QUANTUM MECHANICS Lecture 2

Enrico Iacopini

QUANTUM MECHANICS Lecture 2 The Schrödinger equation The statistical interpretation The probability

Enrico Iacopini

September 4, 2019

D. J. Griffiths: paragraphs 1.1, 1.2 and 1.3

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Why QM ?

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- In the previous lecture we have seen the reasons why Classical Phyics had to be rewieved and a new Mechanics was necessary (⇒ QM).
- We have also said that QM represents a revolutionary departure from classical ideas and in many aspects it appears counterintuitive.
- Nevertheless, up to now, the QM predictions have always been found in perfect agreement with the experiments !

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The Schrödinger equation

In Quantum Mechanics, the particle dynamics is described by the Schrödinger equation, that, in one dimension, reads

 $i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\,\Psi$

This equation allow to evaluate the time evolution of the **"wave-function"** $\Psi = \Psi(x, t)$, that describes the physical state of the system under consideration. QUANTUM MECHANICS Lecture 2

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- The Schrödinger equation is the QM counterpart of the Newton's Lex II:
- 2 given the initial conditions and the force law (the potential energy V(x) ...), in CM, Lex II allow us to find the particle position x = x(t) as a function of time;
- imilarly, in QM, the Schrödinger equation allow us to determine the wave function $\Psi(x,t)$ at any time.
- However, everybody undestands the meaning of the trajectory equation x = x(t); but which is the meaning of the wave-function $\Psi(x, t)$ appearing in the Schrödinger equation ?

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It is precisely in the interpretation of the wave-function that there is **one of the most important differences with respect to the classical world.**

According to Max Born

 $|\Psi(\mathbf{x}, \mathbf{t})|^2$ is proportional to the **probability density** of finding the particle in the position x at time t.

It is the so called **Copenaghen** or statistical interpretation.



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More precisely, according to this interpretation, the probability of finding the particle between a and b at time t is given by

$$P(a, b; t) = \frac{\int_{a}^{b} dx \, |\Psi(x, t)|^{2}}{\int_{-\infty}^{+\infty} dx \, |\Psi(x, t)|^{2}}$$

2 This, in particular, requires that $\Psi(x, t)$ is a square-integrable function, or, in other words, that

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = A(t)$$

for some positive real time function A(t).

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According to QM, a physical state is fully described by its wave-function Ψ; although the correspondence is not one-to-one: an axiom of QM states that wave functions differing only by a complex multiplicative constant (different from zero) describe the same physical state.

 $\Psi(x,t)$ and $K \cdot \Psi(x,t)$ are equivalent

for any (non null) complex constant K.

This aspect has to do with the so-called normalization of the wave function, and we will come on this point later on. QUANTUM MECHANICS Lecture 2

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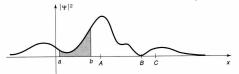
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Consequeces from the statistical interpretation

The most obvious consequence coming from the statistical interpretation is that the physical state af a particle, (fully) described by wave function Ψ, has an intrinsic, unavoidable indeterminacy.



The particle will be found very likely near A and never in B; but if we measure the particle position many times, starting from the same physical state, we will possibly get, each time, different results 1, 1, 1, 1, 2, 2

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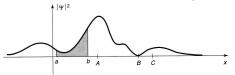
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- Assume now that, after a position measurement, we have got for the particle the position C. Can we say where the particle was just before the measurement ?
- 2 QM states that, before the measurement, since the state described by ψ implies only that there is a non-null probability, but not a certainty, to find the particle in *C*, we cannot say **nothing** about the particle position.
- This looks crazy, but it is like that ! Until a measurement is done, the particle is potentially where the wave function indicates a non-null probability.

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$\Psi \to \Psi'$

- In fact, now, the new wave function Ψ' must be such to give a probability peaked in C, with a virtually absence of spread around this position.
- It is the so called collapse of the wave function, another prediction of QM which was (and still is) not easy to digest.

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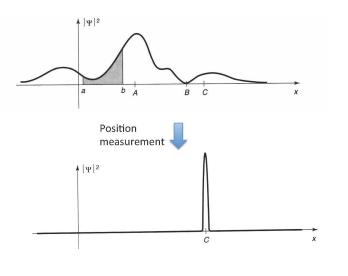
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The w.f. collapse



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The probability

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Because of the statistical interpretation of $|\Psi|^2$, it may be useful some reminder concerning the

Probability Theory ...



