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THE USE OF ALGEBRAIC METHODS IN THE STUDY OF QUANTUM MECHANICS IN HIGHER EDUCATIONAL INSTITUTIONS

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Abstract: *The use of a presentation technique based on the maximum possible standardization of the mathematical language when considering classical and quantum phenomena can significantly improve the quality of studying both the fundamental provisions of theoretical physics and its specific applications. The methodological system of studying quantum mechanics, based on the consistent use of algebraic methods, provides a deeper understanding of physics for students. In this paper, problems on stationary one-dimensional problems in quantum mechanics are posed and solved. In particular, problems of the relativistic Schredinger equation with a constant potential and the problem of a linear harmonic oscillator are considered. An equation based on the expression for the energy of a particle in terms of momentum is obtained. A stationary one-dimensional relativistic Schredinger equation with potential U (x) is obtained. The Stark effect for an oscillator in a constant field is described. The properties of the obtained solutions are analyzed.*
Key words: *algebraic methods, the study of quantum mechanics, Poisson brackets, relativistic quantum mechanics, differential operator, potential well.*

I. Introduction

The modern structure of physics makes new demands on the content and methods of teaching. For courses in theoretical physics, this means the need to create such courses in classical and quantum mechanics, in which certain characteristic moments of the creation and study of properties from models of the studied phenomena would be consistently traced. Let us note some of them.
First, it is the consistency of the fundamental models underlying the theory. As an example, one can point to the concept of the stationary state of an atom in nonrelativistic quantum mechanics, which is determined using the Schrödinger equation and which does not correspond to experimental data regarding the existence of spontaneous radiation. Further development of the fundamental model leads to the conclusion that it is necessary to consider a wider system "atom + electromagnetic field". This model already describes the properties of real atomic systems much more accurately, which, of course, does not prevent us from using the simpler model of an isolated atom to explain and predict various properties of atomic systems.

The second characteristic point is connected with the establishment of exact relationships that connect various characteristics of the system under study within the framework of a certain fundamental model of the phenomenon. Such exact relationships, along with the conservation laws determined by the properties of symmetry, allow a deeper understanding of the physical

mechanism of phenomena, control the conditions for the validity of the model, and determine the limits of its applicability.
The third characteristic point is related to the study of the properties of the mathematical models of the phenomenon in terms of its correspondence to the physical model, which served as the basis for the creation of the mathematical model.

II. Literature review

The development of modern theoretical physics has demonstrated the possibility of using various mathematical methods. In quantum mechanics, variants of Schrödinger, Heisenberg, Dirac, the method of functional integration, and perturbation theory are known, which, within the framework of various mathematical schemes, lead to the same results when considering physical problems. According to the historically established tradition, each section has its own "popular" methods, which are usually preferred when studying theoretical physics at the university. So, in theoretical mechanics, the Lagrange method is usually considered and used in solving problems in practical classes, in quantum mechanics, the consideration is based on the use of the Schrödinger equation [10].
A characteristic feature of existing courses in theoretical physics is the use of different language in describing classical and quantum phenomena. Meanwhile, it is well known that it is possible to use a system of concepts and physical quantities that provide the possibility of a single language in such cases. This includes the correspondence between commutators in quantum mechanics and Poisson brackets in classical mechanics. The use of a presentation technique based on the maximum possible standardization of the mathematical language when considering classical and quantum phenomena can significantly improve the quality of studying both the fundamental provisions of theoretical physics and its specific applications.

III. Analysis

The methodological system of studying quantum mechanics, based on the consistent use of algebraic methods, provides a deeper understanding of physics for students. The main ideas of this system can be formulated as follows.
When considering a harmonic oscillator in quantum mechanics, the so-called Fock representation is introduced, based on the use of operators for the creation and annihilation of oscillation quanta. This representation allows more simplified and more compact calculations. Having developed a certain technique of such transformations in lectures and practical exercises on problem solving, to consider a number of topical problems of modern physics, such as the motion of a particle in an electromagnetic field, the superposition of various quantum states, coherent states, etc. Consider, as an example, some methods for solving one-dimensional problems in practical classes in quantum mechanics.
As is known [1], the application of the Klein-Gordon-Fock equation to the problem of particle states in a space with a deep potential well is associated with significant difficulties. These difficulties also arise in the absence of potential wells. Indeed, it follows from this equation that

