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New Method for Solving Multidimensional Scattering Problem

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A new method is developed for solving the quantum mechanical problem of scattering of a particle with internal structure. The multichannel scattering problem is formulated as a system of nonlinear functional equations for the wave function and reaction matrix. The method is successfully tested for the scattering from a nonspherical potential well and a long-range nonspherical scatterer. The method is also applicable to solving the multidimensional Schrödinger equation with a discrete spectrum. As an example the known problem of a hydrogen atom in a homogeneous magnetic field is analysed.

1. INTRODUCTION

Methods for solving the problem of scattering on a structural scatterer are based on the representation of the wave function of a system, $\psi(X)$, in a multidimensional coordinate space X as an expansion over some basis which would reflect specific features of the problem and would be rather simple. The procedure is known to be as follows: one should choose orthogonal scattering coordinates, compute matrix elements of the Hamiltonian of the problem in a chosen basis, solve a system of integrodifferential (or algebraic) equations, single out the scattering matrix from the wave function asymptotics, and investigate their dependence on the number of basis (or trial) functions. As a rule, this analysis can be made only numerically.

In this paper, an approach is proposed for solving the multidimensional scattering problem without expanding the wave function over the basis in a traditional sense and without calculating matrix elements of the Hamiltonian (a very cumbersome problem). For some of variables, Ω, from $X=\{R, \Omega\}$ characterizing a scatterer, a difference net Ω_i is introduced ($i=0, 1, ..., N$; the distance between nodes is characterized by the step of integration h); those variables are considered discrete, and one variable R (the distance from a particle to the centre of mass of a scatterer) remains continuous. Then the multidimensional Schrödinger equation is approximated by a system of differential-difference equations for the vector $\{\psi_i(R)\}_0^N = \psi(R, \Omega_i)$. For introducing "difference net" procedure for the internal coordinates one can use different approaches (see, for example [1]). The one used here is close to the "discrete variable representation" [2]. At a further step, the scattering

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problem is formulated, following Ref. [3], as a system of nonlinear functional equations

$$F_m^{(v)}(z)=0; \qquad v=0, 1, ..., S\leqslant N; m=1, ..., 5 \tag{1.1}$$

for the vector $z=\{\psi_i^{(v)}(R), \varepsilon, t_{v\alpha}^h\}$, the solution of which for a chosen step h is equivalent to the determination of the wave function of the scattering problem, $\psi_i^{(v)}(R)$, and the scattering matrix $\{t_{v\alpha}^h\}$ corresponding to a given collision energy $\varepsilon=\varepsilon^*$. Components $F_m^{(v)}$ of the operator F define the scattering equations, boundary, and normalization conditions for the searched wave function. In this approach, the problem of accuracy of the solution of the multidimensional scattering problem reduces to the well-elaborated problem of computational mathematics (see, e.g., [4]) on convergence of the solution $\{\psi_i^{(v)}(R), t_{v\alpha}^h\}$ obtained in the space $X_h=\{R, \Omega_i\}$ to the solution of the initial problem, $\{\psi(R, \Omega), t_{v\alpha}\}$, in $X=\{R, \Omega\}$, instead of the convergence in basis. The approximation used in the paper provides the convergence not worse than $\sim h^4$ (here h is less than $\bar{h}$ which depends on problem peculiarities).

In Section 2, the multidimensional scattering problem is reduced to a system of differential-difference equations for the wave function in space X_h and for reaction matrix elements. Solution of the latter is expanded in Appendix A in the form of a sequence of boundary-value problems for iteration corrections to the wave function of the system. In Section 3, the approach is applied to the scattering problem on a nonspherical scatterer. Numerical computations by the method for the potentials

$$V(R, \cos\theta)=\begin{cases} V_0, & R\leqslant R_0+\gamma\cos^2\theta \\ 0, & R>R_0+\gamma\cos^2\theta \end{cases} \tag{1.2}$$

$$V(R, \cos\theta)=\begin{cases} \infty, & R\leqslant R_0 \\ \dfrac{\cos\theta}{R^2}, & R>R_0 \end{cases} \tag{1.3}$$

are presented in Section 4, where convergence of the method is also demonstrated for $h\to 0$ $(N\to\infty)$. Peculiarities of the approach for computation of states of the discrete spectrum of the multidimensional Schrödinger equation are analyzed in Section 5 and the known problem of a hydrogen atom in a homogeneous magnetic field is solved there. In Section 6, the obtained results and possible applications of the method are discussed.

2. Scattering on a Structural Scatterer

Let us consider the solution of the Schrödinger equation in a multidimentional space $X=\{R, \Omega\}$

$$\{H(R, \Omega)-\varepsilon\}\,\psi(R, \Omega)=0 \tag{2.1}$$

with the Hamiltonian

$$H(R, \Omega) = -\frac{1}{2M} \cdot \frac{\partial^2}{\partial R^2} + V(R, \Omega) + H_0(\Omega). \tag{2.2}$$

Where $H_0(\Omega)$ is the Hamiltonian of a scatterer,

$$\{H_0(\Omega) - \varepsilon_n\} \varphi_n(\Omega) = 0, \tag{2.3}$$

whose wave functions $\varphi_n(\Omega)$ satisfy the normalization conditions

$$\int \varphi_n(\Omega) \varphi_{n'}(\Omega) \, d\Omega = \delta_{nn'}, \tag{2.4}$$

$V(R, \Omega)$ is the potential of the interaction between a particle and a scatterer and M is the reduced mass of the system "target-particle."

Let us introduce the difference net Ω_i $(i = 0, 1, ..., N)$ in the space Ω,

$$\psi(R, \Omega) \to \psi(R, \Omega_i) \equiv \psi_i(R) \tag{2.5}$$

and consider the system of differential-difference equations, instead of the partial differential equation (2.1).

