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ELEMENTARY PARTICLE PHYSICS AND FIELD THEORY

METHOD FOR NUMERICAL SOLUTION OF THE STATIONARY SCHRÖDINGER EQUATION

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The aim of this work is to describe a method of numerical solution of the stationary Schrödinger equation based on the integral equation that is identical to the Schrödinger equation. The method considered here allows one to find the eigenvalues and eigensolutions for quantum-mechanical problems of different dimensionality. The method is tested by solving problems for one-dimensional and two-dimensional quantum oscillators, and results of these tests are presented. Satisfactory agreement of the results obtained using this numerical method with well-known analytical solutions is demonstrated.

Keywords: Schrödinger equation, energy eigenvalues, eigenfunctions, numerical solution, fundamental solutions.

INTRODUCTION

The Schrödinger equation is of fundamental importance in the solution of quantum-mechanical problems [1]. Analytical solutions of this equation can be obtained only for an extremely limited set of problems, predominantly one-dimensional. Therefore, a number of approximate methods for solving the Schrödinger equation have been developed, both analytical, using perturbation theory [2–4], and direct numerical methods.

Despite the wide spectrum of numerical methods available for solving the Schrödinger equation, such as the Numerov method [5], the diagonalization method [6, 7], the spectral method [7], and other numerical methods [8–12] for example, the problem of devising effective methods of finding eigenenergies and eigenfunctions for the most basic equation of quantum mechanics, especially in the solution of multidimensional problems, remains an urgent problem. In the present work, we propose a technique for solving the Schrödinger equation that is based on reducing it to an integral equation with subsequent numerical solution.

THE SCHRÖDINGER INTEGRAL EQUATION

Let a particle with mass m perform a finite motion in the force field $V(\boldsymbol{r})$. We write the stationary Schrödinger equation in the form

$$\Delta\psi + \frac{2m}{\hbar^2}E\psi = \frac{2m}{\hbar^2}V(\boldsymbol{r})\psi\,. \tag{1}$$

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In the process of solving Eq. (1), it is necessary to find eigenvalues of the energy E and the corresponding eigenfunctions, i.e., the particle wave functions $\psi(\boldsymbol{r})$. We transform from the homogeneous Schrödinger equation to an inhomogeneous equation by introducing the new unknown function

$$U(\boldsymbol{r}) = \psi(\boldsymbol{r}) - u_0(\boldsymbol{r}), \tag{2}$$

where the prescribed auxiliary function $u_0(\boldsymbol{r})$, as will be shown below, can determine some properties of the solution. We now write the Schrödinger equation as

$$\Delta U + \lambda U = v(\boldsymbol{r})U - (\Delta + \lambda - v)u_0, \tag{3}$$

where $\lambda = \dfrac{2m}{\hbar^2}E$ and $v(\boldsymbol{r}) = \dfrac{2m}{\hbar^2}V(\boldsymbol{r})$.

The right-hand side of Eq. (3) can be considered as the density of some fictitious charge $\rho(\boldsymbol{r})$ generating the field $U(\boldsymbol{r})$ satisfying the inhomogeneous Helmholtz equation

$$\Delta U + \lambda U = \rho(\boldsymbol{r}),$$

where

$$\rho(\boldsymbol{r}) = v(\boldsymbol{r})U(\boldsymbol{r}) - (\Delta + \lambda - v(\boldsymbol{r}))u_0(\boldsymbol{r}). \tag{4}$$

The particular solution of this equation can be represented in the form

$$U(\boldsymbol{r}) = \int_{\Omega} \rho(\boldsymbol{R})\, g(\boldsymbol{r}, \boldsymbol{R})\, d\Omega_R\,. \tag{5}$$

Here $g(\boldsymbol{r}, \boldsymbol{R})$ is the fundamental solution of the Helmholtz equation, which can be considered as a field created at the point $\boldsymbol{r}$ by a unit positive point charge located at the point $\boldsymbol{R}$. The specific forms of the fundamental solutions for the Helmholtz equations of various dimensionalities are well known [13].