the energy of a free particle can be negative. The energy spectrum of a free particle consists of two continuums, upper and lower. In addition, nothing prevents, it would seem, a particle from the upper continuum to "fall" into the lower continuum "fall" endlessly, radiating infinite energy.
However, nothing of the sort appears to be happening. If there are no potential wells anywhere in space with a depth twice the rest energy of the particle, the states of the lower continuum can be ignored, but if there are such wells, the same value of energy in some regions of space belongs to the lower continuum and in others to the upper continuum. Moreover, this should lead to the birth of particles from vacuum. Other difficulties are also known that accompany the application of the Klein-Gordon-Fock equation (complex values of the energy of a hydrogen-like atom with a large nuclear charge, Klein's paradox, and others).
In connection with this, the conviction arose that a relativistic quantum theory should initially be constructed as a theory of many particles or as a theory with an infinite number of degrees of freedom, i.e., as a quantum field theory. However, quantum field theory leads to discrepancies. However, one can understand that all the difficulties that the Klein-Gordon-Fock equations lead to are because, unlike the nonrelativistic Schrödinger equation, this equation is not based on the expression of the particle energy in terms of momentum

$$\varepsilon = \sqrt{m^2 + p^2} \qquad (1)$$

(a system of units is used in which the speed of light c and Planck's constant $\hbar$ are equal to unity), and on the expression of the square of energy in terms of momentum

$$\varepsilon^2 = m^2 + p^2 \qquad (2)$$

The reason for this choice is that if the standard replacement

$$\varepsilon \to i\,\frac{\partial}{\partial t}\,, p \to\ -i\,\nabla$$

to produce in equality (1), then we get a not quite ordinary equation

$$i\frac{\partial \psi}{\partial t} = \sqrt{m^2 - \nabla^2}\,\psi \qquad (3)$$

Of course, this operator (such operators are called pseudo-differential) is not local, since its definition involves integration over coordinates. Nevertheless, it is used in a number of papers, where equation (3) is called the spinless Salpeter equation, but, apparently, it really cannot be considered the basis of relativistic quantum theory. In particular, it is impossible to use this definition for problems with a step potential - it does not allow setting boundary conditions at the points of potential jumps. However, it can be noted that any self-adjoint operator is not local: even a second-order self-adjoint differential operator is not defined on a function equal to zero on $P \subset R3$ if it does not belong to a Hilbert space.

IV. Discussion

Equation (3) can be called the free relativistic Schrödinger equation. In this paper, the relativistic Schrödinger equation is used to solve the problem of the states of a spinless particle in a one-dimensional space with potentials that look like a rectangular potential well.

Stationary one-dimensional relativistic Schrödinger equation with constant potential. It is easy to generalize equation (3) to the case of the presence of a potential (potential energy) U (r):

$$i\frac{\partial \psi}{\partial t} - U(r)\,\psi(r) = \sqrt{m^2 - \nabla^2}\,\psi(r) \qquad (4)$$

If the potential U (r) does not depend on y and z, the dependencies on all variables are separated. Using substitution

$$\Psi(r) = \psi(\varepsilon, x)\, exp\,(-i\varepsilon t)$$

We obtain the stationary one-dimensional relativistic Schrödinger equation with the potential U (x):

$$[\varepsilon - U(x)]\,\psi(\varepsilon, x) = \sqrt{m^2 - \nabla_x^2}\,\psi(\varepsilon, x) \qquad (5)$$

where

$$\nabla_x \equiv \frac{d}{d_x}$$

If U (x)= U_0 for all x ∈ (a, b) ⊂ R, this equation becomes

$$(\varepsilon - U_0)\psi(\varepsilon, x) = \sqrt{m^2 - \nabla_x^2}\,\psi(\varepsilon, x),\ \forall x\ \in (a, b), \qquad (6)$$

It follows from the definition of the operator $\sqrt{m^2 - \nabla_x^2}$ that if ε <U_0, equation (6) is satisfied only by the function ψ(ε,x)= 0, ∀x ∈ (a,b). If 0 < ε – U_0 <m, the solution to equation (5) has the form