To start with, we denote the set of quantum numbers characterizing system (2.3) in the state n by the index α $(\alpha = 0, 1, ..., \infty)$, and the set $\varphi_\alpha(\Omega)$ of eigenfunctions of the Hamiltonian $H_0(\Omega)$ in nodes Ω_i will be represented as a square $(N+1) \times (N+1)$ matrix $\varphi_{i\alpha} \equiv \varphi_\alpha(\Omega_i)$ $(i, \alpha = 0, 1, ..., N)$. Assuming that $\varphi_\alpha(\Omega)$ is a Chebyshev set [5], we introduce the inverse matrix $\varphi_{i\alpha}^{-1}$ (in this case it exists and $\sum_{\alpha=0}^{N} \varphi_{i\alpha} \varphi_{\alpha j}^{-1} = \delta_{ij}$) and represent the searched wave function as the expansion

$$\psi(R, \Omega) = \sum_{j=0}^{N} \left(\sum_{\alpha=0}^{N} \varphi_\alpha(\Omega) \varphi_{\alpha j}^{-1} \right) \psi_j(R). \tag{2.6}$$

At the net points Ω_i for the function $\psi(R, \Omega)$ represented by formula (2.6), expression (2.5) holds automatically and expressions

$$(H_0(\Omega) \psi(R, \Omega))_i = \sum_{j=0}^{N} \left(\sum_{\alpha=0}^{N} \varepsilon_\alpha \varphi_{i\alpha} \varphi_{\alpha j}^{-1} \right) \psi_j(R) \tag{2.7}$$

$$(V(R, \Omega) \psi(R, \Omega))_i = \sum_{j=0}^{N} \left(\sum_{\alpha=0}^{N} (V(R, \Omega) \varphi_\alpha(\Omega))_i \varphi_{\alpha j}^{-1} \right) \psi_j(R) \tag{2.8}$$

are correct.

It is easy to calculate the quantities $(V(R, \Omega) \varphi_\alpha(\Omega))_i$, if the operator $V(R, \Omega)$ contains no differentiation and integration over the variables Ω,

$$(V(R, \Omega) \varphi_\alpha(\Omega))_i = V(R, \Omega_i) \varphi_{i\alpha}.$$

Otherwise, one can obtain

$$(V(R, \Omega)\,\varphi_\alpha(\Omega))_i = \sum_\beta A_{i\beta}(R)\,\varphi_{\beta\alpha},$$

using the finite-difference approximation, where matrix $A_{i\beta}$ is determined by the type of formulas for numerical differentiation and integration and by properties of the basis functions $\varphi_\alpha(\Omega)$.

If in the asymptotic region $R \to \infty$ the interaction potential has the form

$$V(R, \Omega) = \frac{J(J+1)}{2MR^2} + \frac{C}{R^n}, \qquad C = \text{const}, n \geqslant 2, \tag{2.9}$$

the wave function $\psi(R, \Omega)$ as $R \to \infty$ can be represented as

$$\psi^{(\nu)}(R, \Omega) = \sum_{\alpha=0}^{S} \left\{ j_J(k_\alpha R)\,\delta_{\nu\alpha} + \sqrt{\frac{k_\nu}{k_\alpha}}\, t_{\nu\alpha}(\varepsilon)\, n_J(k_\alpha R) \right\} \varphi_\alpha(\Omega) + \sum_{\alpha=S+1}^{\infty} C_\alpha \exp\{-|k_\alpha|\, R\}\, \varphi_\alpha(\Omega), \tag{2.10}$$

where $t_{\nu\alpha}(\varepsilon)$ is the reaction matrix of the scattering problem, with $S+1$ open channels ($\varepsilon - \varepsilon_\alpha > 0$ at $\alpha \leqslant S$), $k_\alpha = \sqrt{2M(\varepsilon - \varepsilon_\alpha)}$ is the momentum of a channel, and C_α are normalization constants. Multiplying (2.10) by $\varphi_\alpha(R)$ and integrating the equation over Ω, one obtains, as $R \to \infty$, $(N+1)$ equations

$$\int \psi^{(\nu)}(R, \Omega)\,\varphi_\alpha(\Omega)\, d\Omega = \begin{cases} j_J(k_\alpha R)\,\delta_{\nu\alpha} + \sqrt{\dfrac{k_\nu}{k_\alpha}} \cdot t_{\nu\alpha} \cdot n_J(k_\alpha R), & \alpha \leqslant S \\ C_\alpha \exp\{-|k_\alpha|\, R\}, & \alpha > S \end{cases}. \tag{2.11}$$

On the other hand, using expansion (2.6) for $\psi(R, \Omega)$ and the conditions of orthogonality for functions $\varphi_\alpha(\Omega)$ (2.4), one obtains

$$\int \psi^{(\nu)}(R, \Omega)\,\varphi_\alpha(\Omega)\, d\Omega = \sum_{j=0}^{N} \varphi_{\alpha j}^{-1} \psi_j^{(\nu)}(R). \tag{2.12}$$

Thus, the multidimensional scattering problem (2.1) and (2.10) is reduced to the system of $(N+1)$ differential-difference equations

$$\sum_{j=0}^{N} \left\{ \delta_{\alpha j} \frac{d^2}{dR^2} + 2M(\varepsilon\delta_{\alpha j} - V_{\alpha j}(R)) \right\} \psi_j(R) = 0, \tag{2.13}$$

where

$$V_{\alpha j}(R) = \sum_{\beta=0}^{N} \{\varepsilon_\beta \varphi_{\alpha\beta} \varphi_{\beta j}^{-1} + (V(R, \Omega)\,\varphi_\beta(\Omega))_\alpha\, \varphi_{\beta j}^{-1}\}$$

with the boundary conditions:

$$\sum_{j=0}^{N} \varphi_{\alpha j}^{-1} \psi_j^{(\nu)}(R) \underset{R\to\infty}{=} \begin{cases} j_J(k_\alpha R)\,\delta_{\nu\alpha} + \sqrt{\dfrac{k_\nu}{k_\alpha}} \cdot t_{\nu\alpha} \cdot n_J(k_\alpha R), & \alpha \leqslant S \\ C_\alpha \exp\{-|k_\alpha|\, R\}, & \alpha > S. \end{cases} \tag{2.14}$$

