

# Multimedia in Physics: Quantum Mechanics

Grzegorz Karwasz  
Katedra Dydaktyki Fizyki  
Instytut Fizyki, UMK Toruń

# MPTL Recommendations

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## **Report on Available Multimedia Material for a Lecture in Quantum Mechanics**

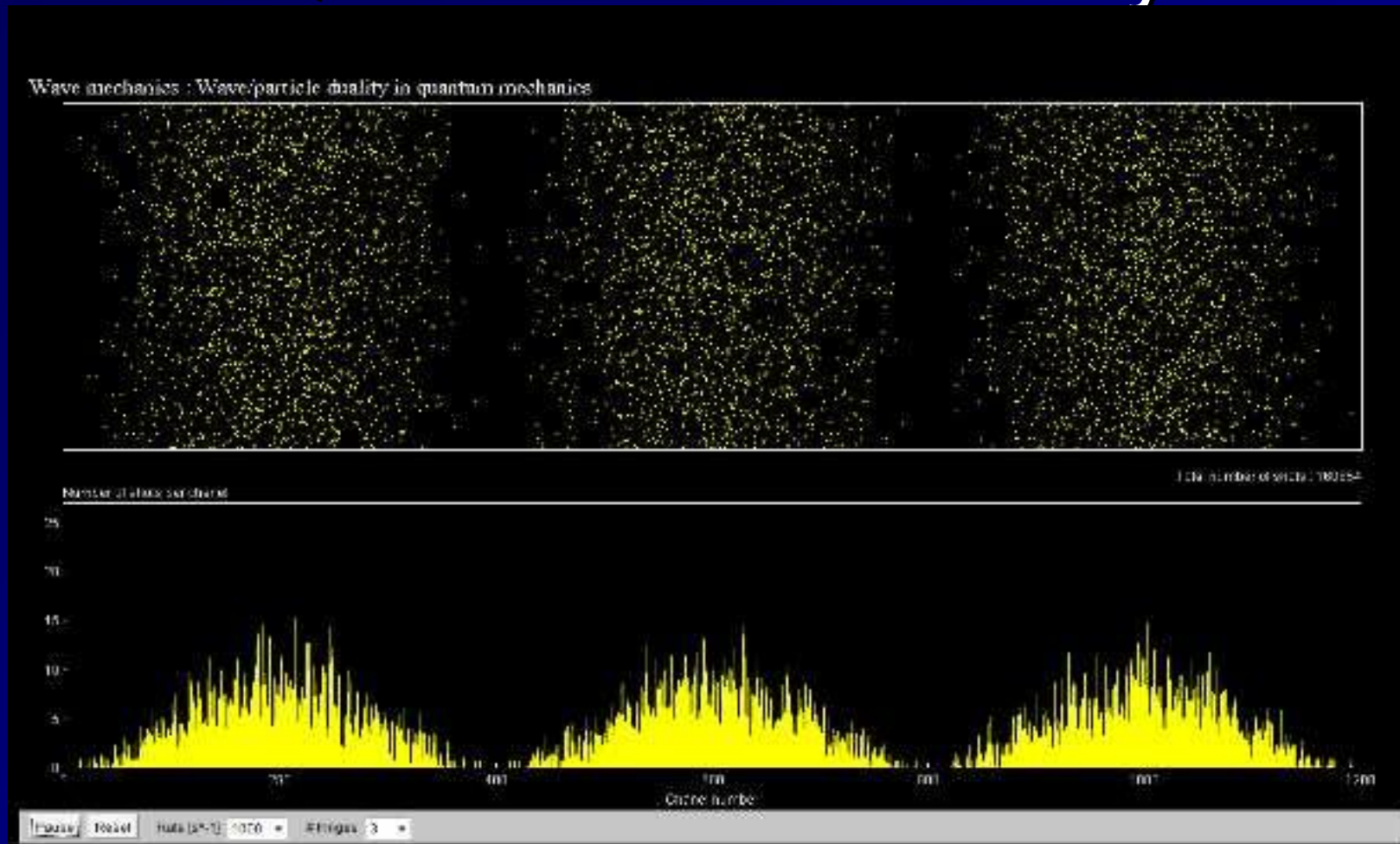
*H. J. Jodl, Department of Physics, University of Kaiserslautern, Germany*

### **Introduction**

Since a few thousand applets to teach physics are nowadays available worldwide, since about ten media server to collect material are now functioning, since a few textbooks for universities already include multimedia material (MM), since individual websites of universities physics professors contain excellent MM for teaching and learning ... it is now time to start a systematic analysis on that matter: to collect what is available, to evaluate this material according to criteria, to recommend and disseminate good material.

One cannot expect from an ordinary professor in physics, mainly involved in research and administration, to perform such an analysis by himself, when he has taken the duty to teach a lecture on topic x.

# Quantum-wave duality



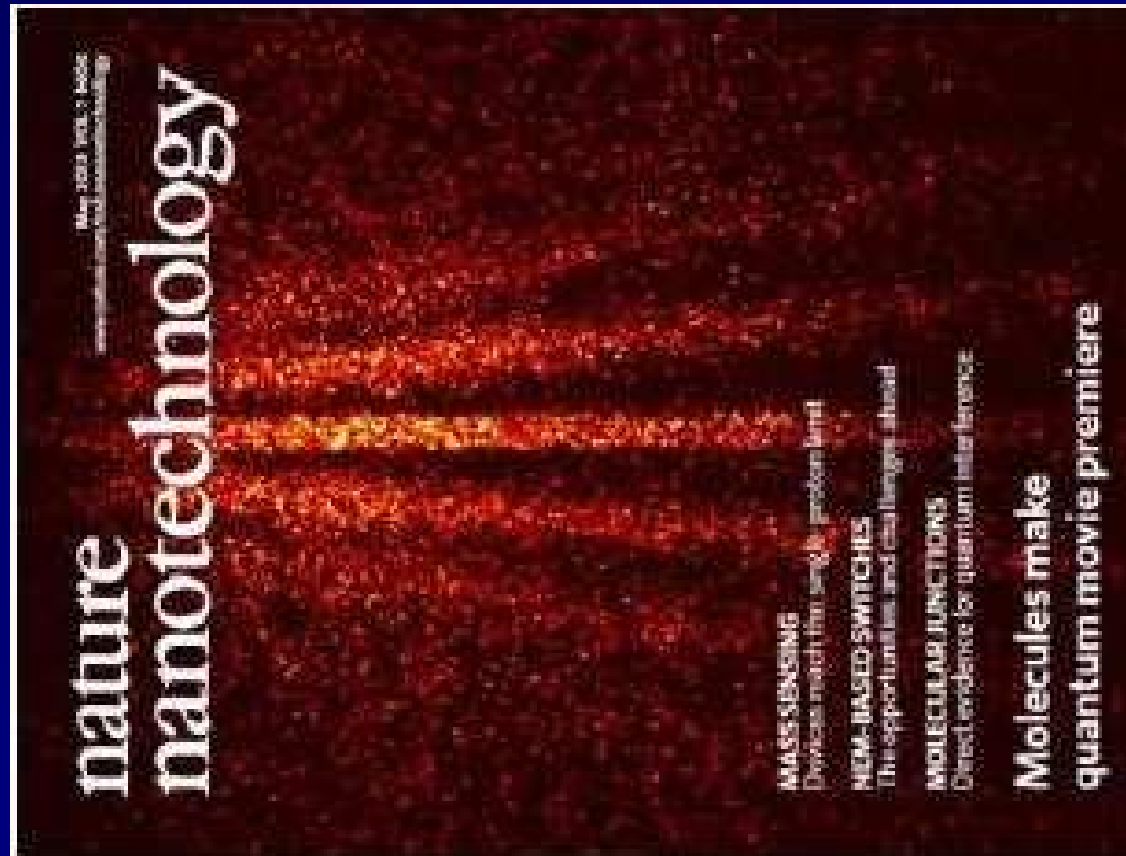
■ <http://www.quantum-physics.polytechnique.fr/>

# Quantum-wave duality



■ <https://www.youtube.com/watch?v=4lcYC2tsDDE>

# Quantum-wave duality

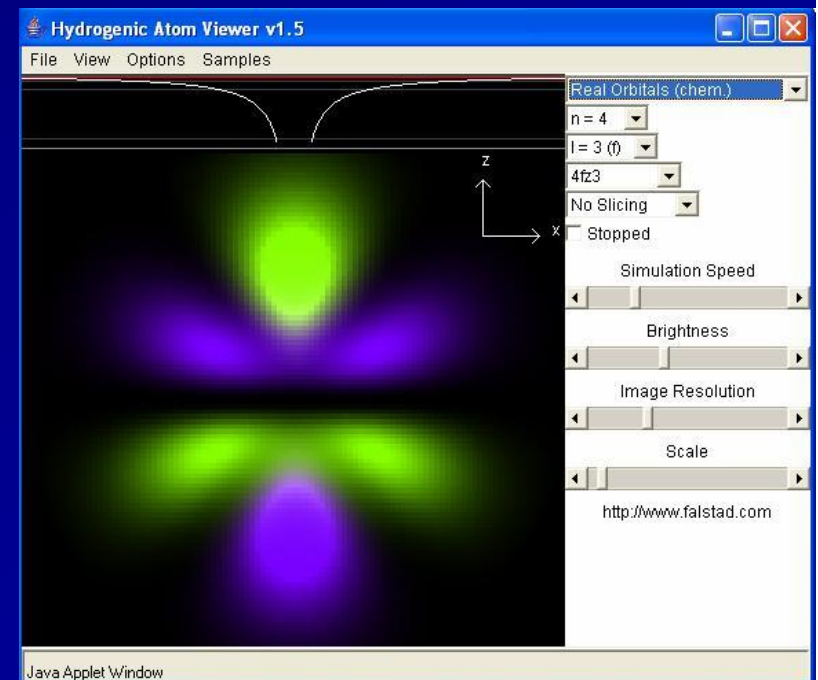
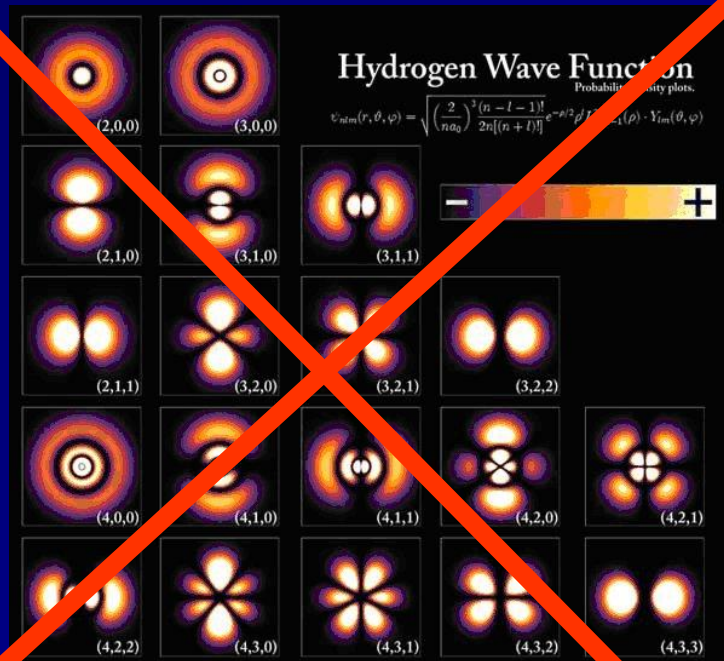