It is physically reasonable to suppose that the integration region Ω in relation (5) is close to, but somewhat larger than, the classically accessible region for a particle, whose boundaries are defined by the equation

$$V(\boldsymbol{r}) = E\,. \tag{6}$$

In the general case, the field corresponding to the Helmholtz equation is equal to the sum of the field corresponding to the particular solution of Eq. (5) and the field created by external *charges* located beyond the limits of the region Ω or on its boundary. Here also, proceeding from physical arguments, it may be posited that the sources of the real physical field and the field of the wave function of the particle are found within the limits of the region Ω, and thus the main component of the wave function $U(\boldsymbol{r})$ satisfies Eq. (5). Now, after substituting charge density (4) into Eq. (5), we obtain the following integral equation for the unknown function:

$$U(\boldsymbol{r}) - \int_{\Omega} U(\boldsymbol{R})v(\boldsymbol{R})\, g(\boldsymbol{r}, \boldsymbol{R})\, d\Omega_R = -\int_{\Omega} (\Delta + \lambda - v(\boldsymbol{R}))u_0(\boldsymbol{R})\, g(\boldsymbol{r}, \boldsymbol{R})\, d\Omega_R\,. \tag{7}$$

Equation (7) is the Schrödinger integral equation. This equation is a consequence of Eq. (3). It can be shown that, conversely, Eq. (3) is a consequence of integral equation (7).

TEST PROBLEM FOR A ONE-DIMENSIONAL WELL POTENTIAL

Equation (7) can be solved numerically. The simplest way to do this, of course, is to solve one-dimensional problems. In this case, with the help of Eq. (6) an interval $[a, b] = \Omega$ is found, within the limits of which the potential energy of the particle does not exceed its total energy E. On the interval $[a, b]$, some number N of grid points (nodes) x_i ($1 \le i \le N$) is laid out, preferably uniformly. We denote the values of the field at these points as U_i. We replace the integrals in Eq. (7) by their approximate values, using some numerical method of integration, for example, the method of rectangles. As a result, for the N unknown quantities U_i we obtain a system of N linear algebraic equations of the form

$$\sum_{j=1}^{N} a_{ij} U_j = b_i \,. \tag{8}$$

The fundamental solution of the one-dimensional Helmholtz equation [14]

$$g(x, X) = \frac{\sin\left(\sqrt{\lambda}\,|x - X|\right)}{2\sqrt{\lambda}} \tag{9}$$

is used to calculate the coefficients of system (8). To start with, let us solve the simplest test problem of the motion of a particle in a one-dimensional well potential of width L. The potential energy of a particle within the potential well is equal to zero, and beyond its limits is equal to infinity. We choose the auxiliary function in the form $u_0(x) = x$. As is well known, the eigenvalues of the energy of the particle in this case are given by the formula $E = \dfrac{\pi^2 \hbar^2}{2mL^2} n^2$, where the quantum number n takes integer values, beginning with $n = 1$. In the numerical solution of the problem, the energy of the particle is given by the last formula, in which the quantum number n is replaced by the test number μ, which can take any value, not only an integer value. The solution is obtained in accordance with the following algorithm. The initial value of the energy of the particle is assigned, for example, $E_0 = 0$, and the energy variation step δε is also assigned. It is desired that this step be much smaller than the distance ΔE between the nearest eigenvalues of the energy: $\delta\varepsilon << \Delta E$. For each successive value of the energy $E = E_0 + k\delta\varepsilon$, $k = 0, 1, 2, \ldots$, system (8) is solved and the values of the wave function at the end-points of the solution region are found. Those values of the energy for which the quantity $e = |\psi_1| + |\psi_N|$ has its smallest possible value, close to zero, are the eigenvalues of the problem. To refine these values, we can narrow the search region and decrease the energy variation step δε. We call the parameter $K = 1/e = 1/\left(|\psi_1| + |\psi_N|\right)$, equal to the inverse of the quantity e, the criterion of the problem of finding the energy eigenvalues. Figure 1 displays a screenshot from the computer, which shows the dependence of the criterion on the value of the test number μ, which in the course of the calculations was varied from 0 to 10 with a step equal to $\delta\mu = 0.1$. The maximum values of the criterion K should correspond to the energy eigenvalues in this case. The number of grid points N in the solution region of the problem was set equal to $N = 100$.

As can be seen from Fig. 1, sharp maxima of the displayed dependence are observed at odd integer values of the number μ. This has to do with the fact that the auxiliary function $u_0(x) = x$ used to solve the problem is odd. If an even auxiliary function is used, for example, $u_0(x) = 1$, then the maxima are observed at even integer values of μ. The wave functions corresponding to the maxima of the criterion K were found to be in exact agreement with the analytical solutions of the problem.