These equations are in a form that is identical to the equations of the multichannel scattering problem; and to solve them, it is natural to use the methods elaborated on earlier for solving this problem (see, for example, [1]), adopted then for the peculiarities of the considered problem. Here, following paper [3], we formulate problem (2.13) and (2.14) as the nonlinear functional equation

$$\begin{gathered} F_m^{(\nu)}(z) = 0; \qquad z = \{\psi_j^{(\nu)}(R),\ \varepsilon,\ t_{\nu\nu}\} \\ \nu = 0, 1, ..., S \leqslant N;\ j = 0, 1, ..., N;\ m = 1, ..., 5, \end{gathered} \tag{2.15}$$

the root of which is a solution of the scattering problem at a fixed collision energy $\varepsilon = \varepsilon^*$. The first two components of the operator $F^{(\nu)}$ define the system of equations (2.13) and the boundary condition for the searched wave functions $\psi_\alpha^{(\nu)}(R)$ at the point $R = 0$:

$$F_1^{(\nu)}(z) = \sum_{j=0}^{N} \left\{ \delta_{\alpha j} \frac{d^2}{dR^2} + 2M(\varepsilon\delta_{\alpha j} - V_{\alpha j}(R)) \right\} \psi_j^{(\nu)}(R) \tag{2.16}$$

$$F_2^{(\nu)}(z) = \psi_\alpha^{(\nu)}(0); \qquad \alpha = 0, 1, ..., N. \tag{2.17}$$

The third component $F_3^{(\nu)}$ defines the boundary condition at the point $R = R_m$ which follows from the asymptotic relations (2.14) (see [3]),

$$F_3^{(\nu)}(z) = \left\{ \mathscr{D}_\alpha^{(\nu)}(t_{\nu\nu}, R) \sum_{j=0}^{N} \varphi_{\alpha j}^{-1} \frac{d\psi_j^{(\nu)}(R)}{dR} - \bar{\mathscr{D}}_\alpha^{(\nu)}(t_{\nu\nu}, R) \sum_{j=0}^{N} \varphi_{\alpha j}^{-1} \psi_j^{(\nu)}(R) \right\}_{R = R_m} \tag{2.18}$$

where

$$\mathscr{D}_\alpha^{(\nu)}(t_{\nu\nu}, R) = \begin{cases} (j_J(k_\alpha R) + t_{\nu\nu} n_J(k_\alpha R))\,\delta_{\nu\alpha} + n_J(k_\alpha R)(1 - \delta_{\alpha\nu}), & \alpha \leqslant S \\ 1, & \alpha > S \end{cases}$$

$$\bar{\mathscr{D}}_\alpha^{(\nu)}(t_{\nu\nu}, R) = \begin{cases} \dfrac{d}{dR}\left[(j_J(k_\alpha R) + t_{\nu\nu} n_J(k_\alpha R))\,\delta_{\nu\alpha} + n_J(k_\alpha R)(1 - \delta_{\nu\alpha})\right], & \alpha \leqslant S \\ -|k_\alpha|, & \alpha > S. \end{cases}$$

In that form, problem (2.15) represents a system of $(N+1)$ second-order ordinary differential equations with boundary conditions at the points $R = 0$ and $R = R_m$ for defining $(N+3)$ unknown values $z = \{\psi_\alpha^{(\nu)}(R), \varepsilon, t_{\nu\nu}\}$. For a unique

solvability of the problem it is necessary to supplement it with two more equations. For this aim let us use the normalization condition for the wave function

$$\int_0^{R_m} dR \int d\Omega \psi^2(R, \Omega) - 1 = 0$$

and the relation

$$\int_0^{R_m} dR \int d\Omega \psi(R, \Omega) \{H(R, \Omega) - \varepsilon^*\} \psi(R, \Omega) = 0$$

fixing the collision energy $\varepsilon = \varepsilon^*$ (see [3]). From expansion (2.6) for $\psi(R, \Omega)$ the expression follows for components $F_4^{(v)}$ and $F_5^{(v)}$ of the operator $F^{(v)}$

$$F_4^{(v)}(z) = \sum_{\alpha j} g_{\alpha j} \int_0^{R_m} \psi_\alpha^{(v)}(R) \psi_j^{(v)}(R)\, dR - 1 \tag{2.19}$$

$$F_5^{(v)}(z) = \sum_{\alpha j} g_{\alpha j} \int_0^{R_m} \psi_\alpha^{(v)}(R) \left\{ \delta_{\alpha j} \frac{d^2}{dR^2} + 2M(\varepsilon^* \delta_{\alpha j} - V_{\alpha j}(R)) \right\} \psi_j^{(v)}(R)\, dR. \tag{2.20}$$

Here $g_{\alpha j}$ is a weight function resulting from the integration over Ω determined by quandrature formulas used and properties of the basis functions $\varphi_\alpha(\Omega)$.

Upon solving the system of Eq. (2.15)–(2.20), one obtains the wave function of the multichannel scattering problem (2.1) and (2.10)

$$\psi^{(v)}(R, \Omega) = \sum_{j=0}^{N} \sum_{\alpha=0}^{N} \varphi_\alpha(\Omega)\, \varphi_{\alpha j}^{-1} \psi_j^{(v)}(R)$$

at $\varepsilon = \varepsilon^*$ and diagonal elements of the reaction matrix $t_{vv}(\varepsilon^*)$.

Nondiagonal matrix elements $t_{v\alpha}$ $(v \neq \alpha)$ are determined by the formula

$$\begin{aligned} t_{v\alpha} &= \frac{(j_J(k_v R_m) + t_{vv} n_J(k_v R_m))}{n_J(k_\alpha R_m)} \cdot \frac{\int \psi_{(Rm,\Omega)}^{(v)} \varphi_\alpha(\Omega)\, d\Omega}{\int \psi_{(Rm.\Omega)}^{(v)} \varphi_v(\Omega)\, d\Omega} \\ &= \frac{(j_J(k_v R_m) + t_{vv} n_J(k_v R_m))}{n_J(k_\alpha R_m)} \cdot \frac{\sum_{j=0}^{N} \varphi_{\alpha j}^{-1} \psi_j^{(v)}(R_m)}{\sum_{j=0}^{N} \varphi_{vj}^{-1} \psi_j^{(v)}(R_m)}. \end{aligned} \tag{2.21}$$

Once the reaction matrix $T(\varepsilon) = \{t_{v\alpha}\}$ is known, it is possible to determine the S-matrix of the problem and the corresponding cross section by the known formulas [6].

