

# Harmonic oscillator

## Notes on Quantum Mechanics

<http://quantum.bu.edu/notes/QuantumMechanics/HarmonicOscillator.pdf>  
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Department of Chemistry, Boston University, Boston MA 02215

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### ■ Classical harmonic motion

The harmonic oscillator is one of the most important model systems in quantum mechanics. An harmonic oscillator is a particle subject to a restoring force that is proportional to the displacement of the particle. In *classical physics* this means

$$F = m a = m \frac{d^2 x}{dt^2} = -k x$$

The constant  $k$  is known as the force constant; the larger the force constant, the larger the restoring force for a given displacement from the equilibrium position (here taken to be  $x = 0$ ). A simple solution to this equation is that the displacement  $x$  is given by

$$x = \sin(\sqrt{k/m} t),$$

since

$$\begin{aligned} m \frac{d^2 x}{dt^2} &= m \frac{d^2}{dt^2} \sin(\sqrt{k/m} t) \\ &= -m(\sqrt{k/m})^2 \sin(\sqrt{k/m} t) \\ &= -k \sin(\sqrt{k/m} t) \\ &= -k x. \end{aligned}$$

The quantity  $\sqrt{k/m}$  plays the role of an angular frequency,

$$\omega = 2 \pi \nu = \sqrt{k/m}.$$

The larger the force constant, the higher the oscillation frequency; the larger the mass, the smaller the oscillation frequency.

### ■ Schrödinger equation

The study of *quantum mechanical* harmonic motion begins with the specification of the Schrödinger equation. The linear restoring forces means the classical potential energy is

$$V = - \int F dx = - \int (-k x) dx = \frac{1}{2} k x^2,$$

and so we can write down the Schrödinger equation as

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} k x^2\right) \psi(x) = E \psi(x).$$

Next, it will be helpful to transform this equation to dimensionless units. We could use the same length and energy units that we have used for the particle in a box and for the one-electron atom, but there is a different set of units that is more natural to harmonic motion.

Since harmonic motion has a characteristic angular frequency,  $\omega = \sqrt{k/m}$ , it makes sense to measure energy in terms of  $\omega$ . It turns out that the choice  $\hbar \omega/2$  works well. (The choice  $\hbar \omega$  would seem more obvious, but the factor of 1/2 simplifies things somewhat.) Next, we can use the energy unit to determine the length unit. Specifically, let's use for the unit of length the amount by which the oscillator must be displaced from equilibrium ( $x = 0$ ) in order for the potential energy to be equal to the energy unit. That is, the unit of length,  $x_0$ , satisfies

$$\frac{\hbar \omega}{2} = \frac{1}{2} k x_0^2 = \frac{1}{2} m \omega^2 x_0^2$$

and so

$$x_0 = \sqrt{\frac{\hbar}{m \omega}}$$

This means we can express energy as

$$E = \frac{\hbar \omega}{2} \epsilon$$

in terms of dimensionless multiples  $\epsilon$  of  $\hbar \omega/2$ , and length as

$$x = \sqrt{\frac{\hbar}{m \omega}} \rho$$

in terms of dimensionless multiples  $\rho$  of  $\sqrt{\hbar/m\omega}$ . In these dimensionless units, the Schrödinger equation becomes

$$\frac{d^2}{d\rho^2} \psi(\rho) = -t(\rho) \psi(\rho),$$

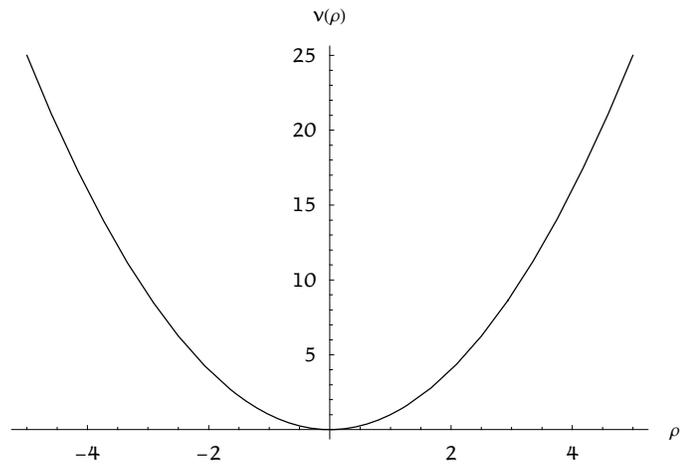
in terms of the dimensionless kinetic energy

