APPLICATIONS OF ORTHOGONAL POLYNOMIALS TO SOLVING THE SCHRÖDINGER EQUATION*

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The article reveals possibilities of using Hermite polynomials and related Hermite–Weber functions to solve a wide range of problems in mathematical physics. The obtained properties of the considered functions allow for constructing solutions for problems of wave dynamics. The solution of the Schrödinger integral equation constructed on their basis is highly accurate since, in this case, waves of matter can freely pass along the entire real axis, and there is no need for "matching" solutions on the finite interval.

Keywords: Hermite polynomials, Hermite functions, orthogonal polynomials, Schrödinger equation.

1. Introduction

Orthogonal polynomials or special functions are used in numerous physical and engineering problems which contain differential and integral equations. Many methods for solving them are based on Hermite polynomials, i.e. a classical sequence of orthogonal polynomials [1]. The fact that a number of Hermite polynomials forms a basis makes it possible to arrange various functions in a series, which facilitates solutions of many problems [2, 3]. Hermite polynomials played a decisive role in the theory of light fluctuations and quantum states and, in particular, in problems of coastal hydrodynamics and meteorology [4].

In addition, the method of decomposition into Hermite polynomials is used in biological and epidemiological sciences. The epidemiological SIR model which estimates the number of people who can become infected was calculated in this way. Hermite polynomials provide a possibility for reducing a three-dimensional system of ordinary nonlinear differential equations to a system of nonlinear algebraic equations [5].

The use of Hermite polynomials has also found a place in economic problems. J. Perote et al. [6–8] use the Hermite polynomial methods to describe behaviour of financial variables.

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Also, these polynomials can model non-Gaussian excitations which reflect models of numerous phenomena surrounding us. The wind pressure in areas of flow separation on the surfaces of buildings usually has non-Gaussian characteristics, as well as modelling wind speed in complex areas [9]. Additionally, polynomials can be applied in the field of engineering marine structures when assessing the reliability of a hull beam for floating, production, storage, and unloading blocks [10]. Such problems are solved using the Hermite impulse model of nonlinear non-Gaussian random oscillations [11].

Expansion in Hermite polynomials greatly facilitates solutions of integro-differential [12] and integral equations. These polynomials are certainly useful for solving any problems in which a solution is defined on the entire real axis. Such problems result from analyzing processes of reflection and passage of waves through given potential barriers. In other words, these are Schrödinger wave dynamics problems. Solving these problems allows to find the probability of passage of atoms and molecules in the form of de Broglie waves through various membranes. Theoretical works [13–20] consider the passage of de Broglie waves through ultrathin membranes based on the solutions determined on the segment and using the "matching" conditions at its ends. Practical works [21–26] on single-layer materials adapt them to quantum screening. The work given in [27] presents a numerical solution of the Schrödinger equation for a tunable potential barrier. The authors of [28] investigate enrichment of helium by resonant tunnelling through biolayers.

2. The Schrödinger differential and integral equations

The differential equation for the Schrödinger wave function $\psi(x)$ in the one-dimensional case is given as

$$\frac{d^2\psi}{dx^2} + \left[k^2 - 2mU(x)\right]\psi = 0, \quad k = \sqrt{2mE}. \tag{1}$$

It describes the passage of a particle with a mass of m and energy E through a potential barrier noted as $U(x)$. The boundary condition at a great distance consists of two parts:

$$\psi \simeq e^{ikx} + Ae^{-ikx}(x \to -\infty), \quad \psi \simeq Be^{ikx}(x \to \infty). \tag{2}$$

This means that for large negative values of x the function $\psi(x)$ represents the sum of the incident and the reflected waves; and for large positive values of x it approaches the plane passing wave. Thus, to solve the problem it is necessary to find two linearly independent solutions of the homogeneous differential equation given in (1) (numerically or analytically) and then match these solutions so that the boundary conditions given in (2) [29–31] are satisfied. This is a common way of dealing with the problem of material particles passing through a potential barrier. In this case, the function $\psi(x)$ appears to be complex; however, it is not this function that has the physical meaning, but the square of its module $\rho = |\psi(x)|^2$ which is equal to the density of probability that the particle is found in the section $x = \text{const}$.

