psi_n \right|^2 \geq 0$$

for real numbers  $c_A, c_B$  and Hermitean operators  $A, B$ . Evaluating it yields

$$\begin{aligned} 0 &\leq \sum_n p_n \left| \left( c_A (A - \langle A \rangle) + i c_B (B - \langle B \rangle) \right) \psi_n \right|^2 \\ &= \sum_n p_n \langle \psi_n | \left( c_A^2 \mathfrak{3}(A - \langle A \rangle)^2 + c_B^2 (B - \langle B \rangle)^2 + i c_A c_B [A, B] \right) | \psi_n \rangle \\ &= (c_A \Delta_\rho A + c_B \Delta_\rho B)^2 - c_A c_B \left( 2 \Delta_\rho A \Delta_\rho B - i \sum_n p_n \langle \psi_n | [A, B] | \psi_n \rangle \right). \end{aligned}$$

Substituting  $c_A = -\Delta_\rho B$  and  $c_B = \Delta_\rho A$  lets the first term vanish. As long as neither  $\Delta_\rho A$  nor  $\Delta_\rho B$  vanish, we have that  $-2c_A c_B > 0$ . This implies the lower bound

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

The absolute value follows since we can repeat the reasoning with  $A$  and  $B$  interchanged. Actually, the relation remains true if  $\Delta_\rho A = 0$  or  $\Delta_\rho B = 0$  as then the ensemble  $\rho$  consists entirely out of Eigenstates to  $A$  or  $B$ , respectively. Indeed, the expectation value of a commutator  $[A, B]$  vanishes in each Eigenstate of  $A$  or  $B$ .

**Correspondence principle.** The *correspondence principle* of Bohr states that to any classical, measurable, quantity an Hermitean (self-adjoint) operator can be assigned. We know from classical mechanics that conjugate quantities such as position  $x$  and momentum  $p$  obey the Poisson bracket relation  $\{x, p\} = 1$ . Dirac postulated that in quantum mechanics, the corresponding observables  $\hat{A}$  and  $\hat{B}$  to classical quantities  $a$  and  $b$  should obey  $[\hat{A}, \hat{B}] = i\hbar\widehat{\{a, b\}}$ . This leads, for example, to the canonical commutation relation  $[\hat{X}, \hat{P}] = i\hbar\mathbb{I}$ . As a consequence, the uncertainty relation for position and momentum reads

$$\Delta X \Delta P \geq \frac{1}{2} \hbar.$$

Here,  $\hbar$  denotes the  $h/(2\pi)$  with  $h$  Planck's constant. It is one of the fundamental constants of Nature. Its physical meaning is most easily understood by the fundamental relation  $E = \hbar\omega = h\nu$  which relates the energy of a photon to its wavelength.

**Caveats.** Much of this formalism with states in an infinite dimensional Hilbert space and operators acting on them is not as simple as it seems. There are many mathematical issues which need careful treatment before quantum mechanics can be considered a mathematical rigorously defined theory. For example, most operators associated to observables are unbounded operators. Let us illustrate this with an example.

Two often used operators are the observables  $X$  for position and  $P$  for momentum. Both admit continuous sets of Eigenstates in the following way:

$$\begin{aligned} \hat{X}|x\rangle &= x|x\rangle, & \hat{P}|p\rangle &= p|p\rangle, \\ \langle x'|x\rangle &= \delta(x - x'), & \langle p'|p\rangle &= 2\pi\delta(p - p'), \\ & & \langle x|p\rangle &= \exp(ipx), \end{aligned}$$

where  $\delta(x)$  denotes the Dirac  $\delta$ -distribution<sup>1</sup>. As these two observables are canonically conjugate to each other, i.e.  $[\hat{X}, \hat{P}] = i\hbar$ , they cannot both have a bounded spectrum. For example, position might be confined to a finite interval, but then momentum will be unbounded. Moreover, these operators cannot obey the canonical commutation relation when acting on a finite dimensional space  $\mathcal{H}$ , since then  $0 = \text{tr}(\hat{X}\hat{P} - \hat{P}\hat{X}) = \text{tr}([\hat{X}, \hat{P}]) = \text{tr}(i\hbar) = i\hbar\text{dim}\mathcal{H} \neq 0$  is a contradiction.

Actually, one often writes  $\psi(x)$  instead of  $\langle x|\psi\rangle$ . One says that  $\psi(x)$  is the coordinate-space representation of the state  $|\psi\rangle$ , called the wave amplitude or probability amplitude. We note here that the whole formalism of quantum mechanics is, for historical reasons, tailored to distinguish coordinate space. The reason is simply that this is closest to our every day experience. The most natural question to ask for a particle is, where it is. In classical physics, the trajectory of a particle is the fundamental object which now is replaced by the quantum mechanical state of it.

