Lecture 10. Distributions and Schroedinger equation

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Schroedinger equation

Schroedinger equation in a simplest form can be written as

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

Here $\hbar$ is a Planck constant, m is a mass of a particle and $V(x)$ is a potential field which defines the behaviour of the particle in a classical mechanics.

- Potential for a free particle is follows:

$$V(x) \equiv 0.$$

- Potential for a linear oscillator is

$$V(x) = k\frac{x^2}{2}.$$

- Potential for an electron of hydrogen atom:

$$V(\vec{x}) = -\frac{e^2}{\varepsilon_0 r}.$$

Typical parameters of quantum systems

- $\hbar \sim 6.62607015 \times 10^{-34}$ J/Hz is the value of the Planck constant;
- $e \sim 1.602 \times 10^{-19}$ C is an electron charge;
- $m \sim 9.1 \times 10^{-31}$ kg is a mass of an electron;
- $r \sim 5.292 \times 10^{-11}$ m is a distance between the kernel and electron (Bohr radius);
- $\epsilon_0 \sim 8.8854 \times 10^{-12}$ F/m is a vacuum permittivity.

Wave motion

When we consider waves and its dependence on time we should understand a direction of wave motion.
let us consider two different solutions of a Schroedinger equation without external field:

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

In the simplest case two different solutions can be written:

$$\Psi_\pm = e^{-i\left(\frac{E}{\hbar}t \pm \frac{\sqrt{2mE}}{\hbar}x\right)}.$$

The wave phase with the sign $+$ is constant at line parallel by a straight-line $x = -t\sqrt{2m/E}$. This means the wave moves in a negative direction with respect to x axis.
In contrast, the wave phase of the solution with $-$ is constant on all lines which are parallel by a straight-line $x = t\sqrt{2m/E}$. This wave moves in a positive direction with respect to the axis x.

A barrier as a potential

Let us consider the potential with a threshold shape.

$$U(x) = \begin{cases} 0, & -l < x; \\ u, & -l \leq x \leq l; \\ 0, & l < x. \end{cases}$$

On left-hand side of the barrier a solution of the Schroedinger equation looks as

$$\Psi = e^{-i\left(\frac{E}{\hbar}t - \frac{\sqrt{2mE}}{\hbar}x\right)} + Re^{-i\left(\frac{E}{\hbar}t + \frac{\sqrt{2mE}}{\hbar}x\right)}.$$

Here first term is a falling wave. This waves move to the barrier. Second term is reflected wave, because this wave moves from the barrier.
On right-hand side of the barrier a solution contains a transmitted wave only:

$$\Psi = Te^{-i\left(\frac{E}{\hbar}t - \frac{x}{\hbar^2}\right)}.$$

Tunnel effect

The wave with the energy E for the Schroedinger equation looks like:

$$\Psi = e^{-i\left(\frac{E}{\hbar}t\right)}\psi(x).$$

In this case the one-dimension Schroedinger equation looks like:

$$\frac{\hbar^2}{2m}\psi'' + (E - U(x))\psi = 0.$$

If $u > E$ this means the energy to overcome this threshold is less that the threshold level. For the classical particle does not be passed through such threshold. Let us find a possibility to pass this threshold for quantum one.

Falling and reflected waves

General solution before the threshold:

$$\psi = e^{i\sqrt{2mE}\frac{x}{\hbar}} + Re^{-i\sqrt{2mE}\frac{x}{\hbar}}.$$

This formula contains the falling wave and reflected one.
At the threshold the solution has another form:

$$\psi = B_1 e^{\sqrt{2(u-E)m}\frac{x}{\hbar}} + B_2 e^{-\sqrt{2(u-E)m}\frac{x}{\hbar}}.$$

After the threshold the solution has transmitted wave only:

$$\psi = Te^{i\sqrt{2mE}\frac{x}{\hbar}}.$$

Our problem is to find the transmitted and reflected waves.
Formally it means one should find the coefficients R and T.

