Numerical Solution of the Schrödinger Equation

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The most basic problem in quantum mechanics is to solve the stationary Schrodinger equation for the energy eigenvalues and the associated energy eigenfunctions. There are number of important cases for which the stationary Schrodinger equation can be solved analytically. In most cases of practical interest exact or approximate numerical methods must be employed. In this project solutions of Schrodinger equation in one-dimensional problems are discussed. Numerov's method which is very elegant fifth-order scheme was derived and used. In dimensions higher than one, if the potential cannot be separated, solving the Schrodinger equation numerically is, in general, quite a complex problem. In practice, variational methods are therefore often used, where the wave function is expanded in an incomplete set of conveniently chosen basis states. This reduces the calculation to an eigenvalue problem in a discrete finite-dimensional space. An example of variational calculation in square-well potential with an internal barrier is shown. The matrix diagonalizations that have to be performed to solve the resulting eigenvalue problem are discussed.

Key words: *Eigenvalue problem, Schrodinger equation*