In Appendix A the solution of problem (2.15)–(2.20) is represented as a sequence of the boundary-value problems for iteration corrections to the searched wave function $\{\psi_\alpha^{(v)}(R)\}$. It is also interesting to consider other representations for the solution of problem (2.15)–(2.20).

Note, that transition from the multidimensional scattering problem to Eq. (2.15) is particularly transparent and it is easily carried out for splitting (2.2) of the initial

Hamiltonian $H(R, \Omega)$. However, the suggested approach does not require the coincidence of $H_0(\Omega)$ with the Hamiltonian of the target, which is demonstrated in the next section using the scattering problem on a nonspherical scatterer as an example. This probem, on the one hand, already reflects peculiarities of the multidimensional scattering problem, and on the other hand, it is quite simple to illustrate the peculiarities of the suggested approach.

For some problems, a more convenient splitting may be introduced as

$$H(R, \Omega) = -\frac{1}{2M}\frac{\partial^2}{\partial R^2} + V(R, \Omega) + H_0(\Omega; R)$$

provided that eigenvalues $\varepsilon_\alpha(R)$ and eigenfunctions $\varphi_\alpha(\Omega; R)$ of the Hamiltonian $H_0(R; \Omega)$ depending on R as a parameter are easily calculated.

3. Scattering on Nonspherical Scatterer

Let us now apply the suggested approach to the scattering problem of a particle with mass M on a nonspherical scatterer $V(\mathbf{R})$. For simplicity we consider the axial-symmetric case $V(\mathbf{R}) = V(R, \cos\theta)$, where θ is the angle between axis $\mathbf{z}$ and the scattering direction. To this end we formulate problem (2.15) for that case.

The Schrödinger equation has the form

$$\frac{\partial^2}{\partial R^2}\psi(R, x) + \frac{1}{R^2}\frac{\partial}{\partial x}(1-x^2)\frac{\partial}{\partial x}\psi(R, x) + 2M(\varepsilon - V(R, x))\,\psi(R, x) = 0, \qquad (3.1)$$

where $R \in [0, \infty)$, $x = \cos\theta \in [-1, 1]$.

We write the asymptotics of its solution as $R \to \infty$ in the reaction-matrix representation

$$\psi^{(\nu)}(R, x) = \sum_{\alpha=0}^{\infty} \{j_\alpha(kR)\,\delta_{\nu\alpha} + t_{\nu\alpha} \cdot n_\alpha(kR)\} \sqrt{(2\alpha+1)} \cdot P_\alpha(x), \qquad (3.2)$$

where $P_\alpha(x)$ are Legendre polynomials with the orthogonality conditions on the segment $[-1, 1]$ $\int_{-1}^{1} P_\alpha(x)\,P_{\alpha'}(x)\,dx = (2/(2\alpha+1))\,\delta_{\alpha\alpha'}$.

A next step is to determine the matrix $T = \{t_{\nu\alpha}\}$, in terms of which it is possible to express the scattering amplitude

$$\begin{aligned} 2ik\hat{f} &= 1 - (1+iT)(1-iT)^{-1}, \qquad \hat{f} \equiv \{f_{\nu\alpha}\} \\ f(\mathbf{n}_k, \mathbf{n}_R) &= \sum_{\alpha,\nu} f_{\nu\alpha} \sqrt{(2\nu+1)(2\alpha+1)}\, P_\nu(\theta_k)\, P_\alpha(\theta_R). \end{aligned} \qquad (3.3)$$

The cross section at the scattering angle θ_k ($\mathbf{n}_k$ and $\mathbf{n}_R$ are unit vectors coinciding with directions $\mathbf{k}$ and $\mathbf{R}$, respectively) equals

$$\sigma(\theta_k) = 2\pi \int_{-1}^{1} |f(x, \theta_k)|^2\, dx \qquad (3.4)$$

and the total cross section averaged over possible orientations of the scatterer is

$$\bar{\sigma}=\frac{1}{2}\int_{-1}^{1}\sigma(x_k)\,dx_k. \tag{3.5}$$

It is easy to see that in the case of spherical potential matrices $\hat{f}$ and T are diagonal.

Let us introduce the net x_i $(i=0, 1, ..., N)$ for the variable x and represent the solution of Eq. (3.1) analogously to (2.6) as

$$\psi(R, x)=\sum_{j=0}^{N}\left(\sum_{\alpha=0}^{N}P_\alpha(x)\,P_{\alpha j}^{-1}\right)\psi_j(R) \tag{3.6}$$

(here $P_{i\alpha}=P_\alpha(x_i)$).