■ <http://www.quantumnano.at/molecular-movies.7005.html>

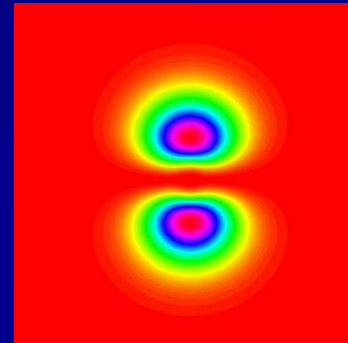
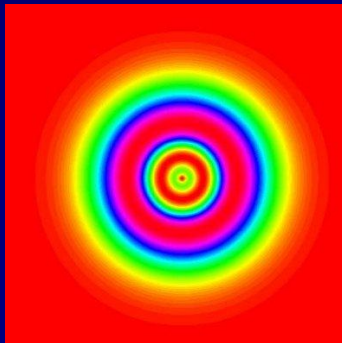
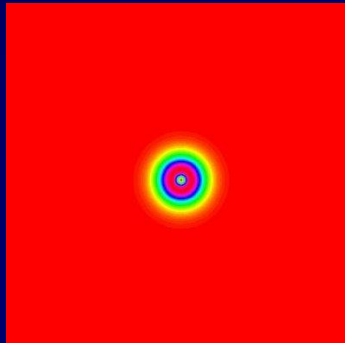


# Hydrogen atom

Orbitals in hydrogen atom [more-or-less]

