Symbolic-Numerical Algorithm for Solving the Time-Dependent Schrödinger Equation

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The modern laser physics and nanotechnologies have stimulated computer simulations for the dynamics of atomic systems in external fields and for control problems of finite dimensional quantum systems [1]. For such subjects symbolic-numerical algorithms based on procedures of normalization and quantization of polynomial Hamiltonians, and numerical methods for solving the time-dependent Schrödinger equation (TSDE) were developed [2–6].

Discrete algorithms for symbolic computation of topological phases in optical interference microscopy are presented and illustrated using a set of test models [5]. The algorithms are implemented using by Maple and Mathematica packages. The basic algorithm AVP is constructed in terms of 3x3 generalized Jones matrices and implemented as a set of subroutines that analytically compute the beam parameters and support the evaluation and visualization of the phases on the sphere of ray directions and/or on the Poincarè sphere. The beam parameters are the generalized Jones 3-vector and the wave 3-vector that determine, respectively, the polarization state and the direction of the beam propagation through a set of optical elements described by the well-known 2x2 Jones matrices. Near-field test models of the systems, that possess both geometrical and dynamical phases in the far-field region, are constructed beyond the ray approximation. These models imply a set of discrete sources with variable parameters and make use of the appropriate set of separable potentials.

A special class of separable potentials in the momentum space is considered, and these potentials are equivalent to 3D "diffused" δ-functions (quantum dots) in the configuration space. They allow obtaining a significant number of exact solutions of the time-dependent and time-independent Helmholtz (Schrödinger) equations. As an example, an intensity of scattering of a plane wave with the wave vector k on the eight "diffused" δ-functions (with the identical strengths $V_n = V$ and diffusion parameters $r_0 = X^{-1}$) disposed in the tops of a cube with the rib d is shown on Fig. 1.

For any numerical method, a pair of requirements is always made: one is stability, and the other is accuracy. From the viewpoint of these requirements, the unitary splitting methods have a big advantage: they preserve the norm of the wave functions, so that the conservation of probability density and robustness of the methods are guaranteed. In spite

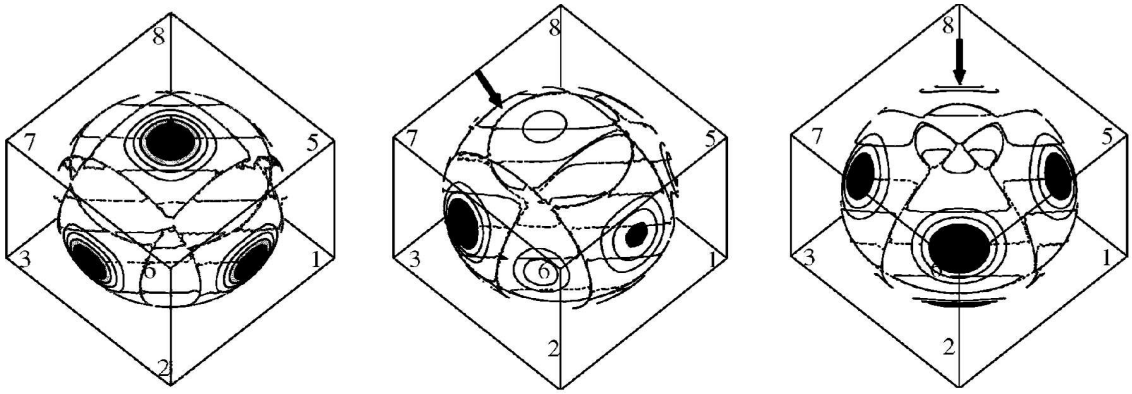

Fig. 1: Isolines of 4π-distribution of intensity of the scattering wave in the far-field region (dark spots correspond to maximums of intensity). The direction of the incident wave is depicted by the fat array: a) incidence in a top of cube b) incidence in a rib of cube c) incidence on a side of cube. Lines of constant values of phase $\varphi = 0, \pi$ and $\varphi = \pm\pi/2$ are shown by continuous and dotted lines respectively. Values of parameters are $s = d/\lambda = 1$, $P = V/(4\pi\lambda) = 1$, $Q = X\lambda = 20\pi$. The top 1 of the cube is disposed in the origin of the coordinate system

of the advantage due to the unitary preserving property, the unitary splitting methods still have had the following problem to be settled: At each time step associated with the splitting, a solution with a certain accuracy has to be determined. As a conventional method to this problem, the expansion of the wave packet of TDSE in a globally defined basis has been considered. Instead of this expansion method, the finite-element method (FEM) is applied together with using suitable interpolation technique connecting solutions given on neighboring spatial grids.