If only the graph of the function $\rho(x)$ is under consideration, it appears to be strongly oscillating in the region where the incident and the reflected waves exist simultaneously. Such a graph complicates the interpretation of calculations since it is practically impossible to correctly separate the amplitudes of the incident and the reflected waves.

However, the differential equation given in (1) is closely related to the Schrödinger integral equation introduced in [32]. It has the following form,

$$\psi(x) - \frac{m}{ik} \int_{-\infty}^{\infty} e^{ik|x-x_0|} U(x_0)\psi(x_0)dx_0 = e^{ikx}. \tag{3}$$

Eq. (3) and (1) are equivalent in the sense that if Eq. (3) is twice differentiated with respect to the variable x, Eq. (1) is obtained. However, the inhomogeneous integral equation given in (3) also contains boundary conditions (2). This can be seen if Eq. (3) is written in a more detailed form,

$$\psi(x) = e^{ikx}\left[1 + \frac{m}{ik}\int_{-\infty}^{x} e^{ikx_0}U(x_0)\psi(x_0)dx_0\right] + e^{-ikx}\left[\frac{m}{ik}\int_{x}^{\infty} e^{ikx_0}U(x_0)\psi(x_0)dx_0\right]. \tag{4}$$

In square brackets there are the amplitudes of the incident and reflected waves:

$$a_{\text{passed}} = 1 + \frac{m}{ik}\int_{-\infty}^{x} e^{ikx_0}U(x_0)\psi(x_0)dx_0,$$

$$a_{\text{reflected}} = \frac{m}{ik}\int_{x}^{\infty} e^{ikx_0}U(x_0)\psi(x_0)dx_0. \tag{5}$$

This corresponds to the boundary conditions in (2) since for large positive values of x the reflected wave disappears, and for large negative values of x the sum of the incident and the reflected waves is obtained. Then the transmission coefficient ρ_{passed} and the reflection coefficient $\rho_{\text{reflected}}$ are defined as follows:

$$\rho_{\text{passed}} = |\mathrm{a}_{\text{passed}}|^2, \quad \rho_{\text{reflected}} = |\mathrm{a}_{\text{reflected}}|^2. \tag{6}$$

In addition, for each value of x the following is true,

$$\rho_{\text{passed}} + \rho_{\text{reflected}} = 1. \tag{7}$$

It is clear that, when interpreting the calculation results, it is preferable to separately construct the graphs of amplitude squares for the incident and the reflected waves. Naturally, in order to use formula (4) it is necessary to obtain the corresponding solution of $\psi(x)$, either with the integral equation given in (3), or with the boundary value problem formulated in (1), (2).

3. Brief information from the theory of polynomials and Hermite functions

Hermite polynomials $\mathrm{He}_n(x)$ were introduced as early as 1864. At present, information concerning them is published in classical monographs and mathematical reference books [33–36]. The polynomial $\mathrm{He}_n(x)$ is a polynomial of degree n in x with integer coefficients which contains only terms of the same parity as x^n. The explicit expressions for the first Hermite polynomials are:

$$\begin{gathered}\mathrm{He}_0 = 1, \quad \mathrm{He}_1(x) = x, \quad \mathrm{He}_2(x) = x^2 - 1, \quad \mathrm{He}_3(x) = x^3 - 3x,\\ \mathrm{He}_4(x) = x^4 - 6x^2 + 3, \quad \mathrm{He}_5(x) = x^5 - 10x^3 + 15x,\\ \mathrm{He}_6(x) = x^6 - 15x^4 + 45x^2 - 15,\\ \mathrm{He}_7(x) = x^7 - 21x^5 + 105x^3 - 105x.\end{gathered} \tag{8}$$

For the generating function and the Rodrigues formula resulting from it we get

$$e^{tx-t^2/2} = \sum_{n=0}^{\infty} \mathrm{He}_n(x)\frac{t^n}{n!}, \quad \mathrm{He}_n(x) = (-1)^n e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}. \tag{9}$$