$$t(\rho) = \epsilon - \rho^2.$$

Verify that the Schrödinger equation has this form in the dimensionless units of energy and length that we have chosen.

Show that the length unit,  $x_0 = \sqrt{\hbar/m\omega}$ , can be written alternatively as  $\sqrt{\hbar\omega/k}$  and  $\sqrt{\hbar/\sqrt{k m}}$ .

Here is a plot of the dimensionless potential energy.



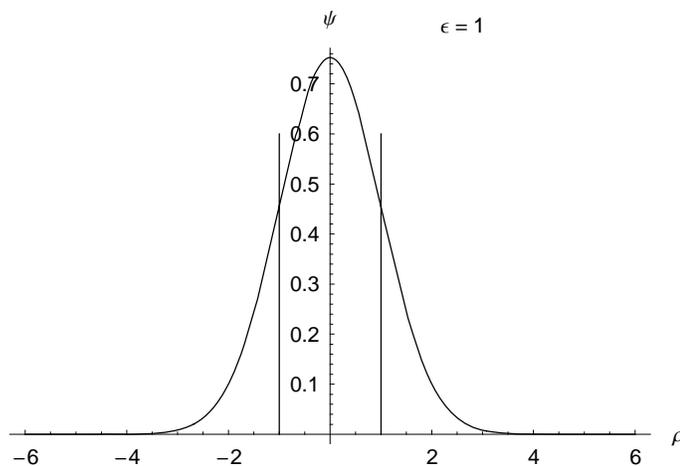
Harmonic potential energy, in units  $\hbar\omega/2$ . Length  $\rho$  is in units  $\sqrt{\hbar/m\omega}$ .

## ■ Energies and wavefunctions

It turns out that the quantal energies in the harmonic potential are

$$\epsilon_j = 2j - 1,$$

where  $j$  is the number of loops in the wavefunction. Here is the lowest energy wavefunction—the wavefunction with one loop. (This and the following example wavefunctions in this part are determined by Numerov integration of the Schrödinger equation.)



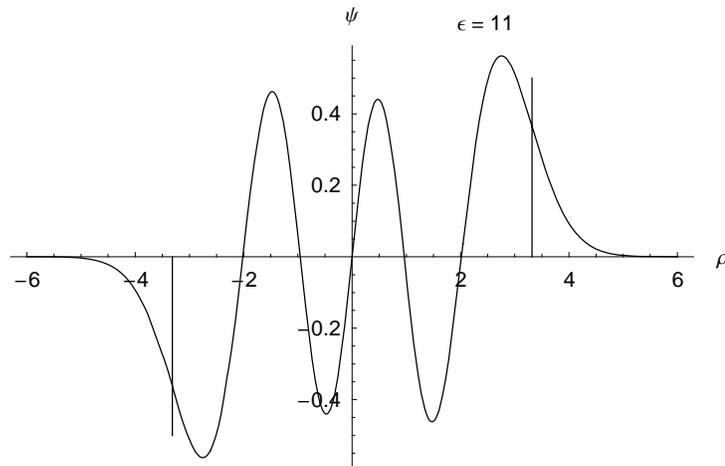
Lowest energy harmonic oscillator wavefunction. The energy is  $2 \times 1 - 1 = 1$ , in units  $\hbar\omega/2$ . Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$ . The vertical lines mark the classical turning points.