A new computational approach is proposed for the solution of the TDSE, in which a symbolic algorithm named GATEO (Generation of Approximations of the Time-Evolution Operator) implemented in Maple and numerical schemes based on the FEM are effectively composed [6]. The second-, fourth-, and sixth-order approximations with respect to the time step are derived for a numerical computation. As for the spatial step, the FEM is applied to construct the numerical schemes with a required accuracy with respect to the spatial step, in which a special gauge transformation of effective Hamiltonians is fixed to ensure a high applicability of the FEM. The efficiency and accuracy of the developed numerical algorithms is confirmed in certain integrable atomic models in external fields.

To illustrate how the above approach allows an efficient solution of the TDSE problem, we consider a Pöschl-Teller atom (PTA) in a pulse field. For the PT model the potential function $V(x) = -\cosh^{-2} x$ supports only one bound state $\psi_0(x) = 1/(2^{1/2}\cosh x)$, and a continuum of the known scattering states. The pulse field $f(t)$ is given by $f(t) = \{\sin^2(\pi t/2), 0 < t < 2; 0, t \geq 2\}$. We choose the corresponding ground state as an initial state. To approximate the solution $\psi_i(x,t), i = 1,2,3,4$ we use 1600 finite elements with sixth order and the finite element grid $\Omega = \{-1500(200) - 300(200) - 20(200) - 1(400)$ $1(200)20(200)300(200)1500\}$, where the numbers in brackets denote the number of finite elements in the intervals. We calculated the above solution over the enclosed time grids $\Omega_i[0,10]$ with four different time steps $\tau_i = 0.01, 0.005, 0.0025, 0.00125$. Fig. 2-3 displays the wave function calculated at time $T = 10$ and behavior of discrepancies $Er(t;i) = ||\psi_i(x,t) - \psi_4(x,t)||, i = 1,2,3$, and Runge's ratios $\alpha_M = \log_2(|Er(t;1) - Er(t,2)|/|Er(t;2) - Er(t,3)|)$ evaluated for generated schemes of $2M = 2,4,6$ order of an accuracy.

We obtained the numerical estimates of $\alpha_M(t)$ and their mean value, α_M, that strongly correspond to theoretical ones.

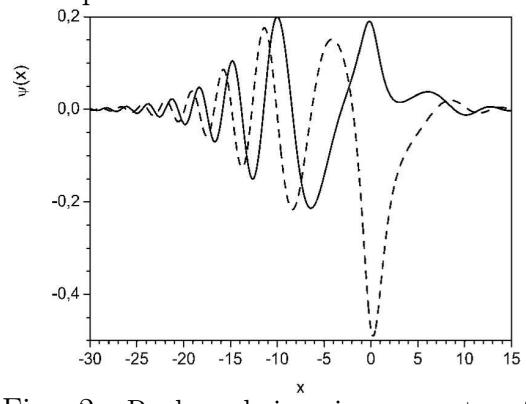

Fig. 2: Real and imaginary parts of solution $\psi(x,t)$ (solid and dashed curves) for PTA atom at $t = T = 10$

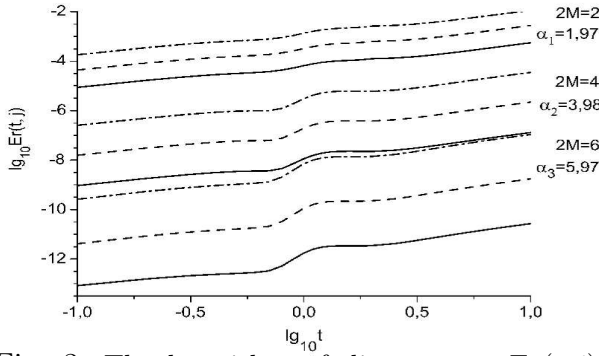

Fig. 3: The logarithm of discrepancy $Er(t;i)$ (dash-dot, dashed and solid curves) for schemes of $2M = 2, 4, 6$ order of accuracy

Our approach would be worth being applied to the quantum control problem, some pre-experimental calculations in the atomic dynamics in traps and/or external-pulse fields and various quantum calculations.

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