A matching of the solutions

These solution and their derivatives of first order should be matched at the point $x = -l$:

$$e^{-i\omega l} + Re^{i\omega l} = B_1\, e^{-lk} + B_2\, e^{kl},$$
$$i\omega\, e^{-i\omega l} - i\omega\, R\, e^{i\omega l} = k\, B_1\, e^{-lk} - k\, B_2\, e^{kl}.$$

The same matching should be made at the point $x = l$:

$$B_1\, e^{kl} + B_2\, e^{-kl} = Te^{i\omega\, l},$$
$$k\, B_1\, e^{kl} - k\, B_2\, e^{-kl} = i\omega\, T\, e^{i\omega l}.$$

Here

$$\omega = \frac{1}{\hbar}\sqrt{2mE}, \quad k = \frac{1}{\hbar}\sqrt{2(u-E)m}.$$

So we have four equations with four unknown values R, T, B_1, B_2. We are interested in R and T only.

The transmission coefficient

One can solve the system of four linear equations by hand or using some computer algebra system.
The transmission coefficient have the following form:

$$T = \frac{1}{\sqrt{\frac{u-E}{E}\sinh^2\left(\sqrt{2m(u-E)}\frac{l}{\hbar}\right) + \cosh^2\left(\sqrt{2m(u-E)}\frac{l}{\hbar}\right)}} \times \frac{1}{\sqrt{\frac{E}{u-E}\sinh^2\left(\sqrt{2m(u-E)}\frac{l}{\hbar}\right) + \cosh^2\left(\sqrt{2m(u-E)}\frac{l}{\hbar}\right)}}.$$

The transmission coefficient exponentially decreases with respect to width l and hight of the barrier $u - E$.

Oscillations in potential well

Let us consider oscillations in an infinite potential well $x \in (0, l)$. The Schroedinger equation with additional boundary conditions is:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}, \quad \Psi|_{x=0} = \Psi|_{x=l} = 0.$$

A special solution which is periodic on time has a form:

$$\Psi(x,t) = e^{-i\frac{E}{\hbar}t}\psi(x).$$

A substitution into the Schroedinger equation yields:

$$\frac{\hbar^2}{2m}\psi'' + E\psi = 0, \quad \psi|_{x=0} = \psi|_{x=l} = 0.$$

Solution can be written for discrete set of energy E_n:

$$\psi = \sin\left(\frac{\sqrt{2\,m\,E_n}}{\hbar}x\right), \quad E_n = \frac{\hbar^2}{2\,m}\frac{\pi^2}{l^2}n^2, \quad n \in \mathbb{N}.$$

A Schroedinger equation for quantum oscillator

A Schroedinger equation for quantum oscillator looks like:

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

A special solution which is periodic on time has a form:

$$\Psi(x,t) = e^{-i\frac{E}{\hbar}t}\psi(x).$$

A substitution into the Schroedinger equation yields:

$$\frac{\hbar^2}{2\,m}\psi'' - \left(\frac{x^2}{2} - E\right)\psi = 0.$$

A connection with parabolic cylinder equation

Let us rewrite this equation in a standard form. For that we substitute new independent variable $\xi = kx$. In this case we obtain the equation in the form:

$$\frac{\hbar^2}{2\,m} k^2 \frac{d^2\psi}{d\xi^2} - \frac{2}{k^2} \left(\frac{\xi^2}{4} - \frac{k^2 E}{2} \right) \psi = 0.$$

Equate the coefficients at the second derivative and at the brackets.

$$\frac{\hbar^2}{2m} k^2 = \frac{2}{k^2}, \quad k^2 = 2\frac{\sqrt{m}}{\hbar}, \quad a = \frac{k^2 E}{2}.$$