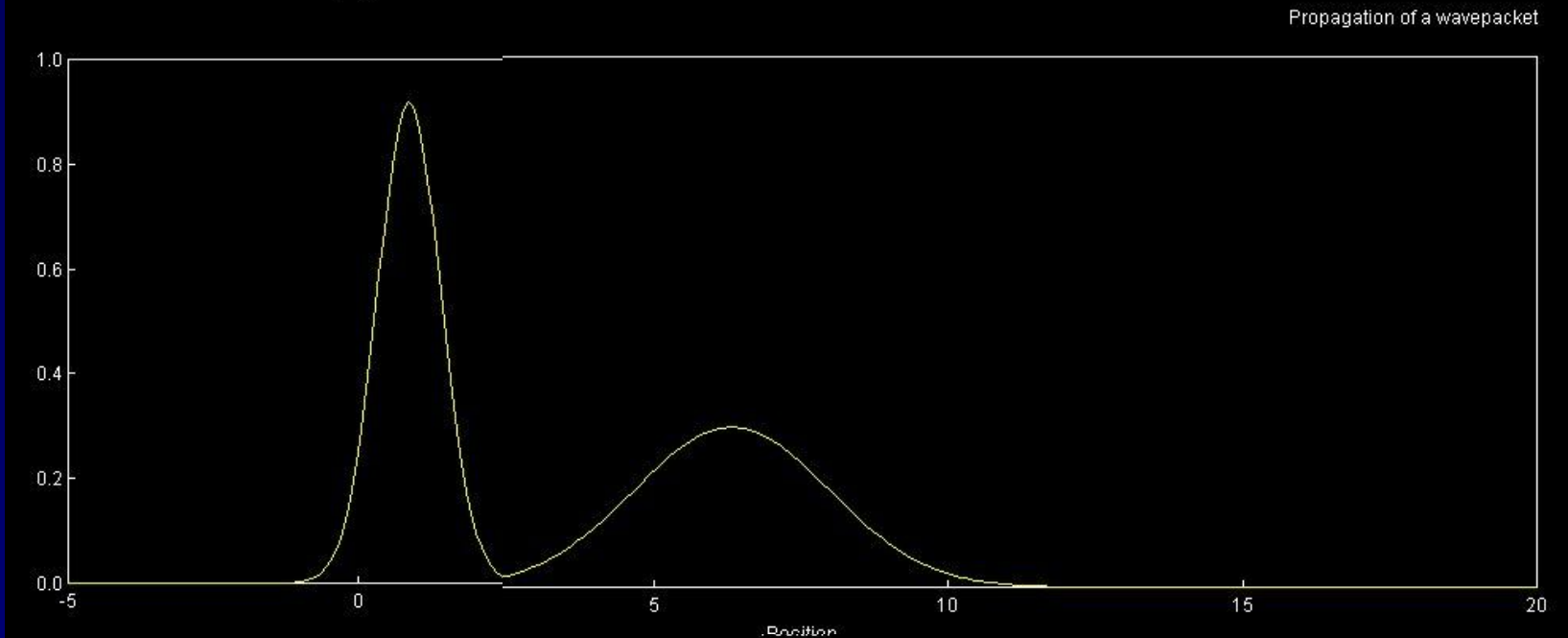


# Hydrogen atom



# Wave packet propagation

Wave mechanics : Propagation of a free wavepacket

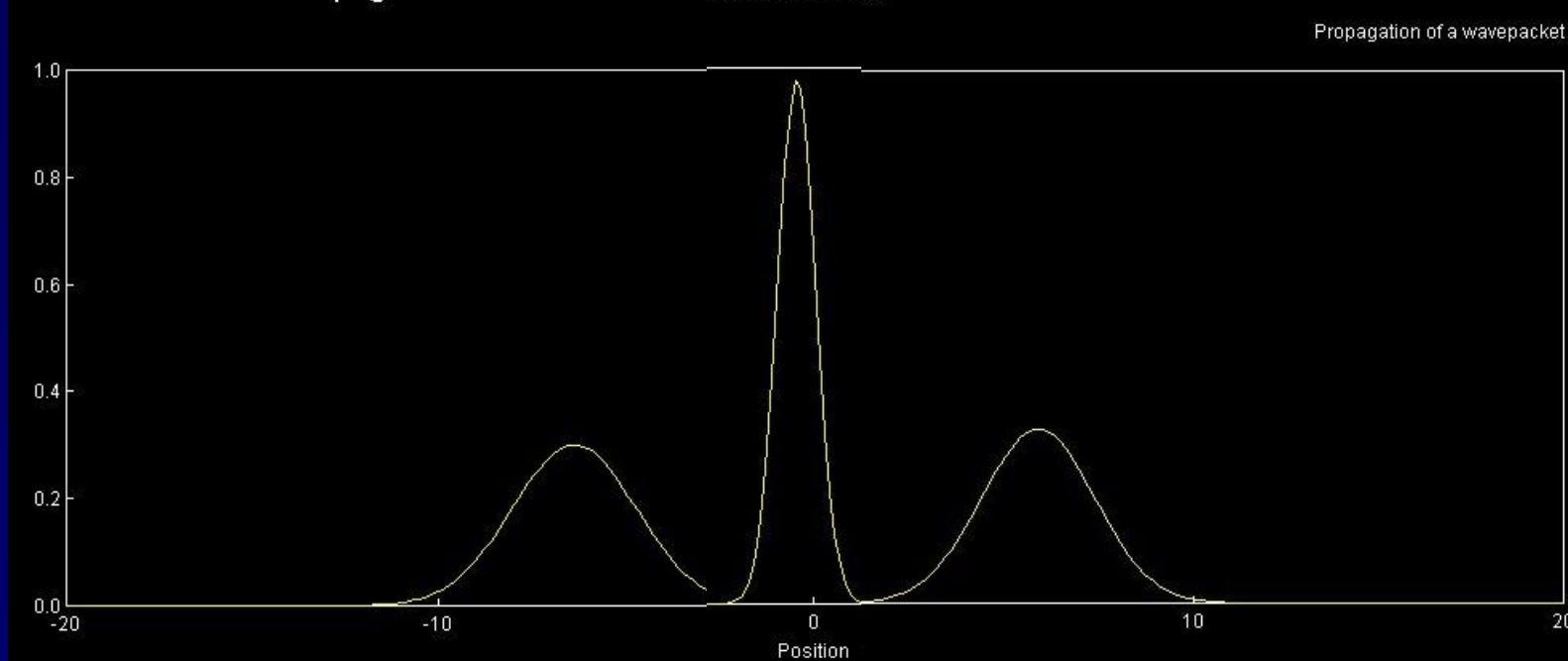


■ <http://www.quantum-physics.polytechnique.fr/>



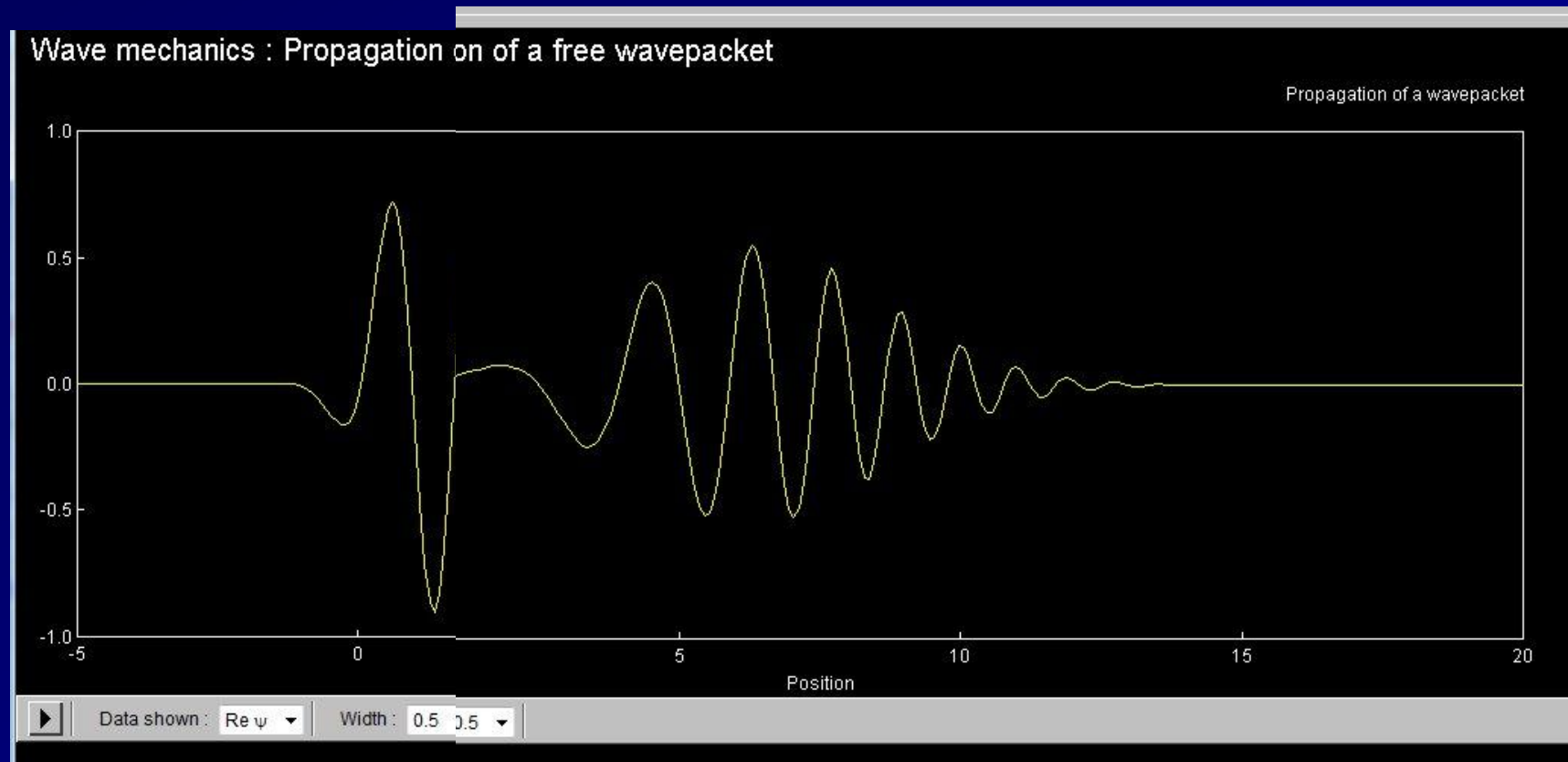
# Wave packet propagation/2

Wave mechanics : Propagation of a non-minimal wavepacket



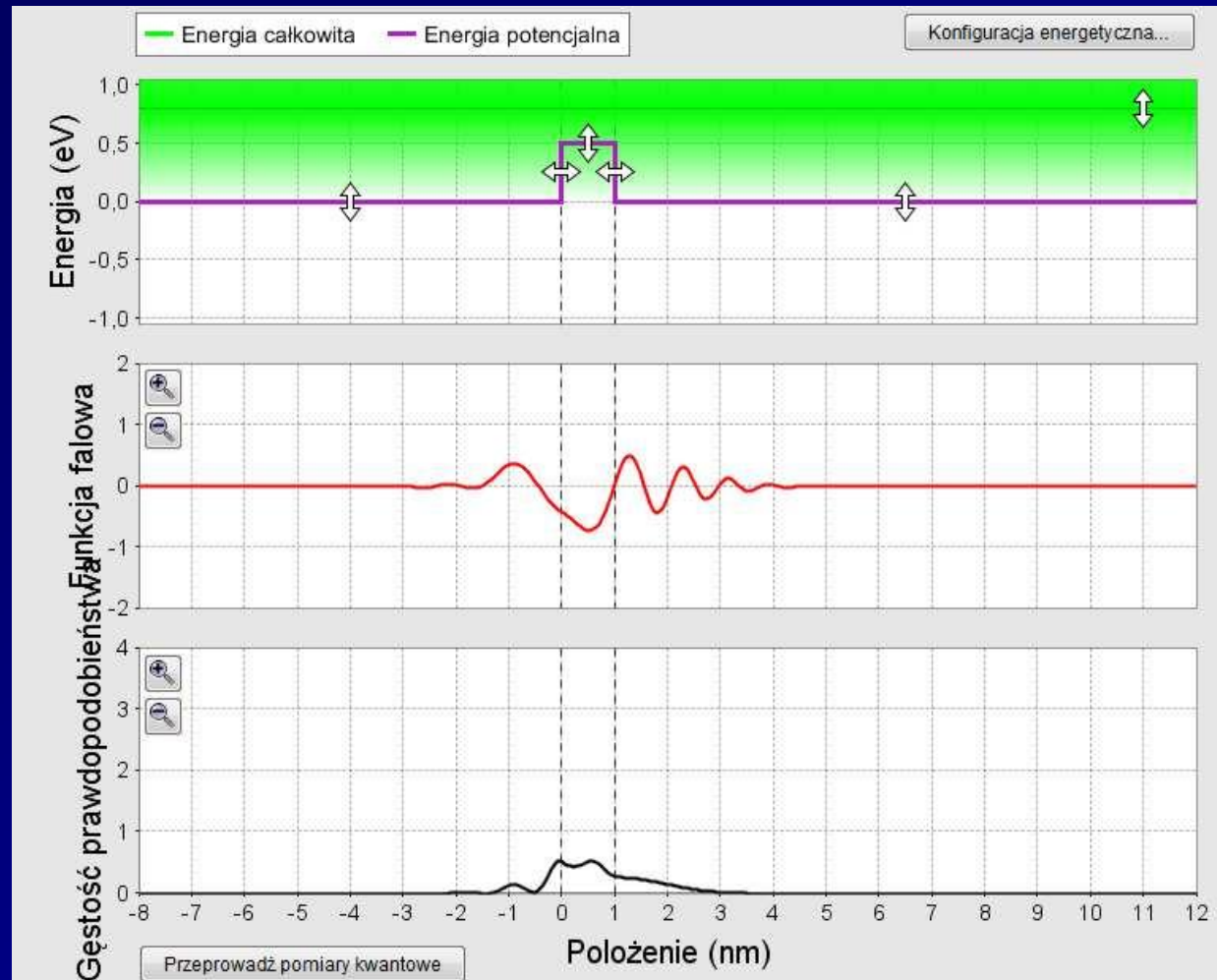
■ <http://www.quantum-physics.polytechnique.fr/>  
(non-minimal packet)

# Wave packet propagation/3



■ <http://www.quantum-physics.polytechnique.fr/>

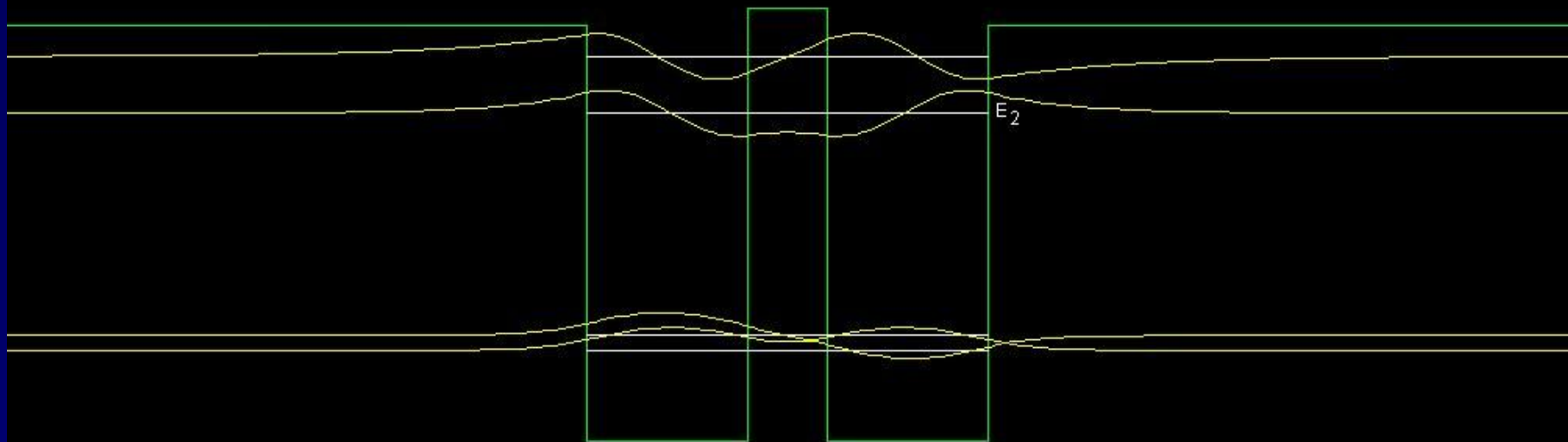
# Potential barrier



■ [http://phet.colorado.edu/sims/quantum-tunneling/quantum-tunneling\\_pl.jnlp](http://phet.colorado.edu/sims/quantum-tunneling/quantum-tunneling_pl.jnlp)

# Double potential well

Quantization in one dimension : Energy levels and eigenfunctions in a one-dimensional potential



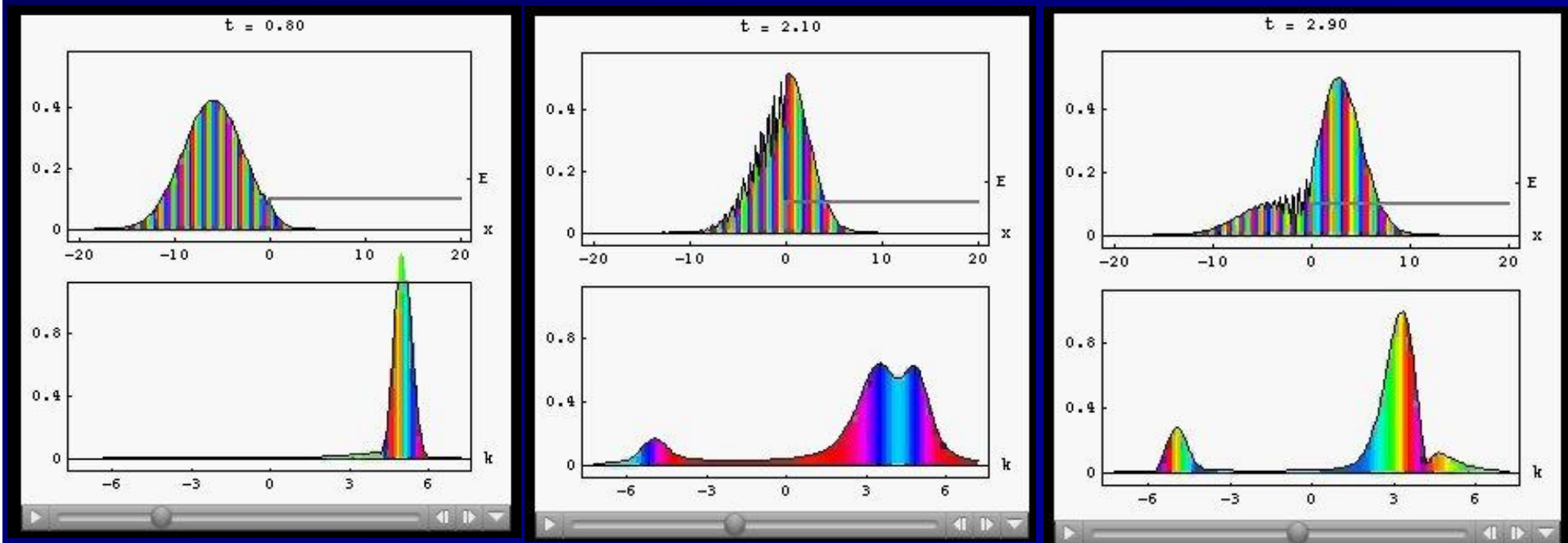
Show eigenstates ▾ Double well ▾ ☒ Symmetric

This simulation shows both energy levels and eigenstates. You can change all the parameters of the simulation, including the potential shape. Note that when you check Symmetrical, the potential will remain an even function. You can use this function to observe the effect of the barrier thickness on the level separation, and in particular how the tunnel coupling between two wells splits the degeneracy.