The vertical lines mark the classical turning points, that is, the displacements for which the harmonic potential equals the energy.

```
turn[j_] := ρ /. Solve[ρ2 == 2 j - 1, ρ] // Evaluate;
turn[j]
```

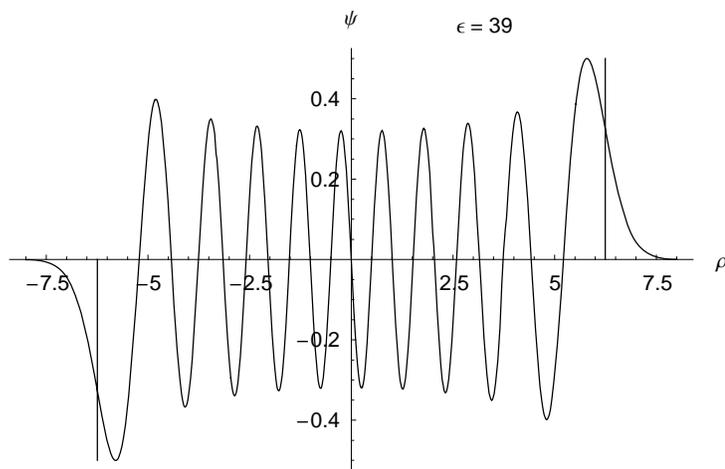
```
{-√(-1 + 2 j), √(-1 + 2 j)}
```

Here is the sixth lowest energy wavefunction,



Sixth lowest energy harmonic oscillator wavefunction. The energy is  $2 \times 6 - 1 = 11$ , in units  $\hbar \omega / 2$ . Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar / m \omega}$ . The vertical lines mark the classical turning points.

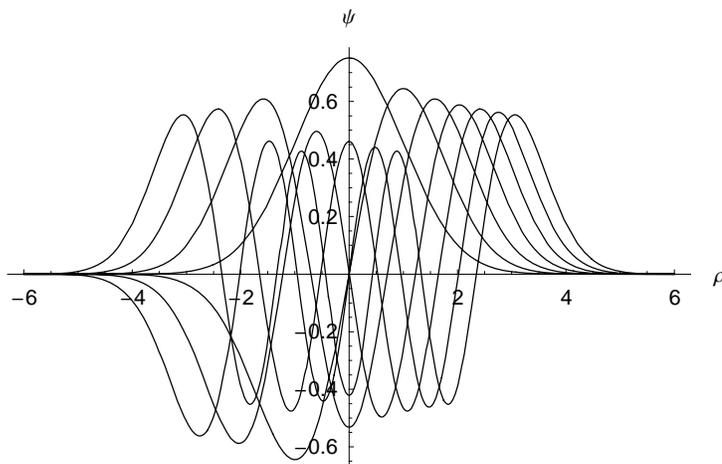
and here is the 20th lowest energy wavefunction,



20th lowest energy harmonic oscillator wavefunction. The energy is  $2 \times 10 - 1 = 19$ , in units  $\hbar \omega / 2$ . Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar / m \omega}$ . The vertical lines mark the classical turning points.

This wavefunction shows clearly the general feature of harmonic oscillator wavefunctions, that the oscillations in wavefunction have the smallest amplitude and loop length near  $\rho = 0$ , where the kinetic energy is largest, and the largest amplitude and loop length near the classical turning points, where the kinetic energy is near zero.

Finally, here are the seven lowest energy wavefunctions.



Seven lowest energy harmonic oscillator wavefunctions. The energies are  $2 \times j - 1 = 1, 3, \dots, 13$ , in units  $\hbar\omega/2$ . Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$ . The vertical lines mark the classical turning points.

## ■ Absolute units

We have expressed energy as

$$E = \frac{\hbar\omega}{2} \epsilon,$$

in terms of dimensionless multiples  $\epsilon$  of  $\hbar\omega/2$ , and length as

$$x = \sqrt{\frac{\hbar}{m\omega}} \rho,$$

in terms of dimensionless multiples  $\rho$  of  $\sqrt{\hbar/m\omega}$ . To get a feeling for these units, let's see how they translate into actual energies and length for particular molecules.

