QUANTUM MECHANICS Lecture 3

Wave function normalization The momentum Linear operators: a first view

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D. J. Griffiths: paragraphs 1.4 and 1.5

The wave function normalization

1. From what we have already seen, it should be clear that the use of a normalized wave function $\tilde{\Psi}$ **makes easier** to draw conclusions through the statistical interpretation.

2. In fact, $|\tilde{\Psi}|^2$ can be interpreted directly as a probability density function.

3. The probability to find the particle between a and b at time $\hat{t}$ is, in fact, simply given by

$$P(a, b; \hat{t}) = \int_a^b |\tilde{\Psi}(x, \hat{t})|^2 \, dx$$

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1. But a wave function which has been normalized at $t = \hat{t}$ **will remain normalized also at any later time or not ?**
2. In other terms, the normalization constant A **changes or not as a function of time ?**
3. If A would change, then to keep the w.f. normalized to one, we would need to put $\tilde{\Psi}(x,t) \equiv \frac{1}{\sqrt{A(t)}}\Psi(x,t)$ **and this function would not anymore solve the Schrödinger equation** satisfied by the original wave function $\Psi(x,t)$, because of the presence of the time dependent factor $\frac{1}{\sqrt{A(t)}}$ ...

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The Schrödinger equation and the w.f. normalization

1. The Schrödinger equation has the relevant property **to preserve the normalization.**
2. To see this, let us start by observing that

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\,dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x,t)|^2\,dx$$

3. But

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi\Psi^*) = \Psi^*\frac{\partial \Psi}{\partial t} + \Psi\frac{\partial \Psi^*}{\partial t}$$

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Now, if we multiply the Schrödinger equation

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

by the quantity $-\mathbf{i}/\hbar$, we obtain

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

But, since the energy potential V is a real function ($V = V^*$), taking the complex conjugate, we have also that

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

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therefore, concerning

$$\frac{\partial}{\partial t}|\Psi|^2 = \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t}$$

since the two terms proportional to V have opposite sign and cancel each other, we have

$$\begin{aligned} \frac{\partial}{\partial t}|\Psi|^2 &= \frac{i\hbar}{2m}\left[\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\partial^2 \Psi^*}{\partial x^2}\right] = \\ &= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right] \end{aligned}$$

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$$\frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = \frac{i\hbar}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]_{-\infty}^{+\infty}$$

2. but, in the limit $x \to \pm\infty$ the w.f. $\Psi(x,t) \to 0$ (otherwise ψ could not be square-integrable ...); therefore

$$\frac{dA(t)}{dt} \equiv \frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = 0$$

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The probability current

1. Before leaving the argument, let us consider again the equation

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right] \quad (1)$$

2. If we define

$$\rho(x,t) = |\Psi(x,t)|^2$$
$$J(x,t) = -\frac{i\hbar}{2m}\left[\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right]$$

3. to the equation (1) we can give the form of a "continuity" equation

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$$\int_a^b dx \, \frac{\partial \rho(x,t)}{\partial t} \equiv \frac{d}{dt}\int_a^b dx \, \rho(x,t) = -\int_a^b dx \, \frac{\partial J(x,t)}{\partial x}$$

$$\Rightarrow \quad \frac{d}{dt} P(a,b;t) = J(a,t) - J(b,t)$$

2. This shows that $J(x,t)$ represents the **probability current** associated to the wave function $\psi(x,t)$.
   In fact, the time derivative of the probability to find the particle between **a** and **b** is the **difference** between the flux of the probability current **entering from** a, minus the one **exiting from** b.

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Consequeces from the statistical interpretation

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Still about the wave function

1. Let us assume to dispose of **many "copies"** of the **same** physical state described by the normalized w.f. $\Psi(x,t)$.
2. If we perform a position measurement on each of the various "copies", we have already said that, a priori, we **will not** obtain always the same result.
3. However, the probabilistic interpretation allow us to predict the exact average value of the position, which will be given by

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

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is called ***the expectation value*** of the observable x at time t.

2. This definition is a bit misleading because it could suggest that the *expectation value* is the most probable value associated to the p.d.f. $|\Psi|^2$, whereas it is not ... **it is its mean value !**

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1. Clearly, we can get the same expectation value $< x(t) >$ starting from very many probability densities $|\Psi(x,t)|^2$ ...
2. One way to measure the **narrowness** of the p.d.f. $|\Psi(x,t)|^2$ is by evaluating the standard deviation (its square ...)

$$\sigma^2(t) = \int_{-\infty}^{+\infty} dx\, |\Psi(x,t)|^2 \left(x - < x(t) >\right)^2$$

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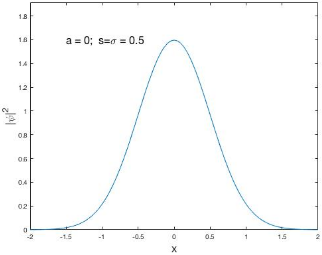
The gaussian case

As an example, consider the wave functions (with s and a real values)

$$\Psi(x,0) = A\, e^{-\frac{(x-a)^2}{4s^2}}$$

which are normalized if $A^2 = \frac{1}{s\sqrt{2\pi}}$.