It yields a standard form of the parabolic cylinder equation:

$$\frac{d^2\psi}{d\xi^2} - \left(\frac{\xi^2}{4} - a \right) \psi = 0.$$

Discrete values of energy of quantum oscillator

The bounded solutions of the parabolic equation with given value of parameter $a = n + 1/2$ look like:

$$\psi(\xi) = (-1)^n \, e^{\xi^2/4} \frac{d^n}{d\xi^n} \left(\frac{e^{-\xi^2/2}}{n!} \right).$$

Therefore the energy of bounded solutions has a discrete set:

$$E_n = -(n + 1/2) \frac{\hbar}{\sqrt{m}}, \quad n \in \mathbb{N}.$$

Semiclassical approach

Let us consider a solution of the Schroedinger equation in the form:

$$\Psi = A(x,t)e^{\frac{i}{\hbar}S(x,t)}.$$

Substitute these formula for the solution into the Schroedinger equation and eliminate the multiplier $e^{\frac{i}{\hbar}S(x,t)}$:

$$-\frac{\partial S}{\partial t}A(x,t) + i\hbar\frac{\partial A}{\partial t} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 A - i\frac{\hbar}{m}\frac{\partial S}{\partial x}\frac{\partial A}{\partial x} - i\frac{1}{2m}\hbar\frac{\partial^2 S}{\partial x^2}A - \frac{1}{2m}\hbar^2\frac{\partial^2 A}{\partial x^2} + U(x)A.$$

Gather terms with power of $\hbar^0$ and eliminate the multiplier A, then:

$$-S_t = \frac{1}{2m}(S_x)^2 + U(x),$$

Terms with an order $\hbar^1$ lead to the following equation:

$$A_t = -\frac{1}{m}S_x A_x - \frac{1}{2m}S_{xx}A$$

An eikonal equation

The non-linear equation for S is called eikonal equation. An approach for solving such equation is used by differentiating and considering an system of quasi-linear equation:

$$S_x = p, \quad -p_t = \frac{p}{m} p_x + \partial_x U$$

Let us assume the dependence $x = x(\tau)$ and $t = t(\tau)$, where τ is new independent variable. This assumption gives for us new form of the equation for $p = p(x(\tau), t(\tau))$:

$$\frac{dp}{d\tau} = \frac{\partial p}{\partial t}\frac{dt}{d\tau} + \frac{\partial p}{\partial x}\frac{dx}{d\tau}$$

The equation for p we will consider as an ordinary differential equation for $p(\tau)$:

$$\frac{dp}{d\tau} \equiv p_t + \frac{p}{m} p_x = -\partial_x U.$$

Hamiltonian equations

This assumption yields the following sysytem of the equations:

$$\frac{dx}{d\tau} = \frac{p}{m}, \quad \frac{dp}{d\tau} = -\frac{\partial U}{\partial x}$$

This system of equations can be derived as Hamiltonian equations for the following Hamiltonian:

$$h(x, p) = \frac{p^2}{2m} + U(x).$$

Recall that Hamiltonian equations for classical mechanics are:

$$\frac{dx}{d\tau} = \frac{\partial H}{\partial p}, \quad \frac{dp}{d\tau} = -\frac{\partial H}{\partial x}.$$

It is easy to see that the equivalence of these two system of equations.

A convection equation

To show the connection between the classical particle and quantum behaviour we show that the localized amplitude of the distribution expanses on a trajectories of this Hamiltonian system. The equation of order $\hbar$ defines an primary order term of amplitude for the distribution:

$$\partial_t A = -\frac{p}{m}\,\partial_x A - \frac{1}{2}\partial_x p\, A.$$

The same assumption $A = A(x(\tau), t(\tau))$ leads to the following equation:

$$\frac{dA}{d\tau} \equiv \partial_t A + \frac{p}{m}\partial_x A$$

and

$$\frac{dA}{d\tau} = -\frac{1}{2}\partial_x p\, A.$$

This shows that the characteristics for the function A are trajectories of motion for the Hamiltonian system.