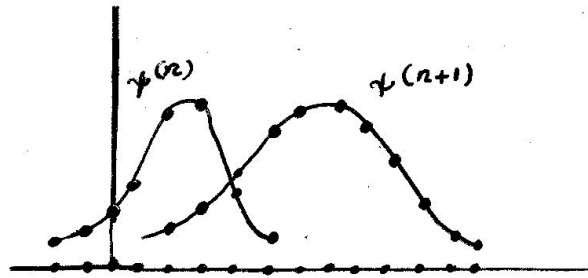


- Fourier method (Koroloff & Kosloff, J. Comp. Phys., 52, 35 (1983))

Discretization of the Schroedinger eq.



$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

$$\frac{\partial \psi^n}{\partial t} = \frac{\psi^{n+1} - \psi^{n-1}}{2\Delta t}$$

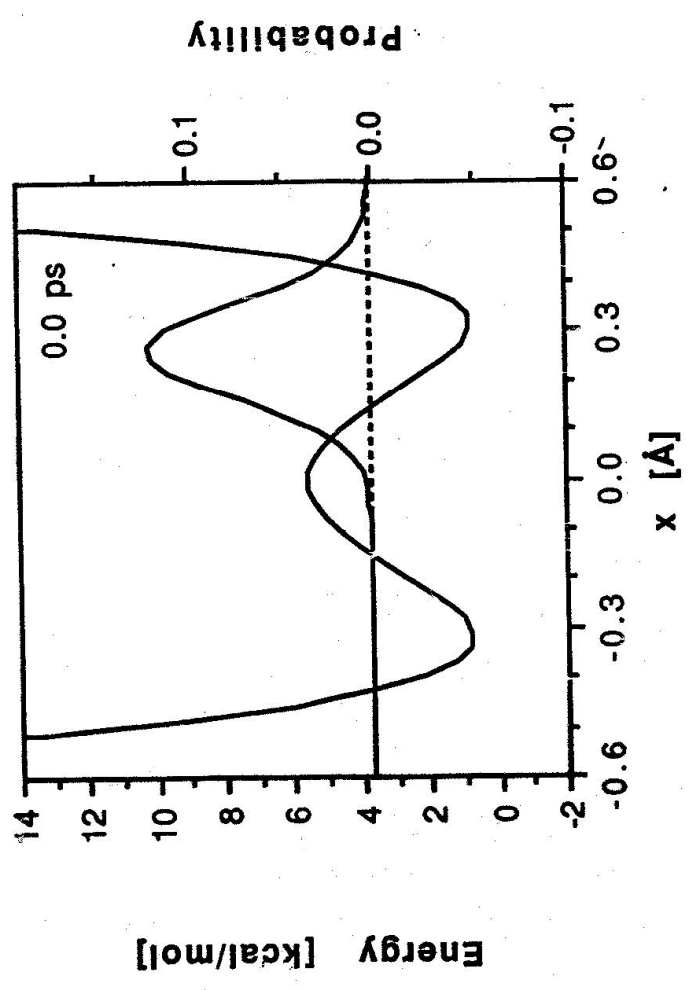
$$\psi^{n+1} = \psi^{n-1} + \frac{2\Delta t}{i\hbar} H\psi^n$$

$$\Delta \psi \Leftrightarrow -k^2 \tilde{\psi}$$

$$\psi \rightarrow \tilde{\psi} \rightarrow -k^2 \tilde{\psi} \rightarrow -k^2 \tilde{\psi}$$

R = 2.85Å

NH3 - H+ - NH3



Probability