Hermite polynomials can also be written in the form of the determinant [38]

$$\mathrm{He}_n(x) = \begin{vmatrix} x & n-1 & 0 & 0 & \dots & 0 \\ 1 & x & n-2 & 0 & \dots & 0 \\ 0 & 1 & x & n-3 & \dots & 0 \\ 0 & 0 & 1 & x & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & x \end{vmatrix}. \tag{10}$$

Moreover, formula (10) is most suitable for practical calculations of coefficients of high-order Hermite polynomials. Algorithmically, formula (10) can be implemented using the following simple program in the MatLab system:

```
function p=He(n)
c=n-1:-1:1; s=ones(1,n-1);
M=diag(c,1)+diag(s,-1);
p=poly(M);
end
```

It lists coefficients p for the Hermite polynomial $\mathrm{He}_n(x)$ of the n-th order. It should be noted that n-th order Hermite polynomials have n simple real roots which are pairwise symmetric with respect to the origin and do not exceed $\sqrt{n(n-1)/2}$ in the absolute value.

In problems of mathematical physics there are applied Hermite functions $D_n(x)$ which are connected with Hermite polynomials and are given by the expression

$$D_n(x) = \frac{e^{x^2/4}\mathrm{He}_n(x)}{\sqrt{n!\sqrt{2\pi}}}. \tag{11}$$

These functions are easily calculated and form a complete orthogonal and normalized system on the entire real axis [37],

$$\int_{-\infty}^{\infty} D_n(x)D_m(x)dx = \begin{cases} 0, n \neq m, \\ 1, n = m. \end{cases} \tag{12}$$

This orthogonality property of the basis elements is not unique to the Hermite polynomials. Some other functions, for instance

$$D_n(x) = \sqrt{\frac{n!}{\Gamma(n+v+1)}}\left(\frac{dy}{dx}\right) e^{-y/2} L_n^v(y),$$

where $L_n^v(y)$ is the Laguerre polynomial with $v > -1$ and $y(x) = e^{x/a}$ have also this property. Another example is

$$D_n(x) = A_n \left(\frac{dy}{dx}\right)(1-y)^{\mu/2}(1+y)^{v/2} P_n^{(\mu,v)}(y),$$

where $P_n^{(\mu,v)}(y)$ is the Jacobi polynomial with $\mu, v > -1$, A_n is a normalization constant and $y(x) = \tanh(\frac{x}{a})$.

This feature of Hermite functions allows determining the expansion coefficients of arbitrary functions in a series with respect to Hermite functions reducing them to calculations of the integral

$$f(x) = \sum_{n=0}^{\infty} C_n D_n(x), \quad C_n = \int_{-\infty}^{\infty} f(\mu) D_n(\mu) d\mu. \tag{13}$$

The functions $D_n(x)$ satisfy the Weber differential equation

$$D_n''(x) = \left[\frac{x^2}{4} - \left(n + \frac{1}{2}\right)\right] D_n(x). \tag{14}$$

The following recurrence relations hold for them:

$$\begin{aligned} &D_{n+1}(x) - xD_n(x) + nD_{n-1}(x) = 0, \\ &2D_n'(x) + xD_n(x) - 2nD_{n-1}(x) = 0. \end{aligned} \tag{15}$$

It is also easy to show that

$$\frac{d^m}{dx^m}\left[e^{-x^2/4} D_n(x)\right] = (-1)^m e^{-x^2/4} D_{n+m}(x). \tag{16}$$

Thus, the derivatives of Hermite functions are expressed in terms of the same functions.

Fig. 1 shows the graphs of the first six Hermite functions which are calculated by the formula (11).

Fig. 2 shows similar Hermite functions of higher order,

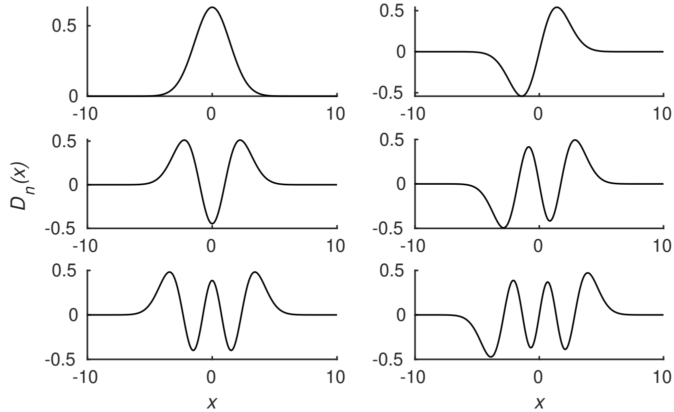

Fig. 1. Graphs of the first six Hermite functions.