# „Visual Quantum Mechanics”

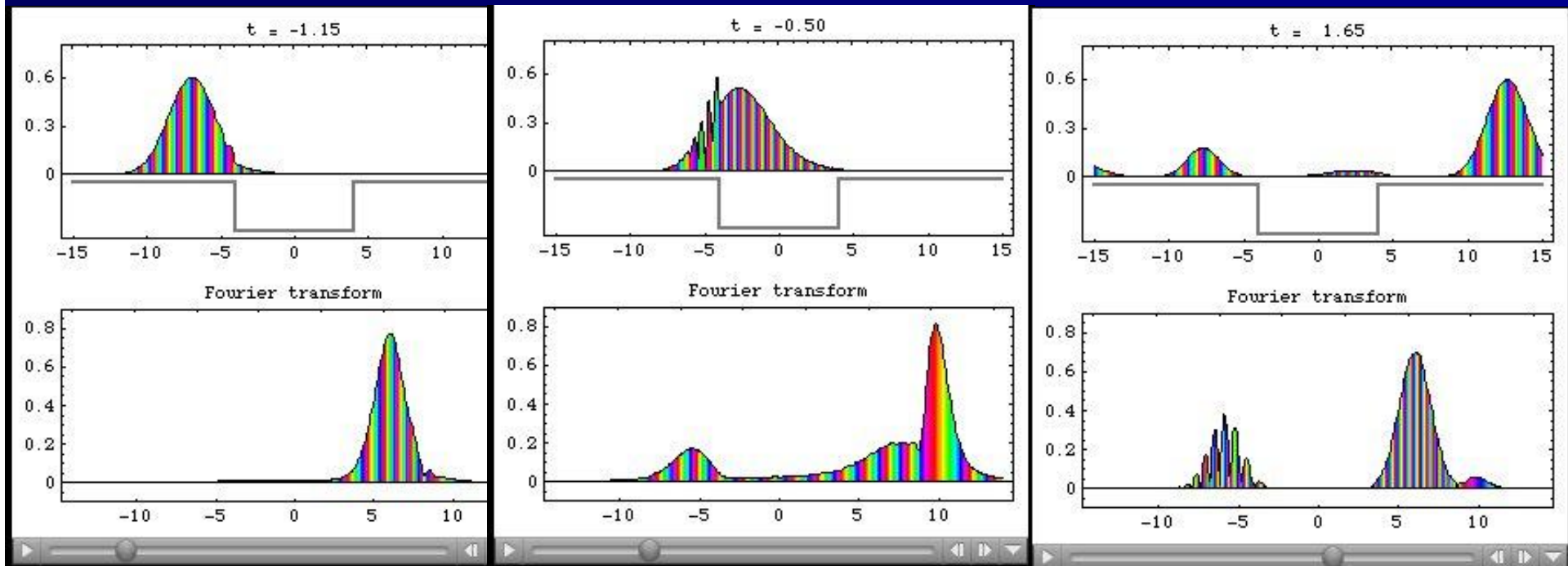
Berndt Teller (Uni Graz)

## Potential barrier in momentum space



# „Visual Quantum Mechanics”

Reflection on both ends of the well

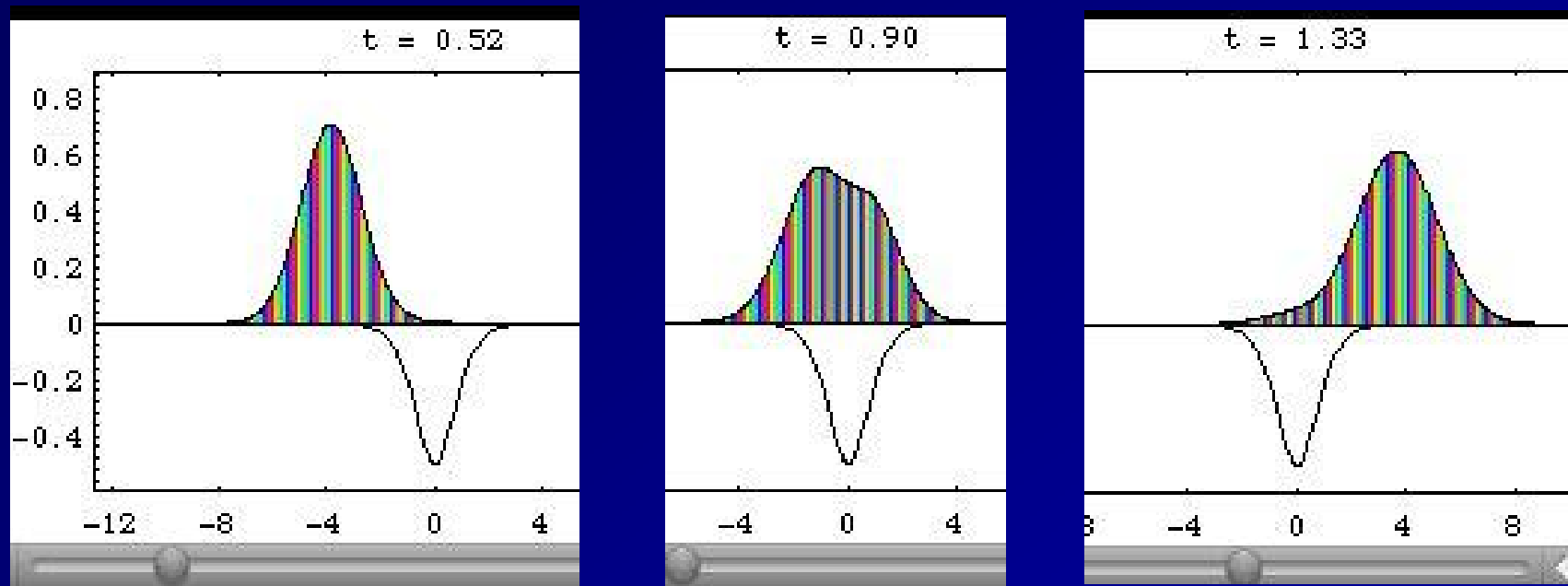


■ [http://vqm.uni-graz.at/pages/supplementary/107S\\_05d.html](http://vqm.uni-graz.at/pages/supplementary/107S_05d.html)



# „Visual Quantum Mechanics”

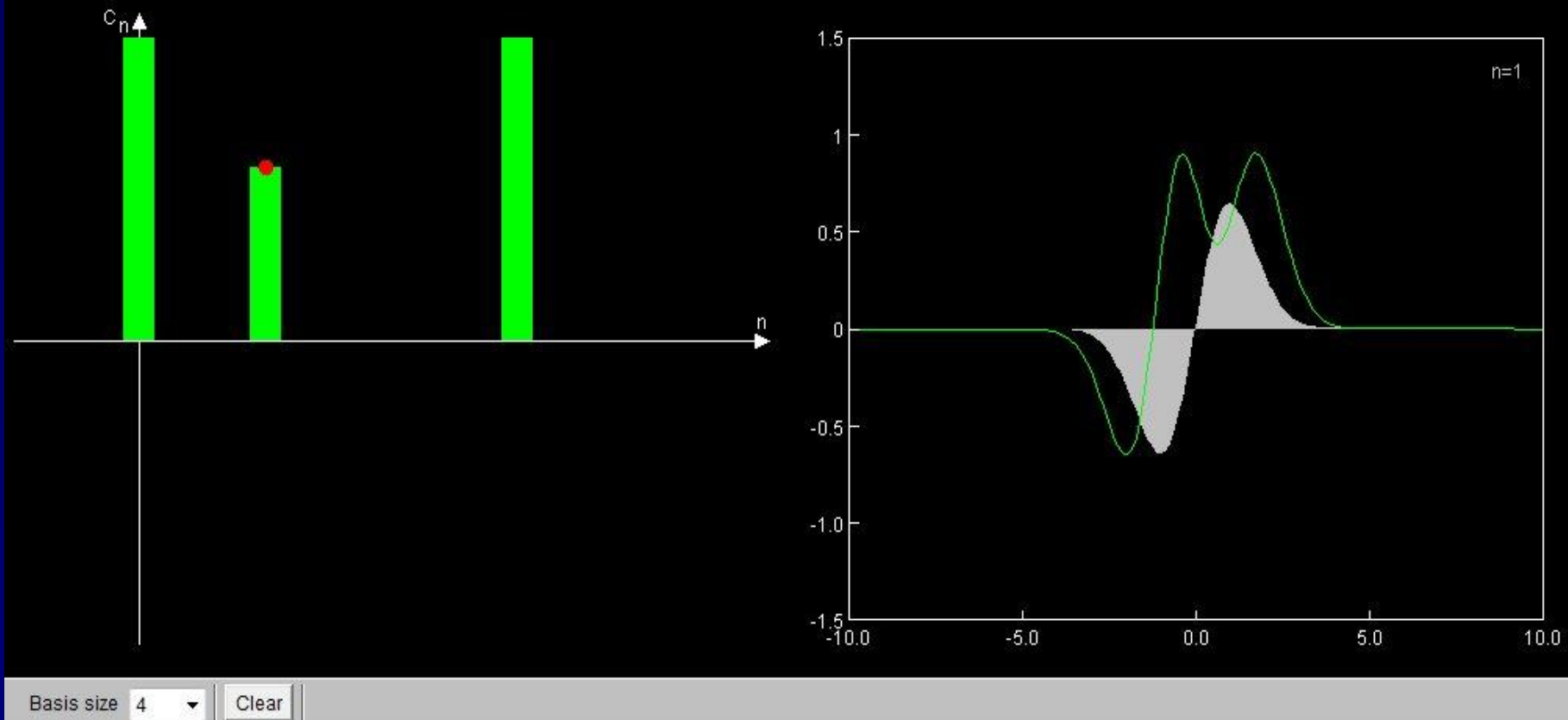
No reflection – soliton-like well



■ [http://vqm.uni-graz.at/pages/supplementary/107S\\_refless.html](http://vqm.uni-graz.at/pages/supplementary/107S_refless.html)