The atoms in hydrogen halide molecules, HF, HCl, etc., vibrate approximately harmonically about their equilibrium separation. The mass undergoing the harmonic motion is the *reduced mass* of the molecule,

$$\mu = \frac{m_a m_b}{m_a + m_b}$$

(I remember that the product of the masses goes in the numerator since the ratio must have units of mass.) To calculate the reduced mass we need to determine the mass of each atom, and to do this, we need to know which isotope of each atom is present in the molecule.

Recall that isotope masses are given in units of atomic mass,  $u$ . The atomic mass unit is defined such that the mass of exactly one gram of carbon 12 is Avogadro's number times  $u$ . This means that the atomic mass unit is

$$u = \frac{1 \text{ Gram / Mole}}{\text{AvogadroConstant}} / . \text{ Gram} \rightarrow 10^{-3} \text{ Kilogram}$$

$$1.66054 \times 10^{-27} \text{ Kilogram}$$

Let's calculate the reduced mass for HCl. If we use the most stable isotope of each atom,  $^1\text{H}$  and  $^{35}\text{Cl}$ , the result is

$$\mu_{\text{H}^{35}\text{Cl}} = \left( \frac{m_{\text{H}} m_{\text{Cl}}}{m_{\text{H}} + m_{\text{Cl}}} \right) / \text{AvogadroConstant} // . \{$$

$$m_{\text{H}} \rightarrow 1.0078 \text{ Gram / Mole},$$

$$m_{\text{Cl}} \rightarrow 34.9688 \text{ Gram / Mole},$$

$$\text{Gram} \rightarrow 10^{-3} \text{ Kilogram}$$

$$\}$$

$$1.62661 \times 10^{-27} \text{ Kilogram}$$

Here are the reduced masses for other combinations of isotopes, together with that for  $^1\text{H}^{35}\text{Cl}$ .

$$^1\text{H}^{35}\text{Cl} \quad 1.62661 \times 10^{-27} \text{ Kilogram}$$

$$^1\text{H}^{37}\text{Cl} \quad 1.62908 \times 10^{-27} \text{ Kilogram}$$

$$^2\text{H}^{35}\text{Cl} \quad 3.1622 \times 10^{-27} \text{ Kilogram}$$

$$^2\text{H}^{37}\text{Cl} \quad 3.17153 \times 10^{-27} \text{ Kilogram}$$

Confirm that these results are correct.

The effect a change in the lighter isotope is larger than the effect of a change in the heavier isotope.

Show why this is so.

The next step is to determine the harmonic angular frequency,  $\omega = 2\pi\nu$ . This is done by measuring the frequency of light that causes the molecule to change its vibrational wavefunction by one loop, since

$$\Delta E_{\text{matter}} = \hbar \omega = h \nu.$$

For  $^1\text{H}^{35}\text{Cl}$  the measured value is  $\tilde{\nu} = 2990 \text{ cm}^{-1}$ . The unit  $\tilde{\nu}$  is the reciprocal wavelength, corresponding to the frequency,

$$\tilde{\nu} = \frac{1}{\lambda} = \frac{1}{c/\nu} = \frac{\nu}{c}.$$

This means that angular frequency is related to wavenumber as

$$\omega = 2\pi\nu = 2\pi \frac{c}{\lambda} = 2\pi c \tilde{\nu}.$$

Hence, the angular frequency of harmonic motion in  $^1\text{H}^{35}\text{Cl}$  is

$$\frac{5.63212 \times 10^{14}}{\text{Second}}$$

Verify this result.

Note that this value properly corresponds to the IR spectral region.

Having determined the oscillator mass and angular frequency, we can evaluate its length unit,

$$x_0 = \sqrt{\hbar/m\omega}.$$

$$0.10729 \text{ \AA}$$

To interpret this result, recall that we have defined the unit of length so that when the oscillator is displaced this distance from its equilibrium point, the potential energy equals the zero-point energy. That is,  $x_0$  is the classical turning point of the oscillation when the oscillator wavefunction has 1 loop. This means that when  $^1\text{H}^{35}\text{Cl}$  is in its ground state its classically allowed region is  $2x_0 = 0.21458 \text{ \AA}$  wide. The equilibrium internuclear distance of HCl is  $1.27 \text{ \AA}$ , and so ground state harmonic motion expands and compresses the bond by a bit less than 10%.