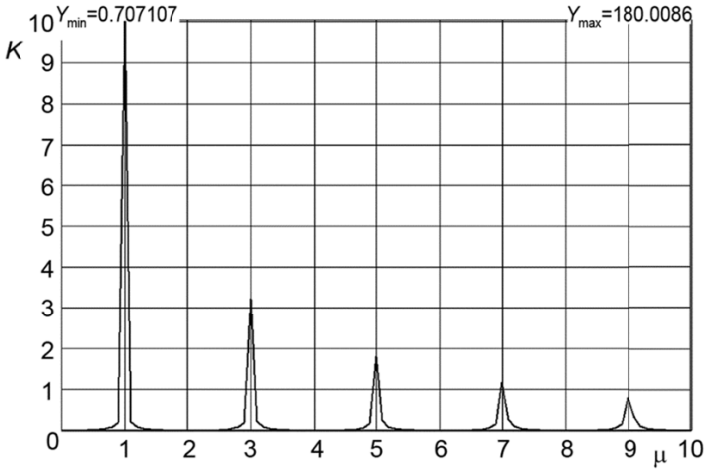

Fig. 1. Dependence of the criterion of the problem, *K*, on the test number μ.

SOLUTION OF A TEST PROBLEM FOR A ONE-DIMENSIONAL OSCILLATOR

Let us next consider the results of a test of the numerical method in the example of solving the problem for a quantum harmonic oscillator. In this case, the potential energy of the particle is given by the formula $V(x) = m\omega^2 x^2/2$, and the solution region is an interval of length $L = 2\sqrt{\frac{2E}{m\omega^2}}$, where ω is the frequency of the oscillator. In order to capture the abrupt falloff of the wave function beyond the limits of the classically allowed region, this interval must be extended somewhat, say, to $L = 3\sqrt{\frac{2E}{m\omega^2}}$. Next, the solution is obtained in accordance with the algorithm described in the preceding section. As a result, we obtain dependences of the criterion *K* on the reduced energy (test eigennumber) $\mu = \frac{E}{\hbar\omega} - \frac{1}{2}$, which in the course of the calculations was varied from 0 to 10 with a step equal to $\delta\mu = 0.1$.

The calculations showed that distinct maxima are observed in the graphs of the dependence of the criterion *K* on the reduced energy at the integer values μ = 1 – 7. For μ = 0 the maximum is expressed quite weakly, and for μ > 7 the positions of the maxima are shifted somewhat toward smaller values and are observed somewhat prematurely at μ = 7.9, 8.9, and 9.8. This is apparently a result of the fact that with growth of the eigennumber corresponding to the energy eigenvalue the number of oscillations of the wave function in the solution region grows. This leads to growth of the error of the numerical solution for the eigenfunction and correspondingly to an increase in the error for the criterion *K*. This problem is eliminated by increasing the number of grid points *N* and decreasing the energy variation step, which in our case is the step $\delta\mu$.

The numerical solution of Eq. (7) turns out to be extremely sensitive to the value of the parameter μ, which determines the value of the energy *E*. Figure 2 displays a graph of the dependence of values of the wave function ψ on the reduced coordinate of the particle *x*/*L*. Curve *1* plots the eigenfunction corresponding to μ = 2. The dependence of the eigenfunction calculated using *N* = 100 grid points coincides with the theoretical dependence calculated using the Hermite polynomials. Curve *2* was obtained for μ = 2.1.

As can be seen from Fig. 2, in the dependence obtained for μ = 2.1, i.e., for a value of the energy not equal to the eigenvalue, apart from a quantitative departure from the dependence of the eigenfunction itself, breaks and jumps are also observed. The presence of these breaks and jumps is one of the signs of a deviation from the eigenvalue of the energy. The main parameter determining the accuracy of the numerical solution is, naturally, the number of grid points