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Assume you have a perfect dice.

Which is the probability of getting, f.i., a 5 after a roll ?



• Everyone knows that this probability is P = 1/6.

The reason of this conclusion is that there are six different possibilities that should appear with the same frequency, and only one corresponds to the 5.

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MECHANICS Lecture 2

Enrico Iacopini

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MECHANICS Lecture 2

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- The probability of the event is identified with the ratio between the number of "positive" cases and their total number.

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- The probability of the event is identified with the ratio between the number of "positive" cases and their total number.
- Clearly, if instead of 5, we bet on any another number between 1 and 6, the probability remains 1/6 ...

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- But what about the probability that, with two dice, we obtain 12 as sum of the two ?

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- But what about the probability that, with two dice, we obtain 12 as sum of the two ?
- 2 Since the possibilities are now $6 \times 6 = 36$, and only in one case we can get 12 (with both dice giving a 6), the probability is 1/36.

QUANTUM MECHANICS Lecture 2

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And in case we bet on 11, the probability still remains 1/36 ?



No.

Because now there are two possibilities out of 36 to get 11, (6, 5) and (5, 6), therefore the probability becomes 2/36 = 1/18.

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Probability

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QUANTUM MECHANICS Lecture 2

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Probability

Probability of obtaining any sum from 2 to 12:



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$$12 : (6, 6) P = 1/36$$

$$11 : (6, 5), (5, 6) P = 2/36$$

$$10 : (6, 4), (4, 6), (5, 5) P = 3/36$$

$$9 : (6, 3), (3, 6), (5, 4), (4, 5) P = 4/36$$

$$8 : (6, 2), (2, 6), (5, 3), (3, 5), (4, 4) P = 5/36$$

$$7 : (6, 1), (1, 6), (5, 2), (2, 5), (4, 3), (3, 4) P = 6/36$$

$$6 : (5, 1), (1, 5), (4, 2), (2, 4), (3, 3) P = 5/36$$

$$5 : (4, 1), (1, 4), (3, 2), (2, 3) P = 4/36$$

$$4 : (3, 1), (1, 3), (2, 2) P = 3/36$$

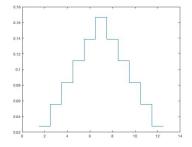
$$3 : (2, 1), (1, 2) P = 2/36$$

$$2 : (1, 1) P = 1/36$$

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Lecture 2

Enrico Iacopini



The probability distribution shows that the most probable value if 7, with a probability equal to $\mathbf{P} = \mathbf{1}/\mathbf{6}$.

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September 4, 2019 19 / 31

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Associated to the probability distribution, we can define the average (mean value) m as

$$m \equiv \sum_{s=2}^{12} s \cdot P(s) \equiv < s >$$

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- It is easy to see that, in our case, we obtain m = 7.
- But be careful: the average and the most probable value are a priori independent !

Take, f.i., the following probability distribution:

$$P(1) = 1/2 P(2) = 1/4 P(3) = 1/8 P(4) = 1/8$$

the most probable value is clearly 1, but the average value is

$$m = \sum_{s=1,4} P(s) \cdot s =$$

= $\frac{1}{2} \cdot 1 + \frac{1}{4} \cdot 2 + \frac{1}{8} \cdot 3 + \frac{1}{8} \cdot 4 = \frac{15}{8}$

QUANTUM MECHANICS Lecture 2

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Together with the average m ≡ < s >, another important quantity, which gives a measure of the spread of the probability distribution, is the variance D defined as

$$D \equiv \sum_{s} P(s) \left(s - \langle m \rangle \right)^2$$

The square root of the variance is called the standard deviation σ or the root mean square (r.m.s.) of the distribution

$$\sigma \equiv \sqrt{D} = \sqrt{\sum_{s} P(s) \left(s - \langle m \rangle\right)^2}$$

