Quantum Wave in a Box

An App for *iPhone* and *iPad*

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Technical details (march 16th 2017)

The time-independent Schrödinger's equation writes in atomic units

$$-\frac{1}{2m}\frac{d^2}{dx^2}\phi(x)+V(x)\phi(x)=E\phi(x) \tag{1}$$

Let $\{\dots, x_{-1}, x_0, x_1, \dots, x_{i-1}, x_i, x_{i+1}, \dots, x_N, x_{N+1,} \dots\}$ be a uniform discretization of the x - axis with step $x_{i+1}-x_i=h$. Using the finite elements method and a 5-point stencil, $\phi(x)$ can be approximated

$$\phi(x)\approx L_i^{(5)}(x) \quad for\ x_{i-2}\le x\le x_{i+2} \tag{2}$$

where $L_i^{(5)}(x)$ is the Lagrange polynomial which passes through the 5 points

$$\{(x_{i-2},u_{i-2}),(x_{i-1},u_{i-1}),(x_i,u_i),(x_{i+1},u_{i+1}),(x_{i+2},u_{i+2})\} \tag{3}$$

and

$$u_i=\phi(x_i) \tag{4}$$

An approximation of the differential part in equation (1) is

$$\phi''(x_i)\approx \frac{d^2}{dx^2}L_i^{(5)}(x)\Big|_{x=x_i}=\frac{-u_{i-2}+16u_{i-1}-30u_i+16u_{i+1}-u_{i+2}}{12h^2} \tag{5}$$

and time-independent Schrödinger's equation (1) leads to a set of linear equations where E and the $\{u_i\}$ are unknown variables

$$-\frac{1}{2m}\left[\frac{-u_{i-2}+16u_{i-1}-30u_i+16u_{i+1}-u_{i+2}}{12h^2}\right]+V_iu_i=Eu_i \tag{6}$$

In matrix form

$$\begin{pmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \iddots \\ \cdots & a+V_{i-2} & b & c & 0 & 0 & \cdots \\ \cdots & b & a+V_{i-1} & b & c & 0 & \cdots \\ \cdots & c & b & a+V_i & b & c & \cdots \\ \cdots & 0 & c & b & a+V_{i+1} & b & \cdots \\ \cdots & 0 & 0 & c & b & a+V_{i+2} & \cdots \\ \iddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ u_{i-2} \\ u_{i-1} \\ u_i \\ u_{i+1} \\ u_{i+2} \\ \vdots \end{pmatrix} = E \begin{pmatrix} \vdots \\ u_{i-2} \\ u_{i-1} \\ u_i \\ u_{i+1} \\ u_{i+2} \\ \vdots \end{pmatrix} \tag{7}$$

with

$$a = \frac{5}{4mh^2}, \quad b = \frac{-2}{3mh^2}, \quad c = \frac{1}{24mh^2}, \quad V_i = V(x_i) \tag{8}$$

If *V(x)* is real, the hamiltonian matrix *H* above is a real symmetric band matrix. To be diagonalizable numerically, it has to be truncated. The x - axis is reduced to the interval $[x_0, x_N]$; the length of this *Box* being a multiple of h .

The *H* matrix is truncated as follows on its left side

$$\begin{bmatrix} V_\infty & b & c & 0 & 0 & \cdots \\ b & a+V_1 & b & c & 0 & \cdots \\ c & b & a+V_2 & b & c & \cdots \\ 0 & c & b & a+V_3 & b & \cdots \\ 0 & 0 & c & b & a+V_4 & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \tag{9}$$

and on its right side

$$\begin{bmatrix} \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & a+V_{N-4} & b & c & 0 & 0 \\ \cdots & b & a+V_{N-3} & b & c & 0 \\ \cdots & c & b & a+V_{N-2} & b & c \\ \cdots & 0 & c & b & a+V_{N-1} & b \\ \cdots & 0 & 0 & c & b & V_\infty \end{bmatrix} \tag{10}$$

with V_∞ being positive and chosen large enough to ascertain $u_0 \approx 0$ and $u_N \approx 0$.

One is limited therefore to work in a subspace of dimension N+1.