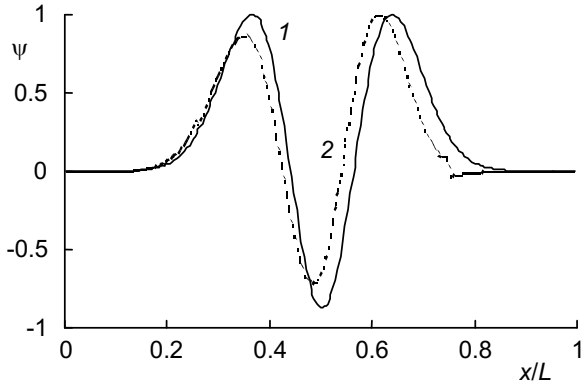

Fig. 2

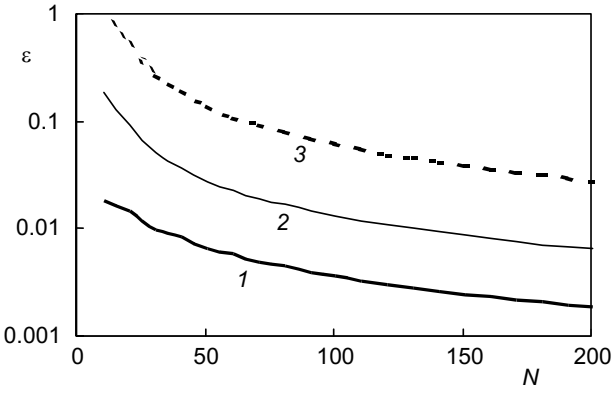

Fig. 3

Fig. 2. Dependence of values of the wave function ψ on the reduced coordinate of the particle, *x*/*L*.

Fig. 3. Dependence of the errors of the numerical solution on the number of grid points *N*: curve *1* corresponds to μ = 0, curve *2* corresponds to μ = 1, and curve *3* corresponds to μ = 2.

N in the solution region of the problem. As a measure of the error in the calculation of the eigenfunctions, we used the quantity

$$\varepsilon = \max_i \left| \psi_i - \varphi(x_i) \right|, \tag{10}$$

where $\varphi(x_i)$ is the value of the analytical solution of the problem at the point with coordinate x_i. In the calculation of the error of the numerical solution, we first normalized the eigenfunctions by dividing them by the maximum of their absolute value in the solution region of the problem. Figure 3 displays a graph of the dependence of the errors of the numerical solution on the number of grid points *N*, for three eigenfunctions: with μ = 0 (curve *1*), μ = 1 (curve *2*), and μ = 2 (curve *3*).

It can be seen from Fig. 3 that the error of the numerical solution for the eigenfunctions falls with growth of *N*, and that with growth of *N* the rate of falloff slows down. It can also be seen that the error of the numerical solution grows with the eigennumber corresponding to the eigenvalue of the energy: the error for the next energy level is increased by almost an order of magnitude. Nevertheless, they can be calculated by increasing the number *N*, to ensure an acceptable calculation accuracy. For example, for the fourth energy level (the energy level with μ = 4) the error of the solution for *N* = 500 does not exceed 2%. It should be noted here that in all cases the mean or root-mean-square error turns out to be significantly less.

The above results were obtained using the auxiliary function $u_0(\boldsymbol{r}) = 1 + x$. This function is the sum of an even and an odd function, which made it possible to obtain solutions possessing different symmetry. If in the development of the algorithm that the numerical solution of the problem is based on, account is taken of certain symmetry properties of the wave functions, it becomes possible to optimize the computer model, limit the number of calculations, and correspondingly increase their accuracy.

SOLUTION OF A TEST PROBLEM FOR A TWO-DIMENSIONAL OSCILLATOR

The main advantage of the method described here for solving the Schrödinger equation is the possibility of applying it, without substantial complication, to the solution of multidimensional problems. Here the main difficulty is

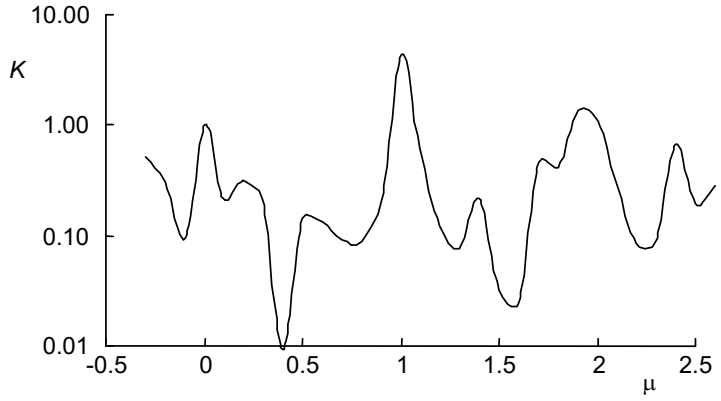

Fig. 4. Dependence of the eigenvalue criterion on the reduced energy of a two-dimensional quantum oscillator.

connected with the abrupt increase in the number of linear equations of type (8) with increase in the dimensionality of the problem. Below we present the main results of solving a two-dimensional test problem for a two-dimensional isotropic quantum oscillator.