$\psi(\varepsilon,x) = A\ exp(\kappa x) + B\ exp(-\kappa x),\ \forall x \in (a, b),$
where $A, B \in C,\ \kappa_k \in R$:

$$k = \sqrt{m^2 - (\varepsilon - U_0)^2}$$

If ε − U_0 >m,

$$\psi(\varepsilon, x) = A\exp(ikx) + B\exp(-ikx),\ \forall x\ \in (a, b),$$

where

$$p = \sqrt{(\varepsilon - U_0)^2 - m^2} \in R.$$

In order to determine the coefficients A, B ∈ C, it is necessary to set boundary conditions. The analogue of the Wronskian of the second-order differential equation in the theory of equation (6) is the function

$$W\left[x, \Psi_1, \Psi_2\right] = \Psi_1(x)(V(\nabla_x)\Psi_2)(x) - \Psi_2(x)(V(\nabla_x)\Psi_1)(x) \qquad (7)$$

and that, if boundary conditions are set under which this function takes the same values at the boundary points, the corresponding boundary value problem is self-adjoint in the sense of the scalar product:

$$(\Psi_1, \Psi_2)_a^b = \int_a^b [\Psi_1{}^*(x)\Psi_2(x) + m^2(g(\nabla_x)\Psi_1{}^*)(x)g(\nabla_x)\Psi_2)(x) +$$
$$(V^*(\nabla_x)\Psi_1{}^*)(x)(V(\nabla_x)\Psi_2)(x)]d_x \qquad (8)$$

Corresponding norm

$$\left||\Psi|\right| = [(\Psi_1, \Psi_2)_a^b]^{\frac{1}{2}}. \qquad (9)$$

The definition of the local operator $\sqrt{m^2 - \nabla_x^2}$ generates an infinite set of self-adjoint boundary value problems, each of which has its own spectrum and its own functions. Each of them can be associated with a self-adjoint operator in the corresponding Hilbert space. J. von Neumann's definition leads directly to a self-adjoint operator, but only to one that corresponds to the only boundary value problem - at (a=-∞), b=∞. The application of this definition, for example, to the problem on the interval (0, ∞), is generally impossible, since our operator must be a function of the operator -$i\nabla_x$, and the latter cannot be defined on functions on this interval as self-adjoint [4].

Linear harmonic oscillator. A linear harmonic oscillator is a particle moving in a potential

pit $V(x) = \frac{m\omega^2 x^2}{2}$ (pic. 1.a),

where m is the mass of the particle, ω is the frequency of the oscillator. In the *classical case*, the particle would move according to the law $x(t) = x_0 \cos(\omega t + \varphi_0)$. The amplitude x0 is uniquely determined by the energy of the oscillator, which, in turn, can take on a continuous series of values in the interval from 0 to ∞.

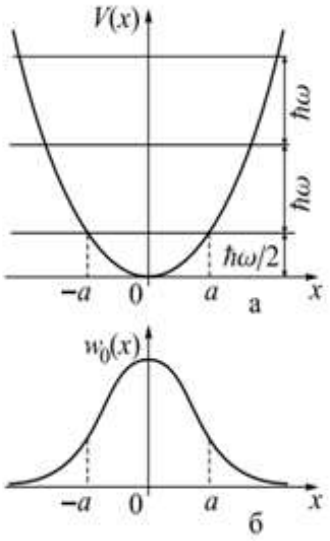


Рис. 1

In the microcosm, the stationary statement of the problem requires the solution of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi_E(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2 \Psi_E(x) = E\Psi_E(x) \qquad (10)$$

with boundary conditions $\Psi_E(\pm\infty) = 0$ due to finite motion.

In accordance with the general theory, the energy spectrum of the oscillator will be *discrete*:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad (11)$$

The levels are equidistant at a distance $\hbar\omega$ from each other. In accordance with the general property of one-dimensional finite motion, they are *not degenerate*, i.e. each corresponds to only one state:

$$\Psi_n(x) = \frac{1}{\sqrt{x_0}}\left(\frac{x}{x_0}\right), \qquad (12)$$

$$x_0 = \sqrt{\frac{\hbar}{m\omega}} \qquad (13)$$

— "natural" unit of length for an oscillator, which allows to significantly simplify all mathematical calculations by passing to dimensionless quantities;

$$\Psi_n^{(osc)}(\xi) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}} H_n(\xi) e^{-\frac{\xi^2}{2}} \qquad (14)$$

$H_n(\xi)$ - Chebyshev-Hermite polynomial. (pic. 1 b). Function (12) normalized to unity and orthogonal on the entire real axis:

$\int_{-\infty}^{+\infty} \Psi_{n'}(x)\Psi_n(x)dx = \delta_{n'n}$ (15)

The ground state of the oscillator has a non-zero energy $E_0 = \hbar\omega/2$ (measured from the "bottom" of the potential well). This is the so-called *zero-point energy*. The presence of zero oscillations does not contradict *the uncertainty principle*, which does not allow the particle to sink to the "bottom". The ground state corresponds to the wave function

$\Psi_0(x) = \frac{1}{\sqrt{x_0\sqrt{\pi}}} exp\left(-\frac{x^2}{2x_0^2}\right)$. (16)

Since the potential energy increases monotonically in a continuous manner as we move away from the equilibrium position, the wave functions will be nonzero even in the classically inaccessible region. The graph of the probability density in the ground state is given as an example in fig. 1.b. It is a Gaussian curve.

