Some equations from previous lecture:

Comments:

1. In the stationary case the general solution of the time dependent Schrödinger equation is the arbitrary linear combination

$$\Psi(\vec{r},t)=\sum_n c_n e^{-\frac{i}{\hbar}E_n t}\psi_n(\vec{r}) .$$

2. In paragraph 13 the above given Schrödinger equation is generalized to the case where an external electromagnetic field is present.

3. Phase transformations. The wave equation is not determined uniquely. Even if normed, the functions

$$\Psi(r,t) \quad \text{and} \quad e^{i\alpha}\Psi(r,t)$$

(where $\alpha \in R$) give the same probability density. Here is no physical contradictions. Therefore these transformations in ordinary quantum mechanics are not physically interesting, but as we see later, analogical phase transformations where the phase factor $\alpha=\alpha(\vec{r},t)$ is a function of space and time are very important in modern particle physics.

4. Microparticles have dualistic properties – they are at the same time both – particles and waves. Free particle is described with the help of de'Broglie wave (one dimensional case), which one can represent in two equivalent forms

$$\Psi(x,t)=e^{-\frac{i}{\hbar}(E\,t-p\,x)}\equiv e^{-i(\omega\,t-k\,x)} ,$$

(particle side is chacterized by energy and momentum, wave side by frequency and wave number). It satisfies the free particle equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=-\frac{\hbar^2}{2M}\frac{\partial^2\Psi(x,t)}{\partial x^2} .$$

De'Broglie wave cannot be interpreted as a classical wave: it has complex values and is not a solution of classical wave equation.

Classical wave equation is

$$\frac{1}{v^2}\frac{\partial^2\Psi(x,t)}{\partial t^2}=\frac{\partial^2\Psi(x,t)}{\partial x^2}\quad ,$$

where v is a velocity of a given wave.

There are different interpretations of the wave function. Is the wave function a real physical object or is it just a mathematical method of describing the properties of microparticles? It doesn't matter if quantum mechanics works well. Do not ask just use.

Problem. Prove that 1) de'Broglie wave is not a solution of classical wave equation; 2) de'Broglie wave must be complex valued function, since its real part $\phi(x,t)=\mathrm{Re}\,\Psi(x,t)=\cos(\omega t-kx)$ does not satisfy the Schrödiner equation.

II.2 Operators

II.2.1 Operator, linear operator, eigenvalue problem.

For stationary problems in quantum mechanics, the eigenvalue problem plays a very important role. Mathematically it is looks like so:

$$\hat{A}\varphi_n = a_n\varphi_n \ .$$

Here A is operator correspond to some physical quantity, a_n-eigenvalues of operator A, are the measurable value of correspond physical quantity.

The set of all eigenvalues is called the spectrum of a given operator. That may be discrete, continuous or both. Eigenfunctions $\phi_1, \phi_2, \dots, \phi_n, \dots$ describe states, where the eigenvalues of $\hat{A}$ are correspondingly $a_1, a_2, \dots, a_n, \dots$.

In the following we mostly treat the cases where the eigenvalues are different and discrete, and to each eigenvalue there is only one eigenfunction, or several eigenfunctions.

All the measurable physical quantities are expressed by the real numbers, therefore we need operators, where all eigenvalues are real numbers.

II.2.2 Hermitean operators. All operators which **correspond** to some physical quantity are Hermitean. In order to define Hermitean operators, we introduce the bilinear form (scalar product) of functions.

Bilinear form of functions φ ja ψ is the following integral

$$\int \varphi * \psi \, dV \quad .$$

Conjugated operator. For each $\hat{A}$ we may write down an integral

$$\int \phi * \hat{A}\, \psi\, dV \quad ,$$

which is the bilinear form of φ and $\hat{A}\psi$.

For each operator $\hat{A}$ there also exists an operator $\hat{B}$, which satisfies

$$\int (\hat{B}\varphi)^{*} \psi\, dV = \int \varphi(\hat{A}\psi) dV \quad .$$

Operator $\hat{B}$ is a conjugated operator for $\hat{A}$ and is denoted $\hat{B} = \hat{A}^{+}$.

Hermitean operator is operator which equals to its conjugated operator (is therefore selfconjugated)

$$\hat{A}^{+} = \hat{A} \quad .$$

Hermitean operaator $\hat{A}$ therefore satisfies

$$\int (\hat{A}\varphi)^{*} \psi\, dV = \int \varphi^{*} (\hat{A}\psi)\, dV \;.$$

Example. X projection of momentum operator $\hat{p}_x = -i\hbar \frac{d}{dx}$ is Hermitean. We assume that both functions $\psi(x)$ and $\phi(x)$ vanish in infinity, we after **integrating by parts**, obtain

$$\langle \phi | \hat{p}\, \psi \rangle = \int_{-\infty}^{+\infty} \phi * (-i\hbar \frac{d\psi}{dx})\, dx \equiv -i\hbar \int_{-\infty}^{+\infty} \phi * \frac{d\psi}{dx}\, dx = -i\hbar \phi * \psi |_{-\infty}^{+\infty} + i\hbar \int_{-\infty}^{+\infty} \frac{d\phi *}{dx} \psi\, dx =$$

$$= i\hbar \int_{-\infty}^{+\infty} \frac{d\phi *}{dx} \psi\, dx \equiv \int_{-\infty}^{+\infty} (-i\hbar \frac{d\phi}{dx})^{*} \psi\, dx = \langle \hat{p}\, \phi | \psi \rangle \quad .$$

II.2.3. Eigenvalues and eigenfunctions of Hermitean operators.