Evaluate  $x_0$  for  ${}^1\text{H}^{81}\text{Br}$  ( $\tilde{\nu} = 2650\text{ cm}^{-1}$ ) and  ${}^1\text{H}^{127}\text{I}$  ( $\tilde{\nu} = 2310\text{ cm}^{-1}$ ), and analyze your results in comparison to the value for  ${}^1\text{H}^{35}\text{Cl}$ .

Here are the answers I get.

	$\mu$	$\omega$	$x_0$
${}^1\text{H}^{35}\text{Cl}$	$1.62661 \times 10^{-27}$	$5.63212 \times 10^{14}$	$0.10729\text{ \AA}$
${}^1\text{H}^{81}\text{Br}$	$1.6529 \times 10^{-27}$	$4.99168 \times 10^{14}$	$0.113055\text{ \AA}$
${}^1\text{H}^{127}\text{I}$	$1.66031 \times 10^{-27}$	$4.35124 \times 10^{14}$	$0.12082\text{ \AA}$

### Comparison of HCl, HBr and HI

Plot, on the same set of axes, the harmonic potential for HCl, HBr, and HI. Measure length in  $\text{\AA}$ . Indicate the first four energy levels of each potential curve. Do this using horizontal lines spanning the allowed region at each energy on each curve. Measure energy in units of the zero-point energy of HCl. In a separate table give energies (in units of the zero-point energy of HCl) and the right side ( $x > 0$ ) classical turning point (in  $\text{\AA}$ ) for the first four energy levels of each molecule.

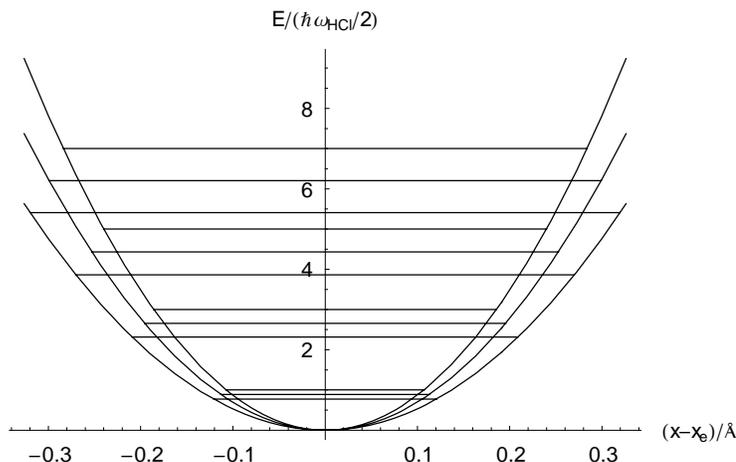
Here are the expressions I get for the potential curve, with distance,  $x$ , in  $\text{\AA}$  and energy in units of the zero-point energy of HCl.

${}^1\text{H}^{35}\text{Cl}$	$86.872 x^2$
${}^1\text{H}^{81}\text{Br}$	$69.3414 x^2$
${}^1\text{H}^{127}\text{I}$	$52.9255 x^2$

Verify that, for HCl, when the displacement is its distance unit,  $x_0 = 0.10729\text{ \AA}$ , the potential energy is 1, since we are using as energy unit the zero-point energy of HCl. *Hint:* Evaluate  $k/2$  in  $\text{J m}^{-2}$ , divide it by the zero point energy,  $\hbar\omega/2$  in J, and then convert the result from  $\text{m}^{-2}$  to  $\text{\AA}^{-2}$ .

These potential energy expressions show that the force constant,  $k$ , decreases going from HCl to HI. Evaluate the force constant for each molecules, in  $\text{J m}^{-2} = \text{kg s}^{-2}$ . Answer: 516.0, 411.9, 314.4.

Here is the plot of the results I get.