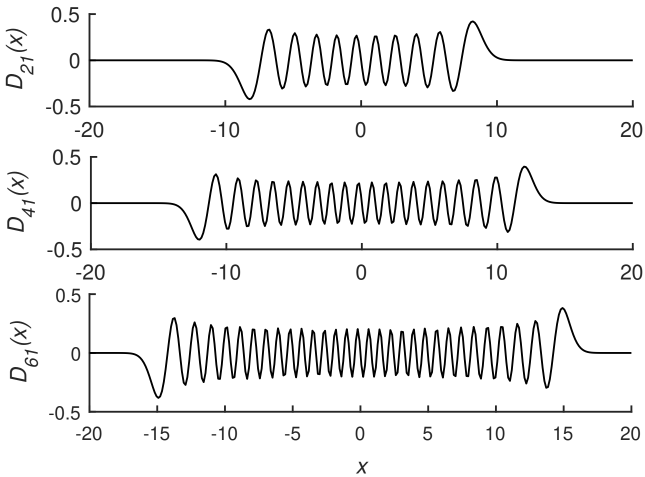

Fig. 2. Graphs of functions $D_{21}(x)$, $D_{41}(x)$ and $D_{61}(x)$.

Considering such graphs of the functions $D_n(x)$ it is rather difficult to imagine that these functions form an orthonormal system on the entire material axis. Nevertheless, a numerical verification shows the correctness of the formula (12).

Note. The formulae given above are taken from the book by J. Kampé de Fériet [38] and they correspond to the so-called mathematical or probability Hermite polynomials. However, it should be borne in mind that in the famous reference book by I. S. Gradshtein and I. M. Ryzhik [39], as well as in the works given in [40–42], instead of the polynomials $\mathrm{He}_n(x)$ they use other polynomials $\mathrm{H}_n(x)$

which are also called Hermite polynomials. Both these Hermite polynomial systems are related by the relation: $\mathrm{H}_n(x) = \sqrt{2^n}\mathrm{He}_n(x\sqrt{2})$.

4. Solving the Schrödinger integral equation

Using the expansion formulae given in (13) we will find a solution to integral equation (3) in the form of a segment of a series with unknown coefficients C_n in Hermite functions:

$$\psi(x) = \sum_{n=0}^{N} C_n D_n(x),$$

$$e^{ik|x-x_0|} = \sum_{n=0}^{N} D_n(x) \int_{-\infty}^{\infty} e^{ik|\mu-x_0|} D_n(\mu) d\mu, \tag{17}$$

$$e^{ikx} = \sum_{n=0}^{N} D_n(x) \int_{-\infty}^{\infty} e^{ik\mu} D_n(\mu) d\mu,$$

N is an integer large enough to approximate the function. Typically there is a maximum integer $N_{\max}$ beyond which numerical calculation will experience convergence problems and the accuracy of the results starts to be reduced. Introducing (17) into integral equation (3) and equating the terms for identical functions $D_n(x)$ we obtain

$$C_n - \frac{m}{ik} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(x_0)\psi(x_0) e^{ik|\mu-x_0|} D_n(\mu) d\mu dx_0 = \int_{-\infty}^{\infty} e^{ik\mu} D_n(\mu) d\mu. \tag{18}$$

Further, with an account of the equality $\psi(x_0) = \sum_{r=0}^{N} C_r D_r(x_0)$, expression (18) takes the form

$$C_n - \frac{m}{ik} \sum_{r=0}^{N} C_r \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(x_0) e^{ik|\mu-x_0|} D_n(\mu) D_r(x_0) d\mu dx_0 \right] = \int_{-\infty}^{\infty} e^{ik\mu} D_n(\mu) d\mu. \tag{19}$$

