Manual for the SuperWave Program

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About SuperWave

SuperWave is an educational program which calculates non-stationary quantumWave functions as a Superposition of stationary Wavefunctions. The result is shown in real time as a moving picture.

Installation

Download Superwave.zip from my Website and place it into any directory (for example C:\SuperWave\. In Windows 10 it seems that it is not even necessary to unzip the zip file. Just look what is inside and double-clisk on SuperWave.exe. Windows needs about 10 second to check whether it does not contain harmful code.

Start **SuperWave.EXE**

Use menu 'Functions' to start animated display

Removing the Program

Simply delete the SuperWave.EXE and SuperWave.HLP files.

SuperWave does not modify any files in your system (in particular it does not make any entries in autoexec, config, INI, and registry files).

Deleting the files thus entirely removes the program from your computer.

How to use SuperWave

- Use menu **Functions** to start animation.

- Vary parameters with Scrollbars. The display reflects changes immediately.

- Real parts of the stationary waves are shown in green.

- A non-stationary wave, calculated as the sum of the stationary waves, is shown above in red.

- Finally, the probability density is shown on the top of the diagram in purple.

- The STOP button terminates the animation.

Theory: Free Electron

The stationary wave functions of the free particle are calculated according to:

$$\varphi_j = A\left(e^{i\frac{p}{\hbar}x} \times e^{-i\frac{E}{\hbar}t}\right)$$

t - time

x - space coordinate

p - impulse

E - total energy, sum of the potential energy E_p and the kinetic energy E_k

The real parts of the stationary waves are shown in green.

A non-stationary wave is then calculated as the sum of the stationary waves:

$$\Psi(x,t) = \sum_j \varphi_j(x,t)$$

The real part of this wave function is shown in red.

Finally, the probability density:

$$P = |\Psi(x,t)|^2$$

is shown on the top of the diagram in purple.

Theory: Harmonic Potential

The stationary wave functions are calculated using the well known formulas:

(parameters correspond to oxygen)

$$u_n(z) = \sqrt[4]{\frac{m\omega}{\hbar\pi}} \frac{e^{-z^2/2}}{\sqrt{2^n n!}} H_n(z)$$

where

$$z = \sqrt{m\omega/\hbar}\, x$$

is the dimensionless coordinate and

Hn is the *Hermite polynomial*

A superposition of the stationary wave functions is then calculated:

$$\psi(x,t) = \sum_{n=0}^{16} c_n \, e^{-i\frac{E_n}{\hbar}} u_n(x)$$

with

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

The real part of this wave function is shown in red.

The coefficients are either selected individually with the Scrollbars, or the 'optimal' coefficients are calculated as

$$c_n = \frac{\alpha^n}{\sqrt{n!}} \, e^{-\frac{|\alpha|^2}{2}}$$

where the parameter α is selected with a scrollbar

Finally, the probability density:

is shown on the top of the diagram in purple.

Two Waves

- The probability density consists of a train of wave packets (that is not of a single packet) because sum is made only two stationary waves.

- Many aspects of the relation of the stationary waves and the resulting wave packet can be visualized and illustrated, however:

just focus your attention on only a single wave packet in the train

- Vary the kinetic and potential energies using the scrollbars and observe the changes of the animated display, in particular look for:

1. DeBroglie wavelength of a the stationary Wave. The wavelength becomes shorter with increasing kinetic energy.

2. Width of the wave packet and its dependence on the difference of the kinetic energies of the two component stationary wave. The wave packet(s) become narrower when the kinetic energies of the two component waves differ more. This

corresponds to the Heisenberg's uncertainty principle - larger uncertainty in energy results in a more precise position information.

3. Dependence of the group velocity on kinetic energy. The wave packets move faster when the two kinetic energies of the stationary waves are increased.

4. The independence of the group velocity of the potential energy: The phase velocity of the two stationary waves varies with the potential energy. (the ridges may even move backward for negative potential energies!) The group velocity, i.e. the velocity of the wave packets, remains constant.

Five Waves

- Five Waves permit to form more localized wave packets - the "gaps" between the individual packets are wider.

- Note that the individual wave packets widen as they propagate.

- Try to vary the mixing coefficient, that is the amplitudes of the component waves, with the Scrollbars. See whether you can form 'nice' wavepackets. Nice packets result when the coefficients lie on a Gaussian.

Harmonic Potential: Instructions

The potential curve is shown green, the stationary wave functions for $n = 0$ - 10 are drawn in the potential.

The real part of the non-stationary wave is shown in brick-red.

The probability density is shown on the top in purple.

The individual mixing coefficients can be entered in two ways:

- chosen by the scrollbars on the right, or

- the 'optimum' coefficients are calculated, based on the parameter α, whose value is entered by the corresponding scrollbar.

(The coefficients are recalculated every time when position of the 'alpha' scrollbar is changed.)

Known Bugs

- The display becomes very slow if you hit the Windows taskbar on the bottom of the screen while animation is running.

   Stop animation and restart it to correct the problem.

- Disable screen savers - they interfere with SuperWave.

- The program crashes from time to time (I am not a professional programmer) - just restart it.

- Use full screen display. Resizing windows does not work well.

References

- R. S. Berry, S. A. Rice, J. Ross, Physical Chemistry (Wiley 1980) page 140. (note that eq. 4.8 is mistyped, however)