In this case at mesh points x_α, formulas (2.7) and (2.8) for $(H_0\psi)_\alpha$ and $(V\psi)_\alpha$ are simplified to[1]:

$$\begin{aligned}(H_0(x)\,\psi(R, x))_\alpha&=\frac{1}{2MR^2}\sum_{j=0}^{N}\left(\sum_{l=0}^{N}l(l+1)\,P_{\alpha l}\cdot P_{lj}^{-1}\right)\psi_j(R)\\ (V(R, x)\,\psi(R, x))_\alpha&=V(R, x_\alpha)\,\psi_\alpha(R).\end{aligned} \tag{3.7}$$

Using (3.2) and (3.7) and orthogonality relations for the Legendre polynomials, we obtain the system of $(N+1)$ equations of form (2.15)–(2.20) with components $F_m^{(\nu)}$ determined by the equations

$$F_1^{(\nu)}(z)=\sum_{j=0}^{N}\left\{\delta_{\alpha j}\frac{d^2}{dR^2}+2M(\varepsilon\delta_{\alpha j}-V_{\alpha j}(R))\right\}\psi_j^{(\nu)}(R), \tag{3.8}$$

where

$$V_{\alpha j}(R)=\frac{1}{2MR^2}\sum_{l=0}^{N}l(l+1)\,P_{\alpha l}P_{lj}^{-1}+V(R, x_\alpha)\,\delta_{\alpha j}$$

$$F_2^{(\nu)}(z)=\psi_\alpha(0); \qquad \alpha=0, 1, ..., N, \tag{3.9}$$

$$F_3^{(\nu)}(z)=\left\{\mathscr{D}_\alpha^{(\nu)}(t_{\nu\nu}, R)\sum_{j=0}^{N}P_{\alpha j}^{-1}\frac{d\psi_j^{(\nu)}(R)}{dR}-\frac{d}{dR}\left[\mathscr{D}_\alpha^{(\nu)}(t_{\nu\nu}, R)\right]\sum_{j=0}^{N}P_{\alpha j}^{-1}\psi_j^{(\nu)}(R)\right\}_{R=R_m}, \tag{3.10}$$

[1] For calculating the inverse matrix P_{ij}^{-1} it is possible to use the relations $\sum_{l=0}^{N}((2l+1)/2)\,P_l(x_\alpha)\cdot P_l(x_j)\approx 1/h\,\delta_{\alpha j}$ which approximate the completeness relations $\sum_{l=0}^{\infty}((2l+1)/2)\,P_l(x_\alpha)\,P_l(x_j)=\delta(x_\alpha-x_j)$. In this case $P_{ij}^{-1}\approx P_l(x_j)\,h((2l+1)/2)$. This formula can be made more accurate if we take x_α as points of N-points Gaussian quadrature and introduce corresponding weights ω_α instead of $h=$ constant. Then $P_{ij}^{-1}\approx\omega_\alpha^{1/2}P_l(x_j)\,\omega_j^{1/2}((2l+1)/2)$, and using formulas (3.7) we obtain Eq. (3.1) in the "*discrete variable representation*" considered in [2].

where

$$\mathscr{D}_{\alpha}^{(\nu)}(t_{\nu\nu}, R) = (j_{\alpha}(kR) + t_{\nu\nu} n_{\alpha}(kR))\,\delta_{\nu\alpha} + n_{\alpha}(kR)(1-\delta_{\nu\alpha})$$

$$F_4^{(\nu)}(z) = \sum_{\alpha j} g_{\alpha j} \int_0^{R_m} \psi_{\alpha}^{(\nu)}(R)\psi_j^{(\nu)}(R)\,dR - 1 \tag{3.11}$$

$$F_5^{(\nu)}(z) = \sum_{\alpha j} g_{\alpha j} \int_0^{R_m} \psi_{\alpha}^{(\nu)}(R) \left\{\delta_{\alpha j}\frac{d^2}{dR^2} + 2M(\varepsilon^*\delta_{\alpha j} - V_{\alpha j}(R))\right\} \psi_j^{(\nu)}(R)\,dR. \tag{3.12}$$

where $g_{\alpha j}$ are the weights of the quadrature formulas of integration over the variable x (see the determination of equations (2.19) and (2.20)).

Nondiagonal matrix elements $t_{\nu\alpha}$ are determined by the formula

$$t_{\nu\alpha} = \sqrt{\frac{2\nu+1}{2\alpha+1}} \cdot \frac{(j_{\nu}(kR_m) + t_{\nu\nu} n_{\nu}(kR_m))}{n_{\alpha}(kR_m)} \cdot \frac{\sum_{j=0}^{N} P_{\alpha j}^{-1}\psi_j^{(\nu)}(R_m)}{\sum_{j=0}^{N} P_{\nu j}^{-1}\psi_j^{(\nu)}(R_m)}. \tag{3.13}$$

As the right-hand side of formula (3.6) is an interpolating polynomial of degree N in the variable x, the accuracy of expansion (3.6), $\delta\psi_N = |\psi - \psi_N|$, can be estimated as follows [15]:

$$\delta\psi_N \lesssim \frac{1}{(N+1)!} \max\left|\frac{\partial^{N+1}}{\partial x^{N+1}}\psi(R,\xi)\right| \left|\prod_{j=0}^{N}(x-x_j)\right|, \qquad \xi \in [-1, 1]. \tag{3.14}$$

Then, it may be shown that the matrix elements $t_{\nu\alpha}$ are also accurate to an order $\sim 1/1(N+1)!$ when Eqs. (3.8)–(3.13) are solved exactly. This provides a rapid convergence of the method with respect to N when highly accurate quadrature formulas are used in (3.11) and (3.12).

4. Numerical Example

As an example of using the suggested approach, we have solved scattering problems for a nonspherical potential well

$$V(R, x) = \begin{cases} V_0, & R \leqslant R_0 + \gamma x^2 \\ 0, & R > R_0 + \gamma x^2 \end{cases} \tag{4.1}$$

and for a long-range nonspherical scatterer,

$$V(R, x) = \begin{cases} \infty, & R \leqslant R_0 \\ \dfrac{x}{R^2}, & R > R_0. \end{cases} \tag{4.2}$$

A potential of type (4.2) has been used, for example, in consideration of the scattering of electrons by polar molecules and hydrogen atoms in excited states [16] ("dipole scattering"). For the solution of problem (3.8)–(3.13) the algorithm [3] had been used (see formulas (A.1)–(A.6) of Appendix A) with the finite-difference approximation in variable R of the order $\sim h_R^2$ [13]. Calculations have been made at $M=1$, $V_0=-0.5$, $R_0=1$.

Results of the calculation of matrix elements $t_{\nu\alpha}$ for the nonspherical potential well (4.1) are presented in Table I at $\gamma=1$ as functions of N ($N+1$ is a number of mesh points in x).