Here the double integral (in square brackets) can be considered as a square matrix $\mathbf{G}$ of order N; and the right-hand side as a column vector $\mathbf{F}$. That is, the following notation should be introduced:

$$\mathbf{G}(k,n,r) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(x_0) e^{ik|\mu-x_0|} D_n(\mu) D_r(x_0) d\mu dx_0, \tag{20}$$

$$\mathbf{F}(k,n) = \int_{-\infty}^{\infty} e^{ik\mu} D_n(\mu) d\mu. \tag{21}$$

In this case, equality (19) is a system of linear algebraic equations for determining the column vector, which is composed of the desired coefficients C_n in the expansion of the function ψ. In the matrix notation, this system of equations has the form

$$\left[\mathbf{E}_N - \frac{m}{ik}\mathbf{G}\right]\mathbf{C} = \mathbf{F}. \tag{22}$$

Here $\mathbf{E}_N$ is the $(N+1)\times(N+1)$ identity matrix.

The question of solving integral equation (3) is, thus, reduced to the most accurate calculation of the integrals in formula (20).

Many integrals containing Hermite functions are calculated explicitly. A list of such integrals is contained in the reference book by I. S. Gradshtein and I. M. Ryzhik [39, p. 851]. Among them is the mentioned above vector $\mathbf{F}$, i.e.

$$\mathbf{F}(k,n) = \int\limits_{-\infty}^{\infty} e^{ik\mu} D_n(\mu)d\mu = \sqrt{4\pi} i^n D_n(2k). \tag{23}$$

Formula (23) is easily verified in various ways and can be derived independently. It shows that the Fourier spectrum of the Hermite function is expressed in terms of the Hermite function of the same order.

The following integral can be explicitly presented in the same way,

$$\int\limits_{-\infty}^{\infty} e^{ik|\mu-x_0|} D_n(\mu)d\mu = \int\limits_{-\infty}^{x_0} e^{ik(x_0-\mu)} D_n(\mu)d\mu + \int\limits_{x_0}^{\infty} e^{ik(\mu-x_0)} D_n(\mu)d\mu. \tag{24}$$

After further transformations, taking into account formula (23), it can be written as

$$\int\limits_{-\infty}^{\infty} e^{ik|\mu-x_0|} D_n(\mu)d\mu = \sqrt{4\pi} i^n D_n(2k)e^{-ikx_0} + 2iS_n(x_0), \tag{25}$$

where $S_n(x_0) = \int\limits_{-\infty}^{x_0} \sin k(x_0-\mu)D_n(\mu)d\mu$. The integral given in (25) is not completely expressed explicitly; the convolution $S_n(x_0)$ is also added and it is usually easily and fairly accurately calculated numerically.

Thus, the elements of the matrix $\mathbf{G}$ and the vector $\mathbf{F}$ of the right-hand side in formula (22) are now represented in the following form:

$$\mathbf{G}(k,n,r) = \int\limits_{-\infty}^{\infty} U(x_0)D_r(x_0)\left[\sqrt{4\pi} i^n D_n(2k)e^{-ikx_0} + 2iS_n(x_0)\right]dx_0,$$

$$\mathbf{F}(k,n) = \sqrt{4\pi} i^n D_n(2k). \tag{26}$$

Here it is necessary to calculate only the one-dimensional integral that takes into account the shape of the potential barrier, which can be solved numerically. However, it can still be calculated with high accuracy since the integration region is limited by the width of the barrier. There are other calculation methods that are very successful in dealing with such regular short-range potentials. For example, the R-matrix method [43], which is nonalgebraic, but also other algebraic approaches like the J-matrix method [44].