To calculate the coefficients of system (8) for positive values of $\lambda = \frac{2m}{\hbar^2}E$, the fundamental solution of the two-dimensional Helmholtz equation, expressed in terms of the zeroth-order Hankel functions of the first kind [13], is used:

$$g(\boldsymbol{r},\boldsymbol{R}) = \frac{i}{4}H_0^{(1)}\left(\sqrt{\lambda}\left|\boldsymbol{r}-\boldsymbol{R}\right|\right).$$

We represent the energy of the oscillator in the form $E = E_x+E_y$, where E_x and E_y are the components of the energy due to motion along the X and Y axes, respectively. The solution region is represented in the form of a rectangle with sides $L_x = 3\sqrt{\frac{2E_x}{m\omega^2}}$ and $L_y = 3\sqrt{\frac{2E_y}{m\omega^2}}$. Of course, the dimensions of the solution region can differ somewhat from these values. However, significant deviations of these lengths from the recommended values lead to a growth of the error of the calculations, which can hinder an analysis of the results of a determination of the energy eigenvalues.

The algorithm for solution of the problem of searching for the energy eigenvalues recapitulates the above-described algorithm for the one-dimensional case. An initial value of the energy of the particle is assigned, for example, $E_0 = 0$, and the energy variation step $\delta\varepsilon$ is also assigned. For each successive energy value $E = E_0+k\delta\varepsilon$, $k = 0, 1, 2, ...$, system (8) is solved and the values of the wave function at the boundaries of the solution region are found. Those values of the energy for which the quantity $e = \sum_l \left|\psi_l\right|$ (here the sum is calculated over the values of the wave function $\left|\psi_l\right|$ at the boundary grid-points of the solution region) has the smallest possible value, close to zero, are the eigenvalues of the problem.

Figure 4 displays a graph of the dependence of the criterion of the problem of finding the energy eigenvalues $K = 1/e = 1/\sum_l \left|\psi_l\right|$ on the reduced energy $\mu = \frac{E}{\hbar\omega} - 1$, which in the course of the calculations was varied from – 0.5 to 2.5 with a step equal to $\delta\mu = 0.1$. The maximum values of the criterion K should correspond to the energy eigenvalues in this case. The number of grid points N in the solution region of the problem was set equal to $N = 24\times 24 = 576$. The calculations were performed for $u_0(\boldsymbol{r}) = 1 + x$.

As is clear from Fig. 4, distinct maxima are observed for μ = 0 and 1. For μ ≈ 2 the maximum is shifted somewhat toward smaller values: to μ = 1.9. These results are in agreement with the exact eigenvalues of the energy of a two-dimensional oscillator $E_m = \hbar\omega(\mu+1)$, $\mu = 0, 1, 2, \ldots$ However, attention should also be given to the presence of several secondary local maxima at values of μ which do not coincide with the theoretically expected results. Increasing the number of grid points from $N = 576$ to $N = 30 \times 30 = 900$ improves the result somewhat; however, the secondary maxima remain, which can lead to errors in the identification of the energy eigenvalues.

Certain difficulties also arise when degeneracy of the energy levels is taken into account. For example, the second energy level (the one with μ = 1) can be put into correspondence with two eigenfunctions. One of them is symmetric with respect to the *X* axis and antisymmetric with respect to the *Y* axis, and the other one, conversely, is symmetric with respect to the *Y* axis and antisymmetric with respect to the *X* axis. To calculate the eigenfunctions in these two cases by the above-described method, it is desirable to use different solution regions (with different ratios of sides) and different auxiliary functions $u_0(\boldsymbol{r})$. In the first case, this can be $u_0(\boldsymbol{r}) = 1 + y$, and in the second, $u_0(\boldsymbol{r}) = 1 + x$.

CONCLUSIONS

The analysis presented above demonstrates the potential of the proposed numerical method for solving quantum-mechanical problems of different dimensionality. It should also be noted that the above-described method for solving the Schrödinger equation can be used to solve different types of elliptical equations of noncanonical form. Additional possibilities also arise when using fundamental solutions, found beforehand by this numerical method, in an integral equation similar to Eq. (7).

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