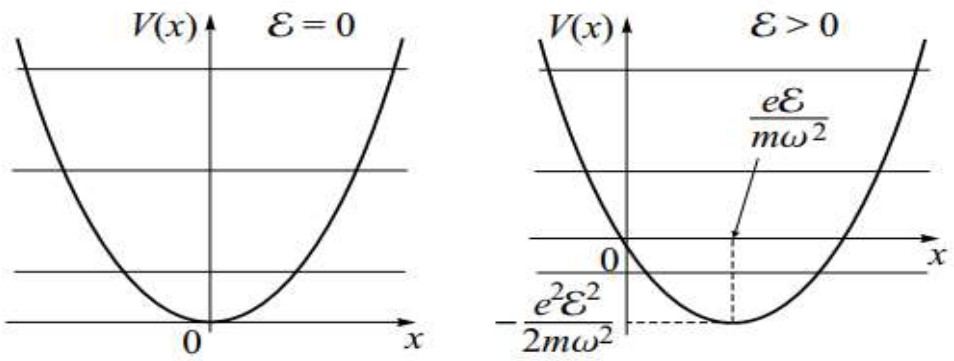
Stark effects are called changes that occur with a connected charged system under the influence of an external electric field. Below we consider the Stark effect for a charged oscillator in a constant electric field.

The Stark effect for an oscillator in a constant field consists in a downward shift of all energy levels by the same amount, which does not disappear in the classical limit.

If the oscillator is affected by a constant uniform electric field of intensity E, directed along the Ox axis. One can find the energies of the stationary states and their corresponding wave functions.

SOLUTION. Schrödinger equation for an oscillator in an electric field

$-\frac{\hbar^2}{2m}\frac{d^2\Psi_E(x)}{dx^2} + (\frac{1}{2}m\omega^2x^2 - e\mathcal{E}x)\Psi_E(x) = E\Psi_E(x)$ (17)



Pic.2

Can be simplified if a full square is selected in the potential well:

$\frac{1}{2}m\omega^2x^2 - e\mathcal{E}x = \frac{1}{2}m\omega^2\left(x^2 - \frac{e\mathcal{E}}{m\omega^2}\right)^2 - \frac{e^2\mathcal{E}^2}{2m\omega^2}$ (18)

After substitutions

$x \to X = x - \frac{e\mathcal{E}}{m\omega^2}; \quad E \to E' = E + \frac{e^2\mathcal{E}^2}{2m\omega^2}; \quad \Psi_E(x) = \Phi_{E'}(X)$ (19)

we go to the equation

$-\frac{\hbar^2}{2m}\frac{d^2\Phi_{E'}(X)}{dX^2} + \frac{1}{2}m\omega^2X^2\Phi_{E'}(X) = E'\Phi_{E'}(X)$ (20)

which in its structure completely coincides with the Schrödinger equation (10) for the same oscillator without a field. The reason for this phenomenon is easy to understand by analyzing (17): the potential curve of the oscillator under the action of an external electric field undergoes only *parallel transfer* (Pic. 2); the shape of the curve that determines the frequency remains unchanged. Thus, the oscillator shifts its equilibrium position and the energy reference point. This is fully reflected in substitutions (18), but not in the final equation (19) and its boundary conditions.
Solution (19) is easily constructed based on (11), (12), and (18):

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{e^2\mathcal{E}^2}{2m\omega^2} \qquad (21)$$

$$\Psi_n(x) = \frac{1}{\sqrt{x_0}}\Psi_n^{(osc)}\left(\frac{x-\frac{e\mathcal{E}}{m\omega^2}}{x_0}\right), \quad n=0,1,2,\ldots\ldots\ldots \quad (22)$$

The Stark effect for an oscillator in a constant field consists in a downward shift of all energy levels by the same amount, which does not disappear in the classical limit[9].

V. Conclusion

A methodological system for the study of quantum mechanics, based on the consistent use of algebraic methods, provides a deeper understanding of theoretical physics for students.

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