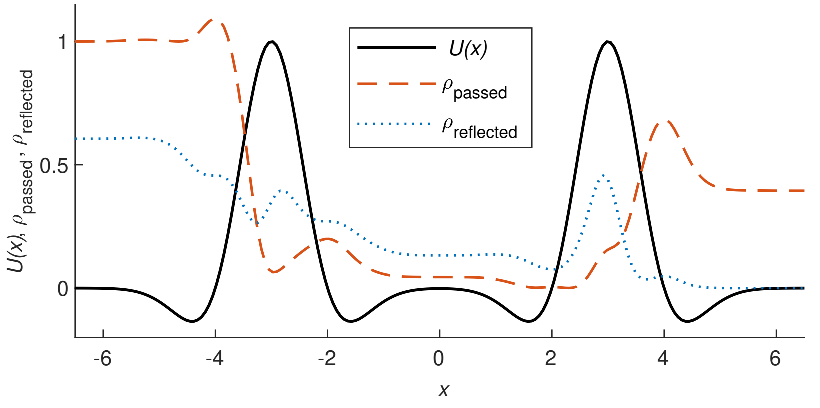

Fig. 3. Graphs of potential barrier $U(x)$ and amplitudes of transmitted ρ_{passed} and reflected $\rho_{\text{reflected}}$ waves. Initial data: $m = 3$, $E = 0.25$, $k = \sqrt{2mE} = 1.2247$.

The mass is expressed in units related to the mass of the hydrogen atom. Therefore, $m = 3$ corresponds to the helium isotope — helion. The dimensionless energy of the passing particle $E = 0.25$ corresponds to temperature of 12.5 K.

Fig. 3 shows one of the results of solving the Schrödinger equation using Hermite functions. First, the matrix $\mathbf{G}$ and the right-hand side of $\mathbf{F}$ are calculated by formulae (4). Then the expansion coefficients C_n are found as a solution of the system of linear algebraic equations (22). After this, the desired function $\psi(x)$ and the density distribution of the incident ρ_{passed} and the reflected $\rho_{\text{reflected}}$ de Broglie waves are obtained using formulae (6).

The graph of the potential barrier shape is indicated in Fig. 3 by a thickened line, and the density distribution of the reflected wave $\rho_{\text{reflected}}$ is represented as a dashed line. Calculations in Fig. 3 show how the dimples at the ends of the potential barrier affect the passage and reflection of particles. In addition, the well-known fact that the sum of the transmission and reflection coefficients is equal to unity is confirmed.

5. Conclusion

An analysis of the available solutions of problems related to the passage of de Broglie waves through given potential barriers shows that all the suggested solutions are connected with the use of numerical procedures implemented on a finite interval of variation of the independent variable. Moreover, the conditions of "matching" the obtained distributions with asymptotic values of the desired function and its derivative are necessarily used.

In such works questions concerning the size of the calculation interval, the correctness of the assumption about the equality of the desired function and its derivative to some external values, as well as the influence of the introduced restrictions and assumptions on the final result remain unsolved.

In the calculation example presented in this paper, there is a consideration of a barrier composed of two "Mexican hats". The mentioned shape of the barrier corresponds to a monolayer of porous graphene or boron nitride which are used in problems of isotope separation. In processes of wave separation of particles that are close in physical properties and differ only in mass, the selectivity of mixture separation can be increased only due to the resonant passage of individual components.

In this case, de Broglie waves move along the entire real axis and the contribution of the errors introduced by the "matching" conditions at the ends of the computational interval can be fatal concerning the selective arrangement of membrane monolayers.

In this regard, the present work suggests a quasi-analytic solution of the Schrödinger integral equation. This equation is defined on the entire real axis and contains a combination of the incident and the reflected waves on the left boundary and the transmitted wave at large positive values of the argument.

The desire for a more accurate description of the solution behaviour is also expressed in the fact that almost all improper integrals in the proposed procedure for constructing the solution are calculated analytically. A particular significance is given to the assertion that the Fourier spectrum of the Hermite function is expressed in terms of the Hermite function of the same order. In addition, the derivatives of Hermite functions are expressed through the same functions of a different order. Moreover, an increase in the order corresponds to the order of the derivative.

The coefficient matrix of the constructed solution includes integrals that depend on the shape of the barrier. In the considered example they are calculated only numerically. However, the accuracy of calculations for these integrals can be arbitrarily high since the nonzero integrands are limited by the width of the barrier under consideration.

Thus, the use of Hermite polynomials greatly simplifies the problem of solving the Schrödinger integral equation and allows for finding a solution that is more accurate than the "matching" method.

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