The quantities

$$\delta_\nu(N)=\frac{t_{\nu\nu}(N)-t_{\nu\nu}(2N)}{t_{\nu\nu}(2N)-t_{\nu\nu}(4N)} \tag{4.3}$$

which characterize the convergence of the method in N are also presented in Table I. In the last column of Table I phase shifts $t_{\nu\nu}$ for the spherical well ($\gamma=0$) (in this case $t_{\nu\alpha}=0$ at $\nu\neq\alpha$) are given, which differ from the exact solution by an order of $\sim 10^{-3}$–10^{-4}. The calculations have been made at $h_R=0.0125$, $R_m=5$ for the collision energy $\varepsilon=0.005$ ($k=0.1$).

In Table II we report results of calculations of the matrix elements $t_{\nu\alpha}$ and quantities $\delta_\nu(N)$ (4.3) for the "dipole" interaction potential (4.2). The calculations have been made at $h_R=0.1$, $R_m=20$ at the collision energy $\varepsilon=0.02$ ($k=0.2$).

In calculations, weight functions of the Simpson formulas have been used in (3.11) and (3.12). As mentioned in Section 3, the convergence of the method in this

TABLE I

Matrix Elements $t_{\nu\alpha}$ and Quantities $\delta_\nu(N)$ for Nonspherical Potential Well (4.1)

		$\gamma=1$					$\gamma=0$
		$t_{\nu\alpha}$					
N	ν \ α	0	1	2	3	$\delta_\nu(2)$	$t_{\nu\nu}$
2	0	0.6460	1×10^{-10}	-0.6714×10^{-3}			
4		0.3817	1×10^{-10}	-0.4004×10^{-3}	1×10^{-14}	529	0.5699×10^{-1}
8		0.3812	1×10^{-10}	-0.3706×10^{-3}	1×10^{-14}		
2	1	1×10^{-10}	0.1191×10^{-2}	1×10^{-13}			
4		1×10^{-10}	0.5131×10^{-3}	1×10^{-12}	-0.2663×10^{-6}	6.2	0.25×10^{-4}
8		1×10^{-10}	0.4034×10^{-3}	1×10^{-12}	-0.2055×10^{-6}		
2	2	-0.1678×10^{-2}	1×10^{-12}	0.1986×10^{-5}			
4		-0.5106×10^{-3}	1×10^{-12}	0.8722×10^{-6}	1×10^{-15}	4.0	0.6×10^{-6}
8		-0.3712×10^{-3}	1×10^{-12}	0.5922×10^{-6}	1×10^{-14}		
2	3						
4		1×10^{-14}	-0.5437×10^{-4}	1×10^{-13}	-0.34×10^{-9}		
8		1×10^{-13}	-0.2290×10^{-6}	1×10^{-13}	-0.21×10^{-9}		

TABLE II

Matrix Elements $t_{\nu\alpha}$ and Quantities $\delta_\nu(N)$ for "Dipole" Scatterer (4.2)

		$t_{\nu\alpha}$					
N	ν \ α	0	1	2	3	4	$\delta_\nu(2)$
2	0	0.3847	0.5916	-0.4902×10^{-1}			
4		0.3095	0.5138	-0.4583×10^{-1}	0.6203×10^{-2}	-0.3290×10^{-3}	376
8		0.3093	0.5134	-0.4581×10^{-1}	0.6163×10^{-2}	-0.3281×10^{-3}	
2	1	0.5916	-0.4253×10^{-3}	0.2466			
4		0.5137	−0.1259	0.2474	-0.1584×10^{-1}	0.7693×10^{-3}	209
8		0.5134	−0.1265	0.2474	-0.1575×10^{-1}	0.7677×10^{-3}	
2	2	−0.1226	0.6164	-0.2522×10^{-1}			
4		-0.4636×10^{-1}	0.2493	0.9181×10^{-2}	0.9243×10^{-1}	0.3617×10^{-2}	
8		-0.4581×10^{-1}	0.2474	0.9150×10^{-2}	0.9210×10^{-1}	0.3611×10^{-2}	
2	3						
4		0.7029×10^{-2}	-0.2356×10^{-2}	0.9200×10^{-1}	0.8515×10^{-2}	0.2174×10^{-1}	
8		0.6163×10^{-2}	-0.1575×10^{-2}	0.9210×10^{-1}	0.6897×10^{-2}	0.2171×10^{-1}	
2	4						
4		-0.3917×10^{-2}	0.4148×10^{-3}	-0.1025×10^{-2}	0.3340×10^{-1}	0.1134×10^{-2}	
8		-0.3278×10^{-3}	0.7670×10^{-3}	-0.3608×10^{-2}	0.2171×10^{-1}	0.8816×10^{-2}	

Note: Matrix elements $t_{\nu\alpha}$ at $\nu, \alpha > 4$ have the order less than 10^{-5}.

case should be better than $\sim 1/N^4$; this means that for all $N > \bar{N}$, where $\bar{N}$ is fixed by the problem peculiarities, the inequality $\delta_\nu(N) \gtrsim \delta_\nu$ theor $= 16$ must hold, which is shown in Tables I and II.

Here we do not consider the well-known question on convergence of the method as $h_R \to 0$ and $R_m \to \infty$ and convergence of the "Newton iterations" (A.1)–(A.6) which were tested in [3, 11–13]. Note only that the convergence up to the quantity $\delta = \|F(z^*)\| \sim 10^{-6}$ has been achieved after five or six iterations for potential (4.1) and after four or five iterations for potential (4.2). The accuracy of the calculations can also be controlled by the accuracy of the relations $t_{\nu\alpha} = t_{\alpha\nu}$ $(\alpha \neq \nu)$ (see Tables I and II where the above relations are fulfilled with a relative accuracy $\sim 10^{-4}$ at $N = 8$).

Note here that a good convergence of the method for both considered examples is found for $N = 2$: δ_ν num$(N) \gtrsim \delta_\nu$ theor.