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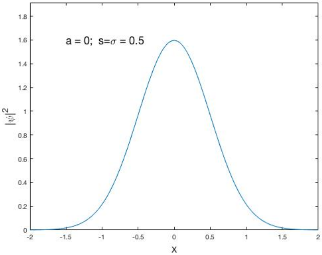

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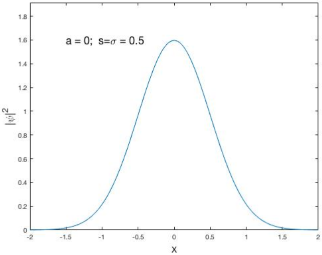

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The momentum

1. The time derivative of the position expectation value

$$< x(t) > \;=\; \int dx\, |\Psi(x,t)|^2 \cdot x$$

gives the expectation value of the particle velocity

$$< v(t) >= \frac{d}{dt} < x(t) >$$

2. This comes from an important **theorem**, due to Ehrenfest, which states that, in QM, **the expectation values of the physical quantities do satisfy the equations of Classical Mechanics.**

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1. Therefore, according to the Ehrenfest theorem, the expectation value of the particle momentum $p = m\,v$ is given by

$$< p >= m\,\frac{d}{dt}\,< x >$$

or, in other words

$$< p > \;=\; m\int x\left[\frac{\partial\Psi^*}{\partial t}\,\Psi + \Psi^*\,\frac{\partial\Psi}{\partial t}\right]dx$$

2. but from the Schrödinger equation multiplied by $\frac{-im}{\hbar}$, we obtain the two cc equations

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

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Therefore, since the terms proportional to V cancel out, we obtain

$$
\begin{aligned}
< p > &= -\frac{i\hbar}{2}\int x\left[\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right]\,dx = \\
&= -\frac{i\hbar}{2}\int x\frac{\partial}{\partial x}\left[\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right]\,dx = \\
&= \frac{i\hbar}{2}\int\left[\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right]\,dx
\end{aligned}
$$

where we made use of the ***integration-by-parts*** and we have assumed that $\Psi \to 0$ when $x \to \pm\infty$. For the same reason, we have

$$\int \frac{\partial\Psi^*}{\partial x}\Psi\,dx = -\int \Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

The momentum

1. In conclusion, for the linear momentum we obtain

$$
\begin{aligned}
< p(t) > &= \frac{i\hbar}{2} \int \left[\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right] dx \\
&= -i\hbar \int dx \;\; \Psi^* \left(\frac{\partial}{\partial x} \Psi \right)
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2. while, let us remember, for the position we have obtained

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Linear operators: a first view

The similar structure of these two results leads us to introduce, now, the concept of
"linear operator" $\mathcal{Q}$,
acting on a generic (wave) function.

Linear operators: a first view

1. In general, the definition requires that $\mathcal{Q}$ is a linear application that associates, in an unique way, the function $\mathcal{Q}(\Psi)$ to the function Ψ.
2. The linearity of $\mathcal{Q}$ means that, if a and b are any complex numbers, then

$$\mathcal{Q}\left(a \cdot \Psi_1 + b \cdot \Psi_2\right) = a \cdot \mathcal{Q}(\Psi_1) + b \cdot \mathcal{Q}(\Psi_2)$$

3. For instance, the **multiplication** by x, $\mathcal{Q}(\Psi) = x \cdot \Psi$ or the **partial derivative** with respect to x, $\mathcal{Q}(\Psi) = \frac{\partial}{\partial x}\Psi$ **do satisfy** the above definitions and, therefore, they are ***linear operators***.

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$$< x(t) > \; = \; \int dx \;\Psi^*(x,t)\; x \cdot \Psi(x,t)$$

$$< p(t) > \; = \; -i\hbar \int dx \;\Psi^*(x,t)\; \frac{\partial}{\partial x}\Psi(x,t)$$

2. If we assign to the position the operator $\mathcal{Q} \equiv \hat{x} = x\cdot$ and to the momentum the operator $\mathcal{Q} \equiv \hat{p} = -i\hbar\frac{\partial}{\partial x}$, then, in both cases, the expectation value of these observables can be obtained by evaluating the integral

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$$< Q(t) >= \int dx\, \Psi^*(x,t)\ \left(\mathcal{Q}\Psi(x,t)\right)$$

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1. But, for a point-like particle, **every mechanical quantity Q can be expressed in terms of position and linear momentum.**

2. Therefore, it is possible to associate to every observable Q a QM operator $\mathcal{Q}$ in this way

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