1 Nonstationary Schrödinger equation

1.1 Crank-Nicholson scheme

One-dimensional Schrödinger equation with a nonstationary potential

$$\frac{\partial\psi}{\partial t} = i\frac{\partial^2\psi}{\partial x^2} - iV(x,t)\psi = -i\hat{H}\psi$$

Discretization: $x = jh$, $t = n\tau$. Crank-Nicholson scheme:

$$(1 + i\tau\hat{H}/2)\psi^{n+1} = (1 - i\tau\hat{H}/2)\psi^n$$

or

$$\psi_j^{n+1} - \frac{i\tau}{2h^2}(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}) + i\frac{\tau}{2}V(jh,(n+1)\tau)\psi_j^{n+1} =$$

$$= \psi_j^n + \frac{i\tau}{2h^2}(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n) - i\frac{\tau}{2}V(jh,n\tau)\psi_j^n$$

$$[-\frac{i\tau}{2h^2}]\psi_{j-1}^{n+1} - [-1 - 2\frac{i\tau}{2h^2} - i\frac{\tau}{2}V(jh,(n+1)\tau)]\psi_j^{n+1} + [-\frac{i\tau}{2h^2}\psi_{j+1}^{n+1}] =$$

$$= \psi_j^n + \frac{i\tau}{2h^2}(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n) - i\frac{\tau}{2}V(jh,n\tau)\psi_j^n$$

We rewrite as

$$A_j\psi_{j-1}^{n+1} - C_j\psi_j^{n+1} + B_j\psi_{j+1}^{n+1} = -F_j$$

where

$$A_j = B_j = -\frac{i\tau}{2h^2}$$

$$C_j = -1 - 2\frac{i\tau}{2h^2} - i\frac{\tau}{2}V(jh,(n+1)\tau)$$

$$F_j = -\psi_j^n - \frac{i\tau}{2h^2}(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n) + i\frac{\tau}{2}V(jh,n\tau)\psi_j^n$$

1.2 Solution of a tridiagonal linear system of equations

Consider a linear system

$$A_jy_{j-1} - C_jy_j + B_jy_{j+1} = -F_j \qquad j = 1,2,\ldots,N-1$$

with boundary conditions

$$y_0 = \kappa_1 y_1 + \nu_1 \qquad y_N = \kappa_2 y_{N-1} + \nu_2$$

Step 1: one calculates supplementary variables α_i, β_i iteratively starting from $i = 1$ to $i = N$ according to

$$\alpha_1 = \kappa_1 \qquad \beta_1 = \nu_1$$

$$\alpha_{i+1} = \frac{B_i}{C_i - \alpha_i A_i} \qquad \beta_{i+1} = \frac{A_i\beta_i + F_i}{C_i - \alpha_i A_i} \qquad i = 1,2,\ldots,N-1$$

Step 2: one calculates y_i iteratively starting from $i = N$ to $i = 1$ according to

$$y_N = \frac{\nu_2 + \kappa_2\beta_N}{1 - \kappa_2\alpha_N}$$

$$y_i = \alpha_{i+1}y_{i+1} + \beta_{i+1} \qquad i = N-1, N-2, \ldots, 0$$