5. Discrete Spectrum of Multidimensional Schrödinger Equation

The proposed approach is used for solving the multidimensional Schrödinger equation both for continuous and discrete spectra. In the latter case, the

problem (2.15)–(2.20) becomes simpler. And the system of equations $F^{(\nu)}(z)=0$ is replaced by one equation $F^{(0)}(z)=0$, where $z=\{\psi^{(0)}(R,\Omega),\varepsilon\}$, and the components of the operator $F_m^{(0)}$ are determined by formulas (2.16)–(2.19) in which $\mathscr{D}_\alpha^{(0)}=0$ and $\bar{\mathscr{D}}_\alpha^{(0)}=1$ for $S=0$ (in this case all channels are closed: $\varepsilon-\varepsilon_\alpha<0$; $\alpha=0, 1, ..., N$). For its solution, as before, formulas (A.1)–(A.6) of Appendix A with the natural condition $\mu_2^n=0$ [3] are applicable.

To demonstrate the possibilities of the method for the discrete spectrum of the Schrödinger equation, it was applied to the well-known problem of a hydrogen atom in a homogeneous magnetic field.

In that case potential $V(R,x)$ in (3.1) equals

$$V(R,x)=-\frac{1}{R}+\frac{R^2\gamma^2}{8}\cdot(1-x^2). \tag{5.1}$$

Here γ is a parameter of the magnetic field intensity (see, for example, [17]).

In Table III calculated energies of the ground state of the hydrogen atom at $N=2, 4, 8, 16$; $h_R=0.0125$, $R_m=10$ are compared for several parameters of the magnetic field γ with the results of papers [17, 18], where an accuracy of an order of $\sim 10^{-4}-10^{-5}$ has been achieved.

Here the quantities $\delta(N)=(\varepsilon(N)-\varepsilon(2N))/(\varepsilon(2N)-\varepsilon(4N))$ which characterize the convergence of the method in N are also presented. Note that for discrete spectra of the Schrödinger equation the convergence of the method in the given variant is more rapid than for the scattering problem, and for $N>\bar{N}$ (here $\bar{N}$ depends on the quantity γ) the convergence is determined only by the accuracy of decomposition (3.6) $\sim 1/(N+1)!$, since in this case numerical integration is performed only for the normalization of the wave function in (3.11). Thus, even for strong field $\gamma=1$, $\delta\,\mathrm{num}(N)\approx\delta\,\mathrm{theor}(N)\simeq(2N)!/N!=12$ for $N=2$.

TABLE III

Energy of the Ground State of the Hydrogen Atom in a Homogeneous Magnetic Field $-\varepsilon$ (in the Units $\varepsilon_0=Ry$)

γ	$N=2$	$N=4$	$N=8$	$N=16$	[17]	$\delta(2)$	$\delta(4)$
0.0	0.999960	0.999960	0.999960		0.999957[a]		
0.1	0.995028	0.995013	0.995013		0.99508		
0.2	0.980923	0.980726	0.980723		0.98076	65.7	
0.5	0.898721	0.894583	0.894380	0.894378	0.89447	20.4	101.5
1.0	0.694082	0.665045	0.662361	0.662291	0.66241 (0.66228[a])	10.8	38.3

[a] The results from paper [18].

6. Conclusion

The method proposed in this paper can be generalized to three-dimensional and multidimensional cases. It is rather effective; the most labour-consuming part of the known methods of solution of the multidimensional Schrödinger equation, the calculation of matrix elements, is replaced here by a simple algorithm of generation of the coefficient matrix for a system of differential-difference equation. An attractive aspect of the approach is its rapid convergence. In the suggested approach the accuracy of expansion (2.6) for the searched wave function is known a priori. For the considered example, (3.6), it equals $\sim 1/(N+1)!$, which provides a rapid convergence of the method when using formulas of a high accuracy for the numerical differentiation and integration of the basis functions $\varphi_\alpha(\Omega)$ over Ω in deriving equations (2.8), (2.19), and (2.20). Note that for simplicity here we only use $h_i = \text{const}$ and optimization by this parameter was not considered. But the suggested approach admits also the use of $h_i \neq \text{const}$ according to some possibly more efficiently weighted integration scheme.

The above two circumstances, in our opinion, make the method attractive for solving essentially multidimensional Schrödinger equations for both continuous and discrete spectra. One of the most interesting problems of that sort is the scattering on a nonrigid rotator, which corresponds to the scattering of a neutral particle on a di-atomic molecule with excitation of the rotational and vibrational degrees of freedom; also we may indicate such problems as the electron scattering on atoms, mesic atomic scattering on nuclei, the hydrogen atom in an inhomogeneous field, etc.

The approach can be generalized to the scattering of a structural complex on a structural target. These problems will be considered elsewhere.

Appendix A

Following paper [3] we represent the solution of problem (2.15)–(2.20) as the iteration procedure

$$\begin{aligned} &F'_{z_n}(z_n)\,\Delta z_n = -F(z_n) \\ &z_{n+1} = z_n + \tau_n \Delta z_n = \{\boldsymbol{\psi}^{(n)} + \tau_n \mathbf{V}^{(n)},\ \varepsilon_n + \tau_n \mu_1^n,\ t_{vv}^{(n)} + \tau_n \mu_2^n\}, \end{aligned} \tag{A.1}$$

where

$$\begin{aligned} &\mathbf{V}^{(n)} = -\boldsymbol{\psi}^{(n)} + \mu_1^n \mathbf{v}^{(n)} + \mu_2^n \cdot \boldsymbol{\omega}^{(n)} \\ &z_0 = \{\boldsymbol{\psi}^{(0)},\ \varepsilon_0,\ t_{vv}^{(0)}\},\ \boldsymbol{\psi}^{(n)} = \{\psi_j^{(n)}(R)\},\ \mathbf{V}^{(n)} = \{V_j^{(n)}(R)\}, \end{aligned}$$