Theorem 1. Eigenvalues of Hermitean opertators are real numbers.

Proof. Let us have some Hermitean operator $\hat{A}$ with its eigenvalues a_n and corresponding eigenfunctions φ_n

$$\hat{A}\varphi_n = a_n \varphi_n$$

Eigenvalue problem for complex conjugated eigenfunction φ_m^{*} is

$$(\hat{A}\varphi_m)^{*} = a_m{}^{*} \varphi_m{}^{*}$$

Taking the scalar product of the first equation with φ_m^{*} we get

$$\int \varphi_m^* \hat{A} \varphi_n dV = a_n \int \varphi_m^* \varphi_n dV \quad .$$

Taking similarly the scalar product of the second equation with φ_n we get

$$\int (\hat{A} \varphi_m)^* \varphi_n dV = a_m^* \int \varphi_m^* \varphi_n dV \; .$$

Since $\hat{A}$ is Hermitean, the last expression may be written as

$$\int (\hat{A} \varphi_m)^* \varphi_n dV = \int \varphi_m^* \hat{A} \varphi_n dV = a_m^* \int \varphi_m^* \varphi_n dV \; .$$

From the above given equations we get the result that

$$(a_n - a_m^*) \int \varphi_m^* \varphi_n dV = 0 \; .$$

At first we take m = n. Then we get

$$(a_n - a_n^*) \int \varphi_n^* \varphi_n dV = 0 \quad .$$

Since $\int |\phi_n|^2 dV \neq 0$, we have

$$a_n{}^* = a_n \quad ,$$

which proves that eigenvalues of Hermitean operator are real numbers.

Theorem 2. Eigenfunctions of Hermitean operator form an orthonormal system of functions.

We consider two different possibilities.
a) We assume that eigenvalues are discrete numbers and different, and for each eigenvalue a_n correspond only one eigenfunction φ_n. Since the eigenvalues are real numbers, we have

$$(a_n - a_n^*) \int \varphi_n^* \varphi_n dV = 0 \; .$$

If we now take $m \neq n$, we have

$$\int \varphi_m^* \varphi_n dV = 0$$

which means that different eigenfunctions are orthogonal. For the same eigenfunctions we have $\int \varphi_n^* \varphi_n dV \neq 0$, therefore the eigenfunctions may be normed to one - $\int \varphi_n^* \varphi_n dV = 1$.

In conclusion $\int \varphi_m^* \varphi_n dV = \delta_{mn}$

b) Eigenvalues are discrete, but to one eigenvalue a_n there corresponds k different eigenfunctions_ $\phi_{n1}, \phi_{n2}, \ldots, \phi_{nk}$ (the case of degenerate state, several eigenfunctions corresponds to only one eigenvalue). It is obvious, that all k eigenfunctions are orthogonal to other eigenfunctions for another eigenvalue. In order to get orthonormed set of eigenfunctions, one must in addition to orthonorme eigenfunctions, corresponding to a_n . We do not give the general proof, but as an example analyse the case of two different eigenfunctions.

We assume, that for some eigenvalue there exists two eigenfunctions which in general are independent, but not orthogonal: therefore we have functions ϕ_1 and ϕ_2 , and assume that $\langle\phi_1|\phi_2\rangle = d \neq 0$. We demonstrate, that we can form two orthogonal functions ψ_1 and ψ_2 (which afterwards may be normed to 1). At first we take $\psi_1 = \phi_1$ and try to find an orthogonal function using linear combination $\psi_2 = a\phi_1 + b\phi_2$. Demanding $\langle\psi_1|\psi_2\rangle = 0$, we have

$$\langle\phi_1|a\phi_1 + b\phi_2\rangle = a\langle\phi_1|\phi_1\rangle + b\langle\phi_1|\phi_2\rangle = 0 \quad .$$

If we choose $b = -a\,\langle\phi_1|\phi_1\rangle / d$, ψ_1 and ψ_2 are orthogonal. (Of course that procedure is not unique, but there are always two orthogonal eigenfunctions.)

Example. Let us consider the free particle moving on x-axis and try to normalize the eigenfunctions of momentum operator. The x-axis is divided to line segments with the length *L.* The eigenfunctions of the momentum operator $\hat{p} = -i\hbar \frac{d}{dx}$ are

$$\varphi_p(x) = e^{\frac{i}{\hbar} p x} \quad .$$

If there are no restrictions, the momentum spectrum is continuous $-\infty \leq p \leq +\infty$.

But by using periodical border conditions we must have (here L is a length of the 1d space)

$$\varphi_p(x) = \varphi_p(x + L) \quad .$$

Now we get discrete eigenvalue spectrum, since from the above given we get

$$e^{\frac{i}{\hbar} p L} = 1 \quad ,$$

and therefore

$$p = \frac{2\pi\hbar}{L} n \, , \quad n = 0, \pm 1, \pm 2, \ldots \quad .$$

Standing wave of probability.

If we choose quite large L the difference between momentum values for n and n+1 may be small (practically continuous).

Wave functions are normed on finite legth L, therefore there are no problems with infinities. Taking $\tilde{\varphi}(x) = Ae^{\frac{i}{h}px}$, we get

$$\int_0^L |\tilde{\phi}(x)|^2 dx = |A|^2 \int_0^L dx = |A|^2 L \quad .$$

If we choose $A = 1/\sqrt{L}$ the wave function is normed to 1.