# Hermite functions/1

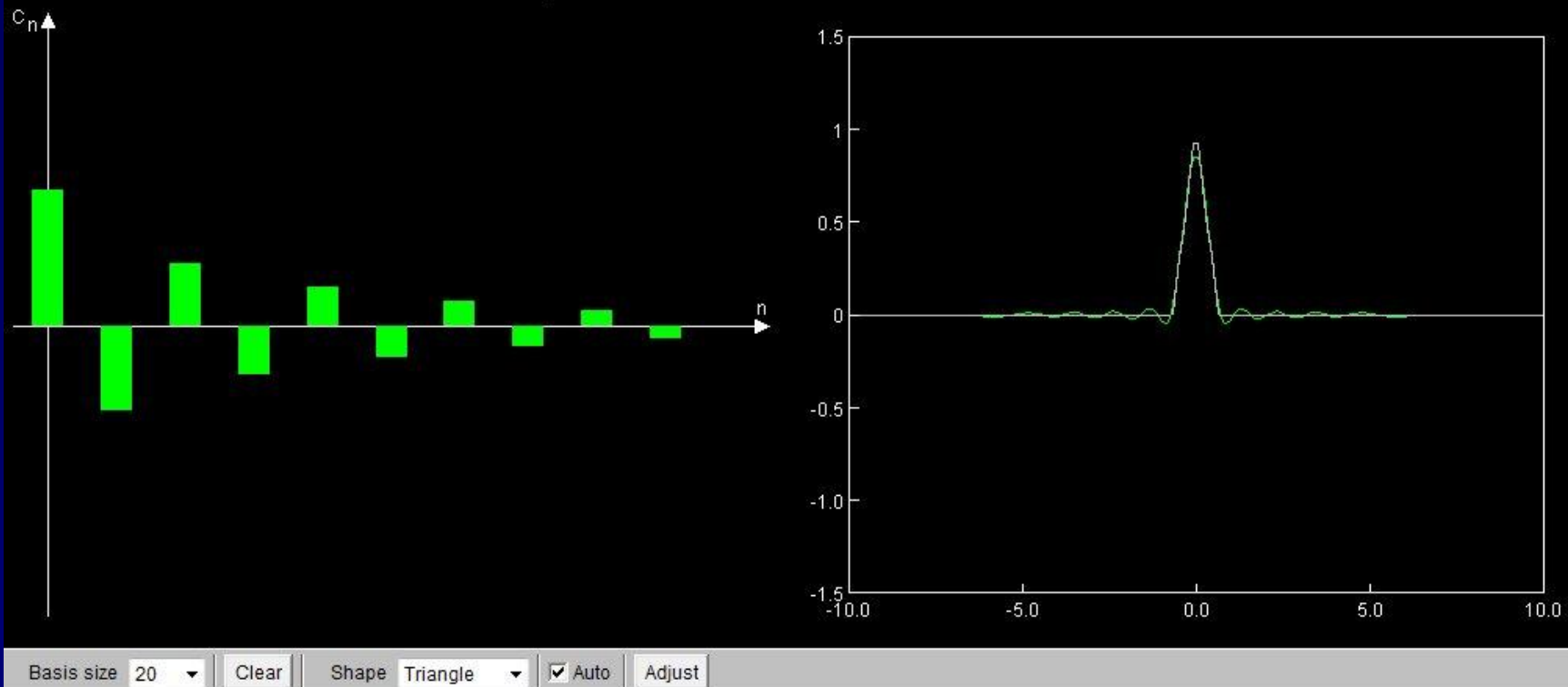
Quantization in one dimension : Superposition of Hermite functions



This simulation allows to sum Hermite functions by changing the coefficient of the sum in the left window. These coefficients are assumed to be real. The obtained function is plotted in green in the right window. Try to generate functions of arbitrary shape.

# Hermite functions/2

Quantization in one dimension : Decomposition on the Hermite basis

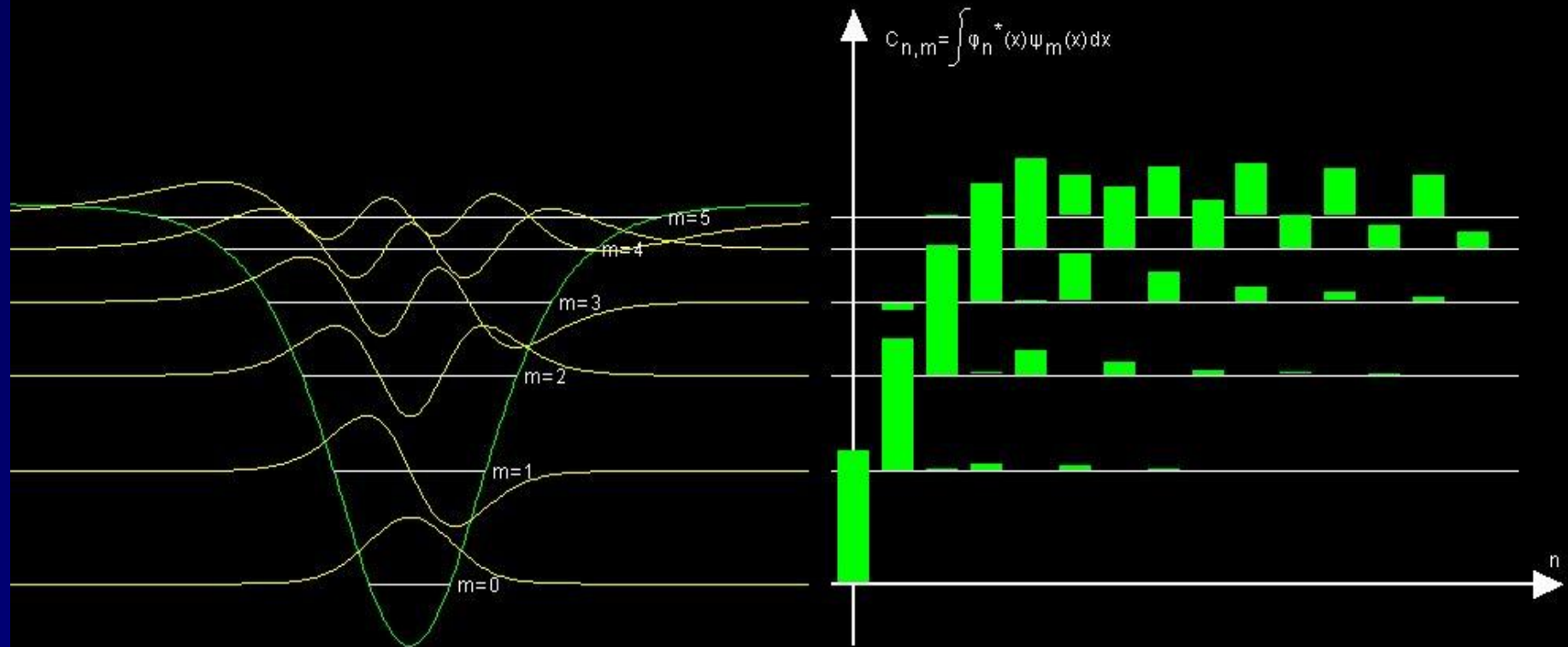


Being the eigenstates of the harmonic oscillator, a set of Hermite functions is a basis of the Hilbert state. This amazing consequence of Hilbert mathematics is illustrated here where you can change a target function chosen among a rectangle, a triangle and a gaussian by changing its center and width.

In fact, the decomposition is exact only when an infinite number of basis functions is used. When truncating the basis to a finite number of element, the decomposition is only approximate.