(F'_{z_n} is a Frechet derivative at the point z_n), which at every iteration step τ_n consists in the solution of boundary-value problems for determination of iteration corrections $\mathbf{v}^{(n)}$ and $\boldsymbol{\omega}^{(n)}$:

$$\frac{d^2}{dR^2}\mathbf{v}^{(n)} + 2M(\varepsilon_n - \hat{V})\,\mathbf{v}^{(n)} = -\boldsymbol{\psi}^{(n)}$$

$$\mathbf{v}^{(n)}|_{R=0} = 0 \tag{A.2}$$

$$\left[\hat{\mathscr{D}}_n \hat{\varphi}^{-1}\frac{d}{dR}\mathbf{v}^{(n)} - \hat{\bar{\mathscr{D}}}_n \varphi^{-1}\mathbf{v}^{(n)}\right]_{R=R_m} = -\left[\frac{\partial \hat{\mathscr{D}}_n}{\partial \varepsilon_n}\hat{\varphi}^{-1}\frac{d}{dR}\boldsymbol{\psi}^{(n)} - \frac{\partial \hat{\bar{\mathscr{D}}}_n}{\partial \varepsilon_n}\hat{\varphi}^{-1}\cdot\boldsymbol{\psi}^{(n)}\right]_{R=R_m}$$

$$\frac{d^2}{dR^2}\boldsymbol{\omega}^{(n)} + 2M(\varepsilon_n - \hat{V})\,\boldsymbol{\omega}^{(n)} = 0$$

$$\boldsymbol{\omega}^{(n)}|_{R=0} = 0 \tag{A.3}$$

$$\left[\hat{\mathscr{D}}_n \hat{\varphi}^{-1}\frac{d}{dR}\boldsymbol{\omega}^{(n)} - \hat{\bar{\mathscr{D}}}_n \hat{\varphi}^{-1}\boldsymbol{\omega}^{(n)}\right]_{R=R_m} = -\left[\frac{\partial \hat{\mathscr{D}}_n}{\partial t_{vv}^{(n)}}\hat{\varphi}^{-1}\frac{d}{dR}\boldsymbol{\psi}^{(n)} - \frac{\partial \hat{\bar{\mathscr{D}}}_n}{\partial t_{vv}^{(n)}}\hat{\varphi}^{-1}\boldsymbol{\psi}^{(n)}\right]_{R=R_m}.$$

In the solution of the system of algebraic equations to search μ_1^n and μ_2^n

$$\begin{aligned} a_{11}^n \mu_1^n + a_{12}^n \mu_2^n &= b_1^n \\ a_{21}^n \mu_1^n + a_{22}^n \mu_2^n &= b_2^n, \end{aligned} \tag{A.4}$$

here, the notation was introduced:

$$\begin{aligned} a_{11}^n &= (\boldsymbol{\psi}^{(n)}, \mathbf{v}^{(n)}), \qquad a_{12}^n = (\boldsymbol{\psi}^{(n)}, \boldsymbol{\omega}^{(n)}) \\ a_{21}^n &= (\boldsymbol{\psi}^{(n)}, \frac{d^2}{dR^2}\mathbf{v}^{(n)} + 2M(\varepsilon^* - \hat{V})\,\mathbf{v}^{(n)}) + (\mathbf{v}^{(n)}, \frac{d^2}{dR^2}\boldsymbol{\psi}^{(n)} + 2M(\varepsilon^* - \hat{V})\,\boldsymbol{\psi}^{(n)}) \\ a_{22}^n &= (\boldsymbol{\psi}^{(n)}, \frac{d^2}{dR^2}\boldsymbol{\omega}^{(n)} + 2M(\varepsilon^* - \hat{V})\,\boldsymbol{\omega}^{(n)}) + (\boldsymbol{\omega}^{(n)}, \frac{d^2}{dR^2}\boldsymbol{\psi}^{(n)} + 2M(\varepsilon^* - \hat{V})\,\boldsymbol{\psi}^{(n)}) \\ b_1^n &= \frac{1}{2}\left[1 + (\boldsymbol{\psi}^{(n)}, \boldsymbol{\psi}^{(n)})\right] \\ b_2^n &= (\boldsymbol{\psi}^{(n)}, \frac{d^2}{dR^2}\boldsymbol{\psi}^{(n)} + 2M(\varepsilon^* - \hat{V})\,\boldsymbol{\psi}^{(n)}), \end{aligned} \tag{A.5}$$

where

$$\hat{V} = \{V_{\alpha j}(R)\}, \qquad (\boldsymbol{\psi}, \boldsymbol{\psi}) = \sum_{\alpha j} g_{\alpha j}\int_0^{R_m} \psi_\alpha(R)\,\psi_j(R)\,dR$$

$$\hat{\varphi}^{-1} = \{\varphi_{\alpha j}^{-1}\}, \qquad \hat{\mathscr{D}}_n = \{\mathscr{D}_\alpha^{(v)}(t_{vv}^{(n)}, R)\,\delta_{\alpha\alpha'}\}.$$

It is convenient to use as an initial approximation $z_0 = \{\boldsymbol{\psi}^{(0)}, \varepsilon_0, t_{vv}^{(0)}\}$ for the solution of problem (2.13)–(2.14) when interaction between a scatterer and a target is absent ($V(R, \Omega) \to J(J+1)/2MR^2$),

$$\boldsymbol{\psi}^{(0)} = \{\psi_\alpha^{(0)}(R)\} = \{j_J(k_\alpha R)\,\delta_{v\alpha}\}, \qquad \varepsilon_0 = \varepsilon^*,\ t_{vv}^{(0)} = 0. \tag{A.6}$$

Formulae (A.1)–(A.5) represent a continuous analog of the Newton solution of Eq. (2.15)–(2.20) (if $\tau_n = 1$, the formulae represent the classical Newton–Kantorovich method) [7, 8].

Convergence of the procedure in that type of problem has been tested theoretically [10] and numerically [11–13].

Note that in transformation of the Schrödinger equation (2.1) into system (2.13) it is important to keep the problem Hermitian, i.e., to symmetrize the matrix of potentials $V_{\alpha j}(R)$, if necessary. For matrix of type (2.13) it is a standard problem [14].

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