An object with the sole property to have a certain momentum is a plane wave propagating in the direction of the momentum and having a frequency given by absolute value of the momentum. This is what the meaning of  $\langle \vec{x}|\vec{p}\rangle = \exp(i/\hbar\vec{p} \cdot \vec{x})$  is<sup>2</sup>. (Often, one works in natural units where  $\hbar = c = 1$ .) Although it seems to be perfectly admissible to define a quantum mechanical object with the sole property of momentum, the resulting wave amplitude is not a square integrable function on  $\mathbb{R}^3$ . Plane waves are examples of non-normalizable states. Strictly speaking, they are not elements of the Hilbert space. One often reads the statement that the Eigenstates of the momentum operator lie on the boundary of the Hilbert space, although this is a mathematically ill-defined concept. One way out is to avoid using the Eigenstates of the momentum operator when working in the coordinate-space picture, and only use the states  $|x\rangle$ . However, we may use the linear functionals  $\langle p|$ , if we think of them as linear functionals instead of Hermitean conjugate states.

**Stone-von-Neumann theorem.** The *Stone-von-Neumann theorem* guarantees that for any pair of operators with canonical commutation relation  $[\hat{A}, \hat{B}] = \alpha\mathbb{I}$ , we can make the choice  $\hat{B} = b\mathbb{I}$ , where  $b$  is a classical variable such as an coordinate, and  $\hat{A} = \alpha\frac{\partial}{\partial b}$  is the partial derivation with respect to  $b$ . Actually, the theorem guarantees the relation between  $\hat{A}$  and  $\hat{B}$  even more generally. Independently of how  $\hat{B}$  is actually represented,  $\hat{A} = \alpha\frac{\partial}{\partial \hat{B}}$  can always be chosen to be the formal partial derivative with respect to the symbol  $\hat{B}$ . Thus, in the coordinate picture,  $\hat{X} = x$  is the classical coordinate,<sup>3</sup> while  $\hat{P} = -i\hbar\partial_x$  is proportional to differentiation with respect to the coordinate.

**Schrödinger equation.** According to the correspondence principle, we should associate to the classical, non-relativistic kinetic energy  $\frac{p^2}{2m}$  the Operator  $\frac{\hat{P}^2}{2m}$ . Note, that mass is a parameter in both, classical and quantum mechanics, and

<sup>1</sup>The  $\delta$ -distribution is a generalization of the Kronecker  $\delta$ -symbol to the continuous case. Its defining property is that for all function  $f(x)$  from a suitable space of test functions,  $\int dx\delta(x)f(x) = f(0)$  as long as zero is contained in the region of integration. Although,  $\delta(x)$  is not a function, one can make perfect sense out of it within the theory of distributions.

<sup>2</sup>Here, we switch to a notation which makes it clear that quantum mechanics usually is a theory for objects in our (three-dimensional) coordinate space. Of course, mathematically, we can define it for any space-dimension

<sup>3</sup>In physics literature, the identity operator is often omitted.

thus not lifted to an operator. The total energy of a system is encoded in the Hamiltonian  $H = \frac{p^2}{2m} + V(x)$  with  $V(x)$  an external potential, in which the mass particle moves. In the same sense as position and momentum are conjugate variables, energy and time are also conjugate to each other. Thus, in the coordinate picture with explicit time, energy gets replaced by the operator  $i\hbar\partial_t$ . Now, classically, we should have  $E = H$ . The correspondence principle demands that one structure should transfer unaltered from the classical to the quantum mechanical world: Namely, conserved quantities. Energy is conserved, and the conservation law is precisely that  $E = H = T + V$ . In the coordinate picture, this implies the Schrödinger equation  $\hat{E}|\psi\rangle = \hat{H}|\psi\rangle$  to take the form

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{x}, t) = \left(-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right)\psi(\vec{x}, t).$$

This equation encodes how the state  $|\psi\rangle$ , or in this case its amplitude  $\psi(\vec{x}, t) = \langle\vec{x}, t|\psi\rangle$ , evolves with time (infinitesimally). Note that we took one more step and changed the notation to the three-dimensional case, where  $\Delta = (\partial_x)^2 + (\partial_y)^2 + (\partial_z)^2$  is the Laplace operator.

Of particular interest are the Eigenstates of  $\hat{H}$ . Their corresponding eigenvalues are their respective energies. Eigenstates of  $\hat{H}$  are called stationary states, as they have a trivial time evolution. Typically, for a non-vanishing potential  $V(x)$ , they are the admissible bound states of the problem. If  $V(x) \equiv 0$ , the Hamiltonian is the one for a free moving particle. Its Eigenstates are, for example, the plane waves discussed above. There is no restriction on the momenta these plane waves may possess. Thus, there is no “quantization”. The so famous fact that energies are quantized in quantum mechanics arises solely due to the requirement that states have to be normalizable. In particular, for  $V(x) \neq 0$ , energy for bound states is quantized because only for certain values of the energy, the solution  $\psi(\vec{x})$  to the partial differential equation

$$E\psi(\vec{x}) = \left(-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right)\psi(\vec{x}).$$

will be square integrable. That alone is the secret of quantization of observable quantities in quantum mechanics.

For today, this must suffice as a first glance on quantum mechanics and its mathematical difficulties.