CRANK-NICOLSON SCHEME TO NUMERICALLY SOLVE TIME-DEPENDENT SCHRÖDINGER EQUATION

M.M. Zathiha[1*] and M.A.A.M. Faham[1]
[1]Department of Mathematical Sciences, Faculty of Applied Sciences, South Eastern University of Sri Lanka, Sammanthurai, Sri Lanka.
[*]zathiha@gmail.com

The Schrödinger equation is one of the fundamentals of quantum theory, which deals with the study of microparticles. The time-dependent Schrödinger equation (TDSE) encodes the information of a non-relativistic quantum mechanical system. In this study, we have investigated the numerical solution techniques to solve TDSE, which involve partial differential equations (PDEs). The Crank-Nicolson scheme is the average of the explicit scheme of forward time-centered space and the implicit scheme of backward time-centered space of finite difference methods. This scheme is derived from the Taylor series expansion of second-order accuracy and given a better approximation with exact solutions. We have chosen this scheme in this study because it is unconditionally stable and attractive for computing unsteady PDE problems. Also, the accuracy of this scheme can be enhanced without losing the stability of the problem at the same computational cost per time step. Further, the scheme converges faster than other numerical methods for the solutions of PDEs. We have examined the complex-valued TDSE using the Crank-Nicolson method with different initial and boundary condition testing examples. We have also used the simulation techniques of the MATLAB software to get the numerical results and two-dimensional graphical representations for the various parameters involving the initial and boundary conditions. When comparing the numerical results obtained, we have observed a pattern that is approximately converging by decreasing the time and space interval steps. Similarly, there is a pattern of increasing the accuracy by increasing the total time values.

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