

QUANTUM MECHANICS

Lecture 6

Still about the Schrödinger equation

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D. J. Griffiths: paragraph 2.2

General solution of the Schrödinger equation

- 1 In the previous lecture we have said that the procedure to find the **general solution** of **the time dependent** Schrödinger equation, for an initial condition $\Psi(x, 0)$, is as follows.
- 2 We solve the time-independent Schrödinger equation, which, in general, has infinite solutions $\psi_1(x), \dots, \psi_n(x), \dots$ corresponding to different energies E_1, \dots, E_n, \dots
- 3 We write $\Psi(x, 0)$ as a linear combination of the above stationary solutions, i.e.

$$\Psi(x, 0) = \sum_n c_n \psi_n(x)$$

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General solution of Schrödinger equation

- 1 We define the function

$$\Psi(x, t) = \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x)$$

- 2 Since it is a linear combination of solutions of the *time – dependent* Schrödinger equation, it is certainly one of its possible solutions.
- 3 At $t = 0$, the w.f. $\Psi(x, t)$ satisfies the initial condition that we have imposed, therefore **it is the solution that we were looking for, because the solution with a given initial condition is unique.**

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About the time dependence

- 1 Let us come again, now, to the argument of the time dependence of the quantum observables
- 2 We have seen that each stationary state describes a physical state which appears "*frozen*" in time: no time dependence of any physical quantity !
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About the time dependence

- ① Suppose that

$$\Psi(x, 0) = c_1 \psi_1(x) + c_2 \psi_2(x)$$

where, for sake of simplicity, c_1 and c_2 are real numbers such that $c_1^2 + c_2^2 = 1$ and ψ_1 , ψ_2 are real *normalized* (orthogonal) stationary solutions, corresponding to the energies E_1 and E_2 , with $E_1 \neq E_2$.

- ② Then the time-dependent solution reads

$$\begin{aligned}\Psi(x, t) &= c_1 \psi_1(x) e^{-iE_1 t/\hbar} + c_2 \psi_2(x) e^{-iE_2 t/\hbar} \equiv \\ &\equiv c_1 \Psi_1(x, t) + c_2 \Psi_2(x, t)\end{aligned}$$

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About the time dependence

Let us see, for instance, how it behaves in time the expectation value of the position x .

If we define $\Delta E \equiv E_2 - E_1$, then we have

$$\begin{aligned}\langle x \rangle &= \int dx (c_1 \psi_1 + c_2 \psi_2)^* x (c_1 \psi_1 + c_2 \psi_2) = \\ &= c_1^2 \langle x \rangle_1 + c_2^2 \langle x \rangle_2 + \\ &+ 2c_1 c_2 \cos\left(\frac{\Delta E t}{\hbar}\right) \int dx \psi_1(x)^* \cdot \psi_2(x) \cdot x\end{aligned}$$

which shows that the expectation value $\langle x \rangle$ evaluated on this state, now, has a term which is oscillating in time, proportional to

$$\int dx \psi_1(x)^* \cdot \psi_2(x) \cdot x$$

Some relevant properties of the time independent solutions ψ

- 1 Let $\psi(x)$ be a solution of the time independent Schrödinger equation for the energy E : we have

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E] \psi(x) \quad (1)$$

- 2 This implies that $\psi(x)$ **admits the second derivative**, therefore $\frac{d\psi}{dx}$ and ψ must be differentiable and, therefore, also **continuous** functions.
- 3 If the potential energy $V(x)$ is differentiable ($\Rightarrow F(x) \equiv -\frac{dV}{dx}$ if a regular function...), from eq.(1) we conclude that also $\frac{d^2\psi}{dx^2}$ is differentiable, and, therefore, continuous.

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- 1 Assume, now, that $V(x)$ changes abruptly between $x_0 - \epsilon$ and $x_0 + \epsilon$ by a relevant quantity ΔV_0 . Consider the identity

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx \frac{d^2\psi}{dx^2} = \int_{x_0-\epsilon}^{x_0+\epsilon} dx \frac{2m}{\hbar^2} [V(x) - E] \psi(x)$$

- 2 The integral on the left side is the difference

$$\int_{x_0-\epsilon}^{x_0+\epsilon} dx \frac{d^2\psi}{dx^2} = \left. \frac{d\psi}{dx} \right|_{(x_0+\epsilon)} - \left. \frac{d\psi}{dx} \right|_{(x_0-\epsilon)}$$

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- ① This means that, also if V presents at $x = x_0$ a step of **finite** amplitude ΔV_0 , $\frac{d\psi}{dx}$ remains continuous in $x = x_0$ (and the same for ψ !).
- ② However, if the discontinuity in $V(x)$ is infinite, we will see later that only ψ remains continuous ...
- ③ In conclusion:

$$V(x) \text{ regular} : \Rightarrow \psi, \frac{d\psi}{dx}, \frac{d^2\psi}{dx^2} \text{ continuous}$$

$$\Delta V_0 \text{ finite} : \Rightarrow \psi, \frac{d\psi}{dx} \text{ continuous}$$

$$\Delta V_0 \text{ infinite} : \Rightarrow \psi \text{ continuous}$$