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QUANTUM MECHANICS Lecture 2

Enrico Iacopini

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We have (remember that
$$\sum_{s} P(s) = 1 \dots$$
)

$$\sigma^{2} = \sum_{s} P(s) \left(s^{2} - 2s < m > + < m >^{2} \right) =$$

$$= \left(\sum_{s} P(s) s^{2} \right) - 2 < m > < m > + < m >^{2} =$$

$$= < s^{2} > - < m >^{2}$$

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In case of a **continuous random variable**. the probability distribution is described by a probability density function (pdf) $\rho(x)$ such that

$$\bigcirc \rho(x) \ge 0$$

$$\int_{x_{min}}^{x_{max}}
ho(x)\,dx=1$$

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In the case of a continuous probability distribution, the average (mean) is defined as

$$m \equiv < x > = \int_{x_{min}}^{x_{max}} dx \;
ho(x) \, \cdot \, x$$

Whereas, for the standard deviation, we have

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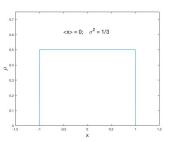
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First example: flat distribution

Assume that $\rho(x)$ is equal to zero for $|x| \ge a$ and that $\rho(x) = \frac{1}{2a}$ when $|x| \le a$



) Clearly $m\equiv <x>=$ 0, but what about σ^2 ? 2) We have

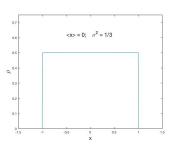
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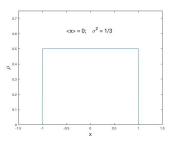
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• Clearly $m\equiv < x>=$ 0, but what about σ^2 ?

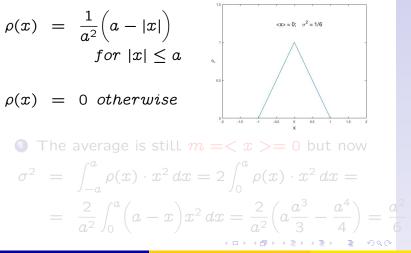
2 We have

1

$$\sigma^{2} = \int_{-a}^{+a} dx \,\rho(x) \, x^{2} = \int_{-a}^{+a} dx \, \frac{1}{2a} \, x^{2} = \\ = \frac{1}{2a} \left(2 \, \frac{a^{3}}{3} \right) = \frac{a^{2}}{3} \implies \sigma = \frac{a}{\sqrt{3}}$$

Triangular prob. density function

Assume now a triangular shape for the p.d.f., such as



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Triangular prob. density function

Assume now a triangular shape for the p.d.f., such as

$$\rho(x) = \frac{1}{a^2} \left(a - |x| \right)$$

for $|x| \le a$
 $\rho(x) = 0$ otherwise

• The average is still $m = \langle x \rangle = 0$ but now

$$\sigma^{2} = \int_{-a}^{a} \rho(x) \cdot x^{2} \, dx = 2 \int_{0}^{a} \rho(x) \cdot x^{2} \, dx =$$
$$= \frac{2}{a^{2}} \int_{0}^{a} \left(a - x\right) x^{2} \, dx = \frac{2}{a^{2}} \left(a \frac{a^{3}}{3} - \frac{a^{4}}{4}\right) = \frac{a^{2}}{6}$$

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So much for the **Probability Theory.**

Let us come back to our wave functions ...

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We have said that the solutions of the Schrödinger equation $\Psi(x, t)$ have to be square integrable, which means that

$$\forall t : \int_{-\infty}^{+\infty} |\Psi(x,t)|^2 \, dx = A(t) > 0$$

where A(t), a priori, can be time dependent (we will see that A is indeed a constant ...).

2 We have also said that, according to QM, two wave functions Ψ_a and Ψ_b that are proportional ($\Psi_a = \mathbf{k} \Psi_b$), they represent the same physical state. QUANTUN MECHANICS Lecture 2

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This allow us to represent any physical state by choosing the^(*) particular wave-function which is "normalized" (at least at some time $t = \hat{t}$):

$$ilde{\Psi}(x,t) = rac{1}{\sqrt{A(\hat{t})}} \Psi(x,t)$$

such that

$$\int_{-\infty}^{+\infty} |\tilde{\Psi}(x,\hat{t})|^2 \, dx = 1$$

(*) The normalized wave function is indeed not unique, but it is determined up to a constant complex phase factor e^{ia}.

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Assume a wave function

$$\Psi(x,t) = A e^{-\mu |x|} e^{i k t}$$

where A, λ and ω are positive real constants.

- i) Normalize ψ ;
- ii) Evaluate $\langle x \rangle$, $\langle x^2 \rangle$ and σ ;

iii) Calculate the probability to find the particle outside the interval $\langle x \rangle \pm 2\sigma$.