QUANTUM MECHANICS
Lecture 11

The free particle
The group velocity

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October 8, 2019

D. J. Griffiths: paragraph 2.4

The free particle

1. In Classical Mechanics, a free particle is simply characterized by a motion with a **constant velocity** in any inertial frame.

2. **How this fact translates in QM ?**

3. Let us start again from the time-independent Schrödinger equation, that, for a free particle ($V(x) = 0$), reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\,\psi \quad \Rightarrow \quad \frac{\mathbf{d^2}\psi}{\mathbf{dx^2}} = -\mathbf{k}^2\,\psi$$

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1. It is the same equation that we have found for the infinite square well.
   Its solutions are

$$\psi(x) = A\,e^{ikx} + B\,e^{-ikx}$$

   with A and B arbitrary integration constants.

2. However, now we do not have to satisfy any boundary condition and, as a consequence, **all the $k \in \Re$ are possibile.**

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1. The time-dependent solutions can be written as

$$\Psi(x,t) = A\,e^{i(kx - E_k t/\hbar)} = A\,e^{ik(x - \frac{\hbar k}{2m} t)}$$

with k any positive or negative real quantity.

2. The wave propagates with a **phase velocity** defined by the equation

$$x - \frac{\hbar k}{2m} t = const. \quad \Rightarrow \quad \frac{dx}{dt} \equiv v_{ph} = \frac{\hbar k}{2m}$$

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2. In QM, since $E = \frac{\hbar^2 k^2}{2m}$, this classical velocity becomes

$$v_c = \pm\sqrt{\frac{2E}{m}} = \pm\sqrt{\frac{2}{m}\frac{\hbar^2 k^2}{2m}} = \frac{\hbar k}{m} = 2\, v_{ph}$$

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1. Concerning the particle speed, **are we sure** that the w.f. $\Psi(x,t) = A\, e^{i(kx - E_k t/\hbar)}$ **represents at all** the state of a moving particle ?
2. For such a state, the p.d.f. should describe the motion and, therefore, $|\Psi|^2$ should be **time dependent**, but the w.f. that we are considering is a stationary solution of the Schrödinger equation and therefore, $|\Psi|^2$ is **time independent !**
3. Moreover, there is another very important aspect of these solutions that we have to face: **they cannot be normalized**, in fact $\int dx |\Psi|^2 = |A|^2 \int dx = \infty$...

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2. Does this mean that the stationary solutions concerning the free particle **are useless ?**
3. **No !**
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We have already said that, for any given potential, the general solution of the Schrödinger equation can be written in terms of the normalized stationary states $\psi_n(x)$ as

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

where

$$c_n = \int dx \, \psi_n^*(x) \, \Psi(x,0)$$

The free particle

In this case, the stationary solutions are not numerable but labelled by the continuous variable k. For this reason we need now to use an integral instead of a summation and we have

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \phi(k)\, \mathbf{e^{i(kx-\frac{\hbar k^2}{2m}t)}}$$

where the function $\phi(k)$ takes the place of the coefficients c_n and we have

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-ikx}\, \Psi(x,0)$$

which shows that $\phi(k)$ is simply the Fourier transform of $\Psi(x,0)$.

The free particle

1. The factor $\frac{1}{\sqrt{2\pi}}$ has been introduced only for normalization reasons.

2. In fact, with the above definition of $\phi(k)$, similarly to the numerable case where we had

$$\int dx \, |\Psi(x,t)|^2 = \sum_n |c_n|^2$$

in agreement with the Fourier theory, now we have

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1. The only possible normalizable states of a free particle **must involve a suitable range of k** and, therefore, **a suitable range of energies.**

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Let us consider, now, a generic wave-packet

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int dk\, \phi(k)\, e^{i(kx - \frac{\hbar k^2}{2m} t)} \equiv$$
$$\equiv \frac{1}{\sqrt{2\pi}} \int dk\, \phi(k)\, e^{i(kx - \omega t)}$$

where $\phi(k)$ is square-integrable and we have defined

$$\omega = \omega(k) \equiv \frac{\hbar k^2}{2m}$$

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1. Let us assume that the function $\phi(k)$ is narrowly peaked at $k = k_0$.
   Since the integrand is negligible far from k_0, we can expand $\omega(k)$ around k_0 and retain only the leading terms:

$$\omega(k) \approx \omega(k_0) + (k - k_0) \left.\frac{d\omega}{dk}\right|_{k=k_0} \equiv$$
$$\equiv \omega_0 + (k - k_0)\omega_0^{'}$$

2. Let us put, now, $s \equiv k - k_0$: we have

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int ds\, \phi(k_0 + s)\, e^{i\left[(k_0+s)x - (\omega_0 + \omega_0^{'} s)t\right]}$$

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2. For $t \neq 0$, the phase present in the exponential can be rewritten as

$$(k_0 + s)x - (\omega_0 + \omega_0^{'} s)t =$$
$$= (k_0 + s)x - \omega_0\, t - s\, \omega_0^{'}\, t + k_0\, \omega_0^{'}\, t - k_0\, \omega_0^{'}\, t =$$
$$= (k_0 + s)x - t(\omega_0 - k_0 \omega_0^{'}) - \omega_0^{'} t(s + k_0) =$$
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1. Therefore, we obtain

$$\Psi(x,t) \approx \frac{1}{\sqrt{2\pi}} e^{-i(\omega_0 - k_0\,\omega_0^{'})t} \cdot \int ds\,\phi(k_0+s)\; e^{i\left[(k_0+s)(x-\omega_0^{'}\,t)\right]} = $$

$$= e^{-i(\omega_0 - k_0\,\omega_0^{'})t}\;\Psi(x-\omega_0^{'}\,t, 0)$$

2. Since the phase factor $e^{-i(\omega_0 - k_0\,\omega_0^{'})t}$ will not contribute to $|\Psi(x,t)|^2$, we can conclude that **the p.d.f.** associated to the wave-packet under consideration **describes a free particle motion at the speed** $\omega_0^{'}$.

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1. This quantity $\omega_0^{'}$ is called **group velocity** and it represents the velocity of the whole group of travelling waves constituting the wave packet.

2. It is indeed the ***group velocity***

$$\omega_0^{'} = v_g = \left.\frac{d\omega}{dk}\right|_{k=k_0}$$

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$$v_g = \frac{\hbar k}{m} = \frac{p}{m} = v_c$$

2. whereas, for the phase velocity, we had found

$$v_{ph} = \frac{\omega}{k} = \frac{\hbar k}{2m} = \frac{1}{2} v_c$$

3. As an example, in **Appendix 2** we show the **free evolution of a gaussian wave-packet**.

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