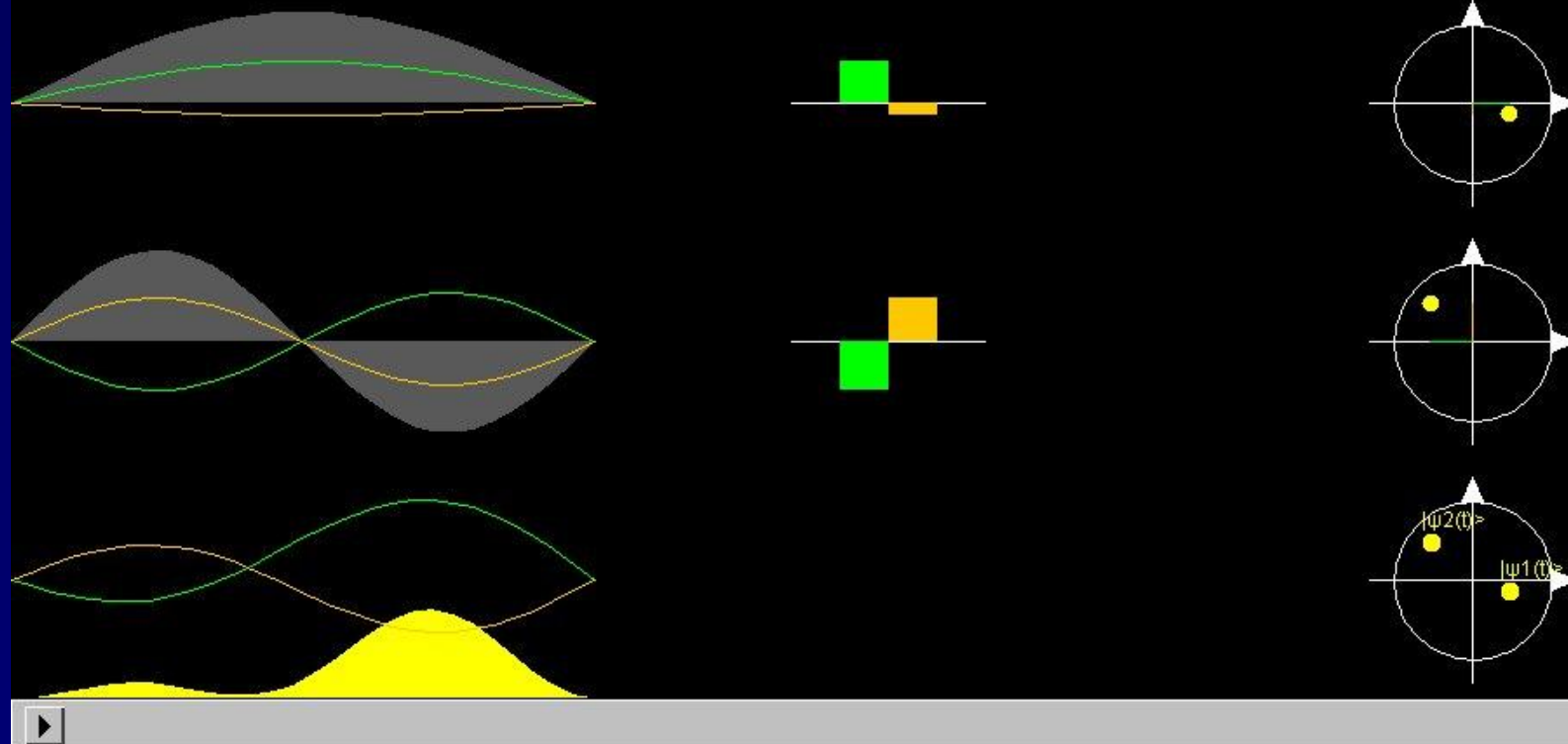
# Hermite functions/3

Quantization in one dimension : Decomposition of an eigenbasis



# Superposition in 1D

Quantum superposition in one dimension : Superposition of two stationary states

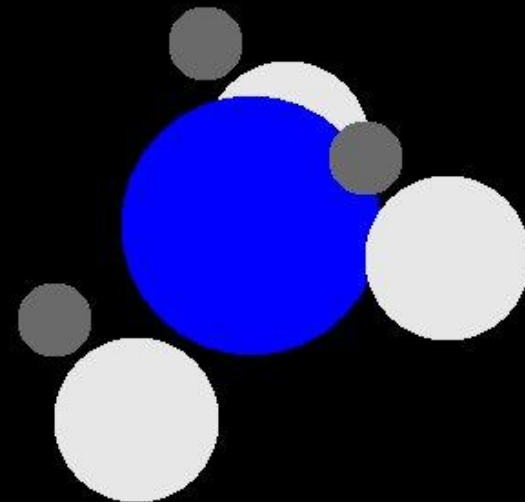
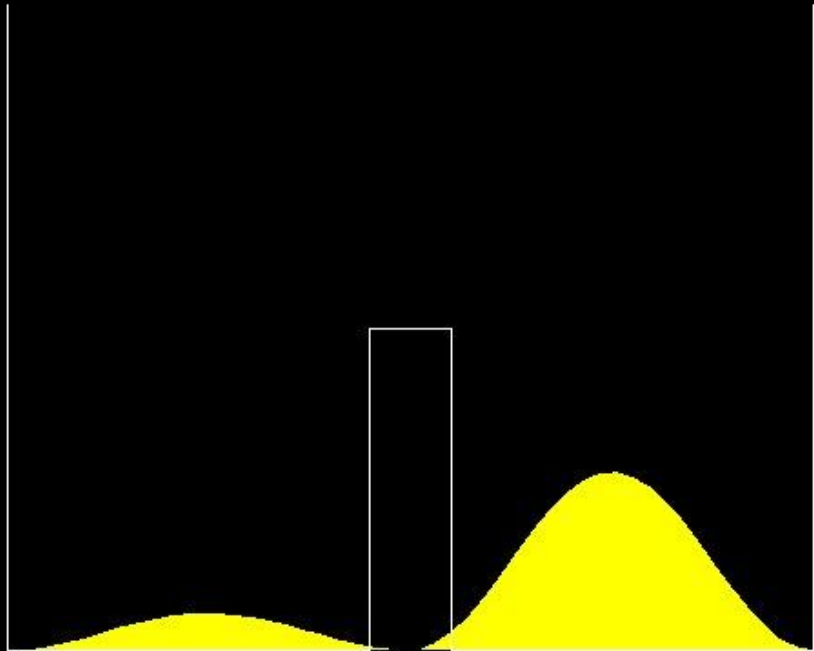


Let us now consider the linear superposition of the two previous stationary states:  $\psi(x,t) = C_1(t) \psi_1(x) + C_2(t) \psi_2(x)$ . By manually changing  $C_1$  and  $C_2$  you can observe that when the two coefficients are in phase, the eigenfunctions interfere constructively on the left side while they interfere destructively on the right side, because  $\psi_1(x) + \psi_2(x)$  takes greater values on the left side. The particle has a greater probability to be detected on the left side. In contrast, when  $C_1$  and  $C_2$  are in opposition, the eigenfunctions interfere destructively on the left and constructively on the right, because  $\psi_1(x) - \psi_2(x)$  takes greater values on the right. The particle has a greater probability to be detected on the right side.

By starting the animation, you can observe that  $C_1(t)$  and  $C_2(t)$  are alternatively in phase and in opposition, which result in an oscillation of the average position at frequency  $\omega_2 - \omega_1$ . The linear superposition of two stationary states of different energies is no longer a stationary state.

# Ammonia oscillations

Quantum superposition in one dimension : NH<sub>3</sub> oscillations



Other vision

This applet shows the evolution of NH<sub>3</sub> when its state is a linear superposition of the first two eigenstates with equal weights. On the left is a double-well model of the molecule oscillations, while the right panel attempt to show a representation of the molecule itself.

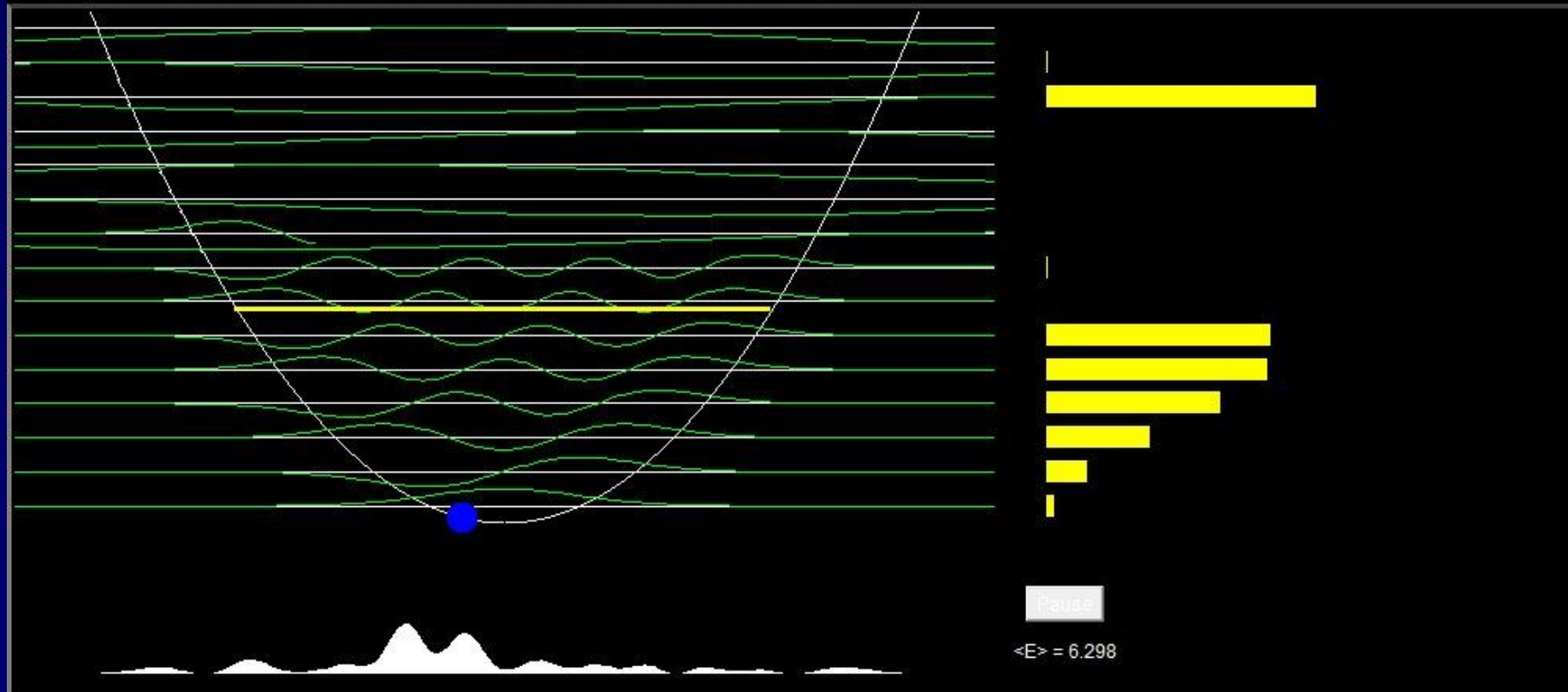
Of the two representations which you can choose by pushing the button on the toolbar, which do you think is closer to the truth ?



# Harmonic oscillator

3.6

## Quantum superposition in one dimension : Harmonic oscillator



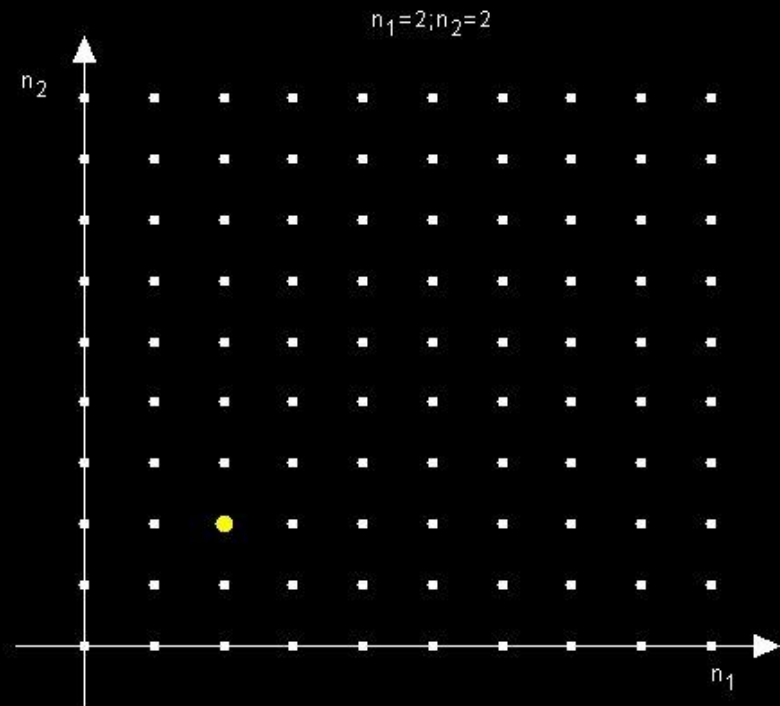
This simulation shows the evolution of a harmonic oscillator when the initial state is a linear superposition of several stationary states. You can change the relative weights of the different levels directly by dragging the horizontal bars with the mouse. The program then shows the average energy (horizontal yellow line), the average position (blue dot), and the probability density. According to the Ehrenfest theorem, the blue dot undergoes a classical harmonic motion, corresponding here to a sinusoidal oscillation in an harmonic potential.

