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A method for numerical solution of a time-dependent Schrödinger equation based on the Lee-Trotter-Suzuki formula

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The talk is devoted to the results of investigation of methods for numerical solution of a non-stationary Schrödinger equation. A review of a family of numerical methods based on the application of the Lee-Trotter-Suzuki product formula to the approximation of an evolution operator is presented. The problem of reducing the number of exponential operators in high-order accuracy approximation schemes by optimizing the sequence of multipliers is discussed. Two tenth-order accuracy algorithms to approximate the evolution operator are constructed based on the idea proposed by Yoshida. The results of numerical tests that demonstrate the stability of the algorithms and their order of accuracy are presented. The constructed algorithms make it possible to significantly reduce the number of exponential factors in the numerical scheme compared to the Lee-Trotter-Suzuki formula.