The truncated *(N+1)x(N+1)* hamiltonian matrix *H* is diagonalized using standard numerical routines. Numerically the energy levels $\left\{ \left(E_i, \vec{e_i} \right) \right\}$ where $i = 0,1,\cdots,N$ append to be non-degenerated. The matrix of passage P to the new basis of vectors $\{ \vec{e_i} \}$ being orthonormal, its inverse $P^{-1} = P^T$.

After diagonalization the hamiltonian is represented by a diagonal matrix Λ so that

$$\Lambda = P^{-1}HP \tag{11}$$

Finally one gets the evolution operator $U(t)$ in matrix form

$$U(t) = e^{-iHt} = e^{-itP\Lambda P^{-1}} = P\ e^{-i\Lambda t}P^{-1} \tag{12}$$

where

$$e^{-i\Lambda t} = \begin{pmatrix} e^{-iE_0 t} & & 0 \\ & \ddots & \\ 0 & & e^{-iE_N t} \end{pmatrix} \tag{13}$$

is a diagonal matrix with energies $E_0, E_1, \cdots, E_N$ sorted in ascending order.

The solution of the time-dependent Schrödinger's equation can then easily be calculated on the grid for any time value

$$\begin{bmatrix} \psi(x_0,t) \\ \psi(x_1,t) \\ \vdots \\ \psi(x_i,t) \\ \vdots \\ \psi(x_N,t) \end{bmatrix} = U(t) \begin{bmatrix} \psi_0(x_0) \\ \psi_0(x_1) \\ \vdots \\ \psi_0(x_i) \\ \vdots \\ \psi_0(x_N) \end{bmatrix} \tag{14}$$

where

$$\psi_0(x) = \left(\frac{1}{2\pi\alpha}\right)^{\frac{1}{4}} e^{\frac{-(x-x_0)^2}{4\alpha}}\ e^{ik_0(x-x_0)} \tag{15}$$

is a gaussian wave-packet centered on x_0 , with group velocity $v_0 = k_0 / m$ and standard deviation $\sigma = \sqrt{\alpha}$. In expression (15) $\psi_0(x)$ has been normalized as a continuous function

$$\int_{-\infty}^{+\infty} \left|\psi_0(x)\right|^2 dx = 1 \tag{16}$$

Since the evolution operator conserves the norm, at time t

$$\int_{-\infty}^{+\infty} \left|\psi(x,t)\right|^2 dx \approx h\sum_{i=1}^{N-1}\left|\psi(x_i,t)\right|^2 \approx 1 \tag{17}$$

if N is large enough and the potential *V(x)* has no imaginary part. Moreover the initial wave-packet at *t = 0* has to be far enough from the boundaries of the Box.

Since the solution $\psi(x,t)$ of the time-dependent Schrödinger's equation is *known*, through the calculation described above, only for the $x_0, x_1, \cdots, x_N$ of the grid, a natural cubic spline will be used, if necessary, to evaluate $\psi(x,t)$ for any x value within the box $[x_0, x_N]$ for the purpose of displaying a smooth curve on the screen of the device.

Appendix

- 3-point stencil

$$\phi''(x_i) \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{h^2}$$

- 5-point stencil

$$\phi''(x_i) \approx \frac{-u_{i-2} + 16u_{i-1} - 30u_i + 16u_{i+1} - u_{i+2}}{12h^2}$$

- 7-point stencil

$$\phi''(x_i) \approx \frac{2u_{i-3} - 27u_{i-2} + 270u_{i-1} - 490u_i + 270u_{i+1} - 27u_{i+2} + 2u_{i+3}}{180h^2}$$

- 9-point stencil

$$\phi''(x_i) \approx \frac{-9u_{i-4} + 128u_{i-3} - 1008u_{i-2} + 8064u_{i-1} - 14350u_i + 8064u_{i+1} - 1008u_{i+2} + 128u_{i+3} - 9u_{i+4}}{5040h^2}$$

- 11-point stencil

$$\phi''(x_i) \approx \frac{8u_{i-5} - 125u_{i-4} + 1000u_{i-3} - 6000u_{i-2} + 42000u_{i-1} - 73766u_i + 42000u_{i+1} - 6000u_{i+2} + 1000u_{i+3} - 125u_{i+4} + 8u_{i+5}}{25200h^2}$$