You can also directly change the average energy by dragging the horizontal line to the target value. The simulator then puts the system in the quasi-classical state, or coherent state, with the energy you have set. Such a state, usually called  $|\alpha\rangle$ , exhibits the following properties:

- This is an eigenstate of the annihilation operator:  $a|\alpha\rangle = \alpha|\alpha\rangle$ . - The product  $\Delta n \Delta \phi = \hbar/2$ , i.e. the smallest possible value according to the

# 2D harmonic oscillator

Quantum superposition in two dimensions : Two-dimension harmonic oscillator

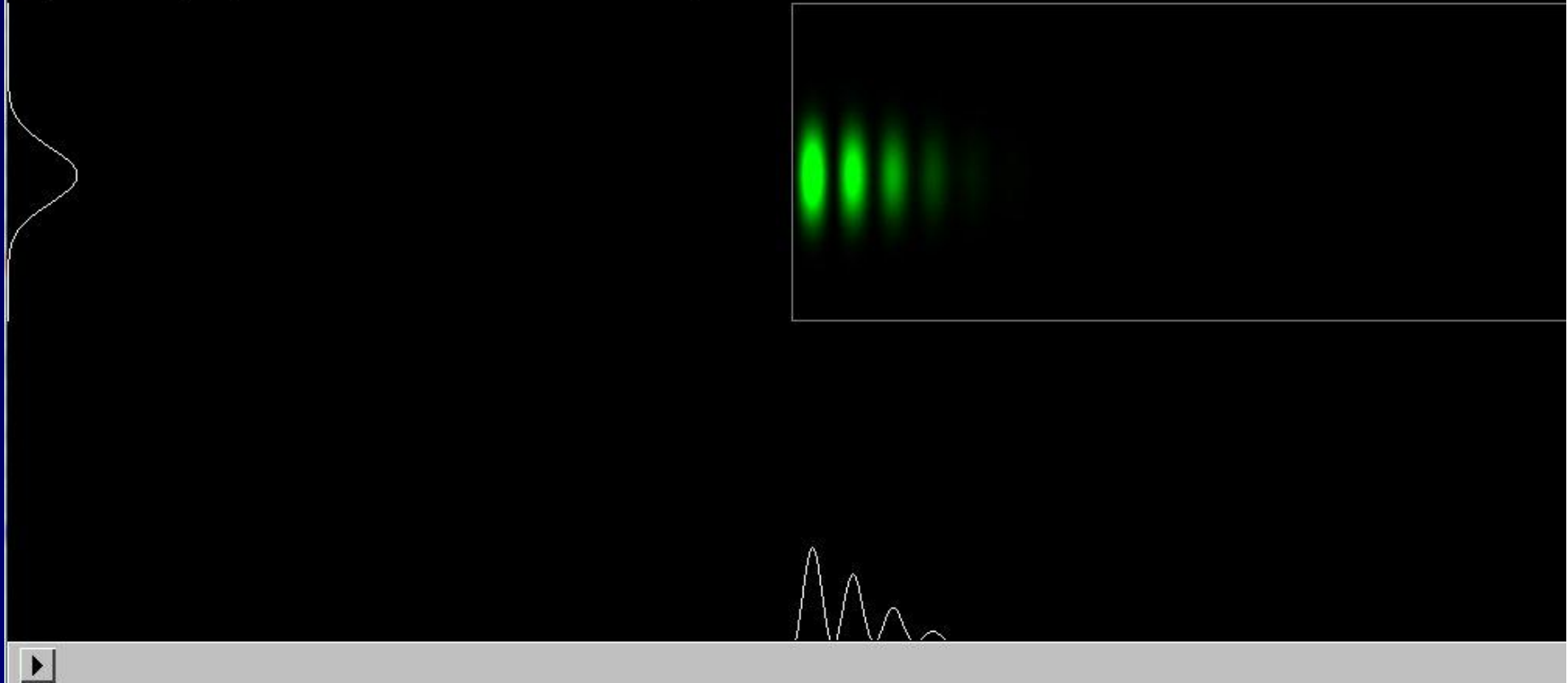


The potential is now a two-dimension harmonic potential. As in the previous case, you can select the eigenstate by clicking in the right panel.

# 2D quantum box

4.5

Quantum superposition in two dimensions : Wavepacket in a box

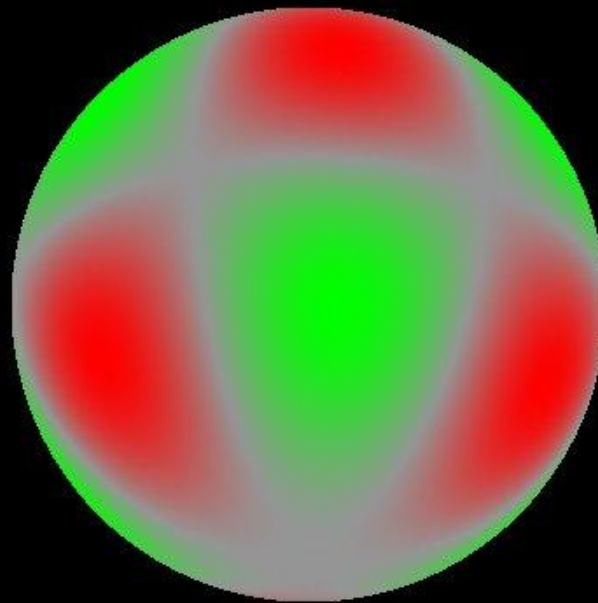


Propagation of a gaussian wavepacket in a 2D box. In agreement with the Ehrenfest theorem, the wavepacket center moves like a classical particle, bouncing on the walls of the box. Quantum mechanics manifests itself through the interferences between the incident and reflected waves, and through the spreading of the wavepacket, similarly to what we observed in one dimension.

NB: The parameters of the simulation are not quite right. In reality, such a wavepacket would need a much smaller value of the wavelength in order to spread so slowly. The size of the wavelength has been enlarged so that interferences could be seen on such a low-resolution image.

# 3D - spherical harmonics

Quantization in three dimensions : Spherical harmonics



☐ Complex    L = 4    +    -    M = 3    +    -

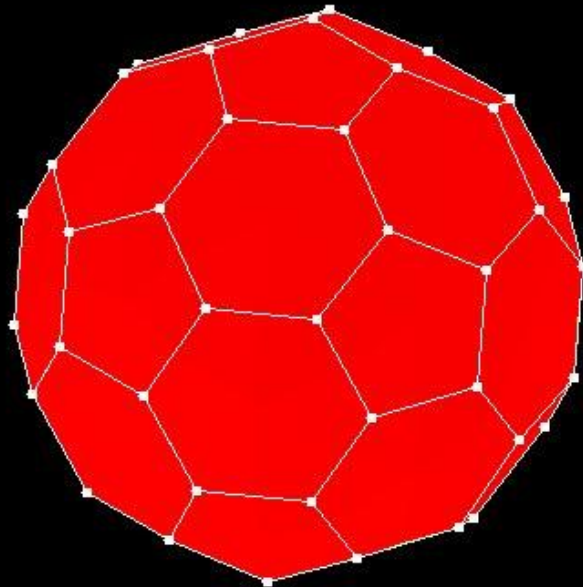
This simulator shows spherical harmonics plotted on a sphere. For each point of spherical coordinates  $(\theta, \phi)$ , the corresponding value of the spherical harmonic  $Y(L,M)$  is plotted. In real mode, the real quantity  $Y(L,M)+Y(L,-M)$  is plotted, in red or blue depending on its sign. Note the analogy with a sine wave rolled round the sphere. A spherical harmonic is the spherical equivalent of a Fourier series.

In complex mode,  $Y(L,M)$  is directly shown, the phase being color coded.

The orientation of the sphere can be set using the mouse.

# 3D - Fullerene

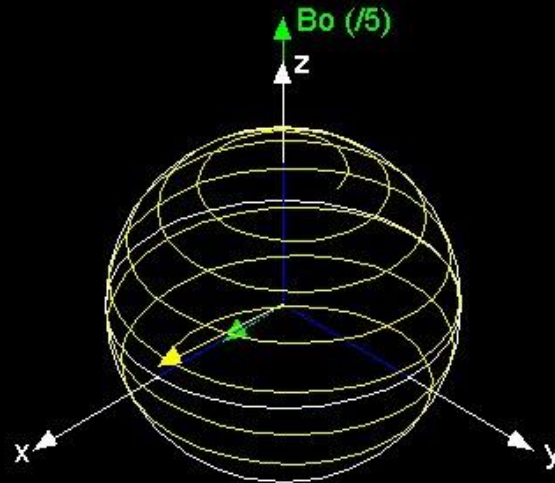
Quantization in three dimensions : Carbon 60



The electronic states of C60 can be simulated using the Hückel model. The corresponding 60x60 matrix is shown on the right side. The non-zero elements, shown by a yellow dot, correspond to two nearest neighbors. As each carbon atom has three neighbors, there are three non-zero elements per line. This matrix can be diagonalized numerically by clicking on the button. The energy levels are then shown on the right side.

# NMR

## Spin 1/2 : Magnetic resonance



$\omega_1/\omega_0$  0.05

$\omega/\omega_0$  1.0

This animation illustrates magnetic resonance, namely the evolution of a spin in a strong magnetic field  $B_0$  applied additionally to a rotating magnetic field  $B_1$ , perpendicular to  $B_0$ . When the frequency  $\omega$  of the rotating field is exactly equal to Larmor frequency, magnetic resonance is achieved. The spin then goes slowly but surely from state  $|-\rangle$  to state  $|+\rangle$ , and vice-versa. In contrast, if the frequency of the rotating field is not tuned to Larmor frequency,  $\langle S_z \rangle$  oscillates only a tiny little bit around its average value (try for example  $\omega/\omega_0 = 3.5$ ).

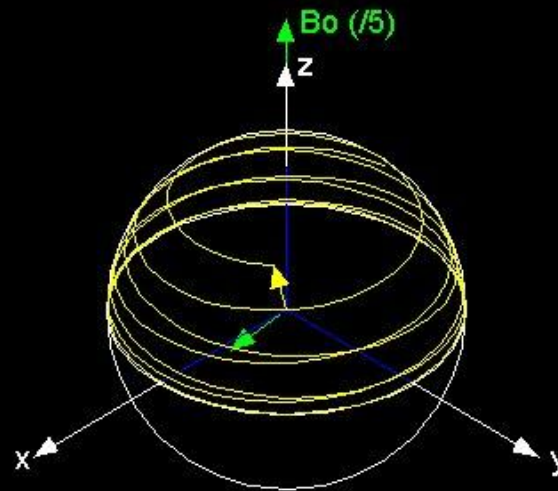
Note that the field magnitudes are expressed in frequency units according to the relations  $\hbar\omega_0 = \gamma B_0$  and  $\hbar\omega_1 = \gamma B_1$ , where  $\gamma$  is the gyromagnetic ratio. You can change the ratios  $\omega_1/\omega_0$  and  $\omega/\omega_0$  by entering new values with the keyboard and pressing the Enter key.



# NMR

Spin 1/2 : Magnetic resonance

Spin 1/2 : Magnetic resonance



$\omega_1/\omega_0$  0.05

$\omega/\omega_0$  1.1

This animation illustrates magnetic resonance, namely the evolution of a spin in a strong magnetic field  $B_0$  applied additionally to a rotating magnetic field  $B_1$ , perpendicular to  $B_0$ . When the frequency  $\omega$  of the rotating field is exactly equal to Larmor frequency, magnetic resonance is achieved. The spin then goes slowly but surely from state  $|-\rangle$  to state  $|+\rangle$ , and vice-versa. In contrast, if the frequency of the rotating field is not tuned to Larmor frequency,  $\langle S_z \rangle$  oscillates only a tiny little bit around its average value (try for example  $\omega/\omega_0=3.5$  ).

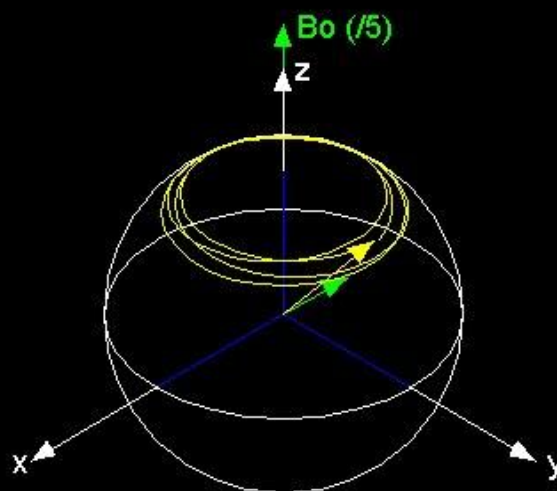
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# NMR

Spin 1/2 : Magnetic resonance

Spin 1/2 : Magnetic resonance

Spin 1/2 : Magnetic resonance



$\omega_1/\omega_0$  0.05

$\omega/\omega_0$  1.6

This  
field  
spin  
fre  
No  
Yo

This

This animation illustrates magnetic resonance, namely the evolution of a spin in a strong magnetic field  $B_0$  applied additionally to a rotating magnetic spin field  $B_1$ , perpendicular to  $B_0$ . When the frequency  $\omega$  of the rotating field is exactly equal to Larmor frequency, magnetic resonance is achieved. The spin then goes slowly but surely from state  $|-\rangle$  to state  $|+\rangle$ , and vice-versa. In contrast, if the frequency of the rotating field is not tuned to Larmor frequency,  $\langle S_z \rangle$  oscillates only a tiny little bit around its average value (try for example  $\omega/\omega_0 = 3.5$ ).

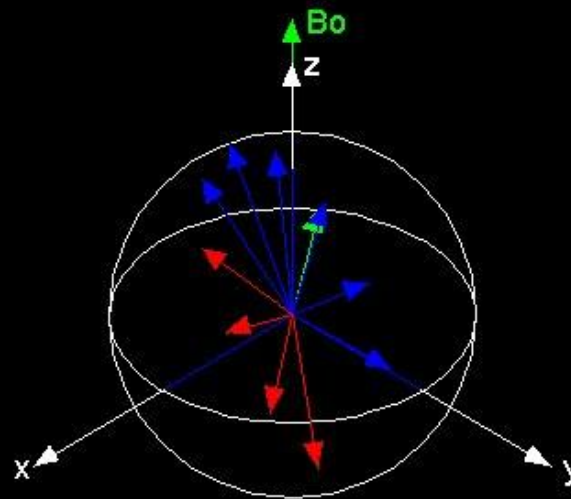
Note You Note that the field magnitudes are expressed in frequency units according to the relations  $\hbar\omega_0 = \gamma B_0$  and  $\hbar\omega_1 = \gamma B_1$ , where  $\gamma$  is the gyromagnetic ratio. You can change the ratios  $\omega_1/\omega_0$  and  $\omega/\omega_0$  by entering new values with the keyboard and pressing the Enter key.

# NMR

Spin 1/2 : Magnetic resonance

Spin 1/2 : Magnetic resonance

Spin 1/2 : Spin echo



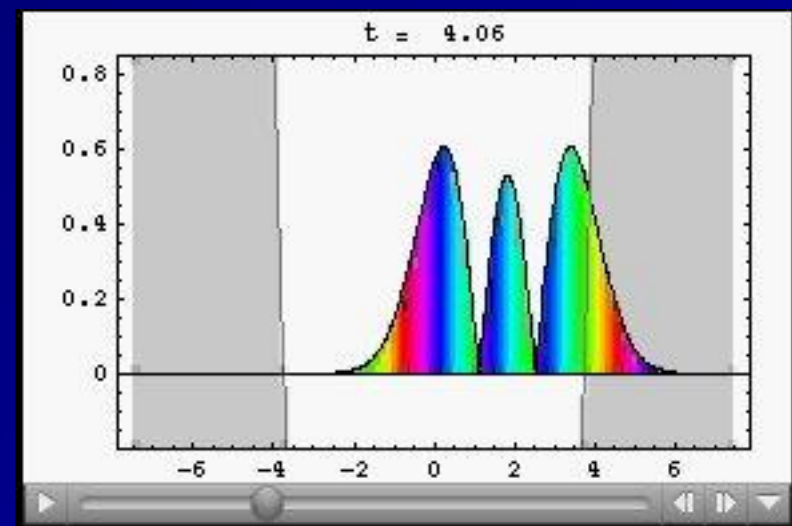
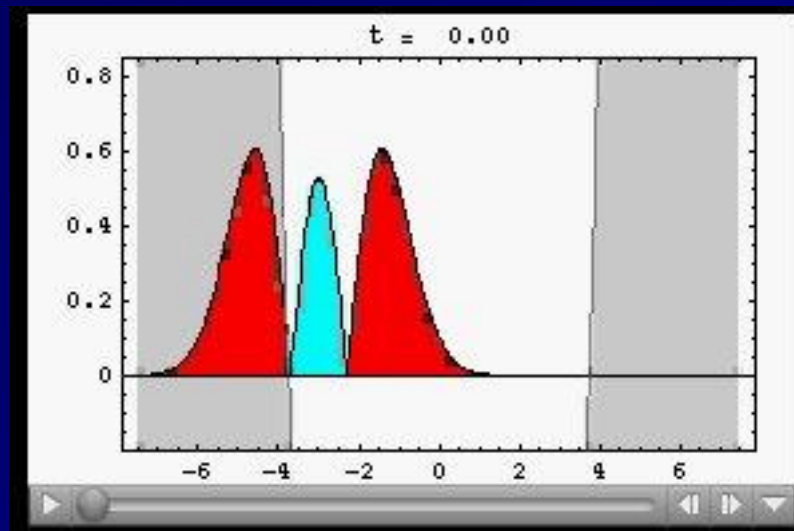
Stop Pi

Spin echo consists of applying a sequence of two magnetic pulses to an inhomogeneous spin assembly, as described below.

- 1) You first apply a  $\pi/2$  pulse, which puts the system in a superposition of states  $|-\rangle$  and  $|+\rangle$ .
- 2) Due to Larmor precession, the spin average value rotates around the vertical axis. However, due to a spatial inhomogeneity - for example in the applied  $B_0$  field - the Larmor frequency is not the same for all spins. Some of them (shown here in blue) precess more slowly than others (shown in red). Consequently, the total magnetization induced in the sample decays.
- 3) After a time delay  $T$ , a  $\pi$  pulse is applied to the spin assembly. The resulting  $\pi$  precession flips the spin in the equatorial plane. The faster spins are now behind the slower ones.

# „Visual Quantum Mechanics”

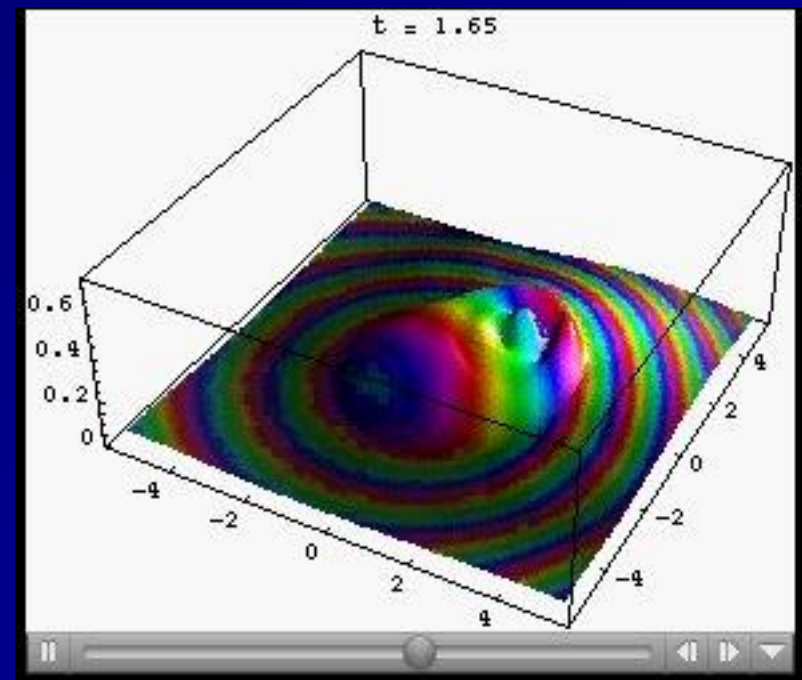
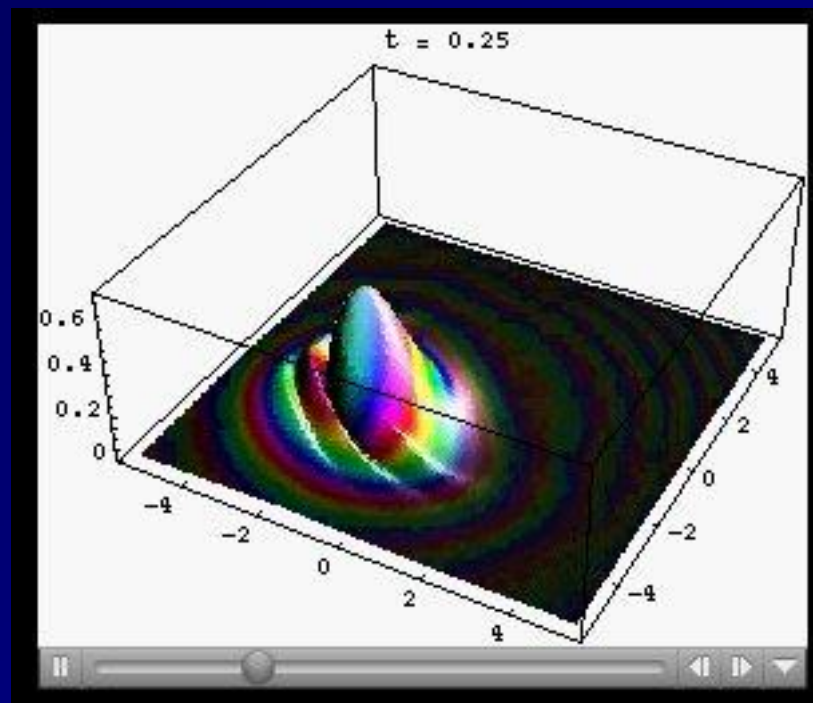
## Eigen state in harmonic potential



■ [http://vqm.uni-graz.at/pages/samples/105\\_19b.html](http://vqm.uni-graz.at/pages/samples/105_19b.html)

# Visual Quantum Mechanics

## Scattering on a cylindrical barrier



■ [http://vqm.uni-graz.at/pages/samples/107\\_17s.html](http://vqm.uni-graz.at/pages/samples/107_17s.html)



# Ionization of H by electron impact

etc., etc.