Harmonic potential energy curves and lowest four harmonic energy levels (horizontal lines) for  $^1\text{H}^{35}\text{Cl}$  ( $\bar{\nu} = 2990\text{ cm}^{-1}$ ),  $^1\text{H}^{81}\text{Br}$  ( $\bar{\nu} = 2650\text{ cm}^{-1}$ ) and  $^1\text{H}^{127}\text{I}$  ( $\bar{\nu} = 2310\text{ cm}^{-1}$ ). Energy is in units of the zero-point energy of  $^1\text{H}^{35}\text{Cl}$ ,  $2.969 \times 10^{-20}\text{ J}$ .

Here is the tabulation of energies and right side turning points for the lowest four levels of each molecule.

	loops (j)	$E_j / (\hbar\omega_{\text{HCl}}/2)$	$x_{\text{tp}}/\text{\AA}$
$^1\text{H}^{35}\text{Cl}$	1	1.	0.10729
	2	3.	0.185832
	3	5.	0.239908
	4	7.	0.283863
$^1\text{H}^{81}\text{Br}$	1	0.886288	0.113055
	2	2.65886	0.195818
	3	4.43144	0.252799
	4	6.20401	0.299116
$^1\text{H}^{127}\text{I}$	1	0.772575	0.12082
	2	2.31773	0.209266
	3	3.86288	0.270161
	4	5.40803	0.319659

Lowest four harmonic energy levels and right side classical turning points for  $^1\text{H}^{35}\text{Cl}$  ( $\bar{\nu} = 2990\text{ cm}^{-1}$ ),  $^1\text{H}^{81}\text{Br}$  ( $\bar{\nu} = 2650\text{ cm}^{-1}$ ) and  $^1\text{H}^{127}\text{I}$  ( $\bar{\nu} = 2310\text{ cm}^{-1}$ ). Energy is in units of the zero-point energy of  $^1\text{H}^{35}\text{Cl}$ ,  $2.969 \times 10^{-20}\text{ J}$ .

The results reflect the effects of the decreasing harmonic frequency going from HCl to HI: The force constant decreases, and so the harmonic potential energy curve rises less steeply on either side of its minimum, with the result that turning points are farther apart and so a wider allowed region at a given total energy. The effect is an increase in loop length and so a lowering of energy for a given number of loops, analogous to the energy lowering in an infinite well when the well width is increased.

Now, here are two final questions to consider.

Show that the decrease in harmonic frequency,  $\omega$ , and so in the force constant,  $k$ , going from HCl to HI *cannot* be due to the increasing reduced mass alone. Hint: Compare the change in harmonic frequency expected due to mass alone to the actual change in harmonic frequency. Answer: Relative frequency expected due to reduced mass: 1, 0.9920, 0.9898; actual relative frequency: 1, 0.8863, 0.7726.

What do you suppose the decrease in force constant *is* due to?

## ■ Analytic wavefunctions

It turns out that the harmonic oscillator Schrödinger equation can be solved analytically. The wave functions have the general form

$$\psi_j(\rho) = \frac{1}{\sqrt{2^{j-1} (j-1)! \sqrt{\pi}}} H_{j-1}(\rho) e^{-\rho^2/2}$$

in terms of *Hermite polynomials*,  $H_{j-1}(\rho)$ . Here are the first few Hermite polynomials.

loops	Hermite polynomial
1	1
2	$2\rho$
3	$-2 + 4\rho^2$
4	$-12\rho + 8\rho^3$
5	$12 - 48\rho^2 + 16\rho^4$
6	$120\rho - 160\rho^3 + 32\rho^5$
7	$-120 + 720\rho^2 - 480\rho^4 + 64\rho^6$

First several Hermite polynomials  $H_{j-1}(\rho)$ . When the polynomials are multiplied by the factor  $e^{-\rho^2/2}$  the resulting function has the number of loops given in the first column. Polynomial corresponding to even numbers of loops are even about  $\rho = 0$ ; polynomials corresponding to odd numbers of loops are odd about  $\rho = 0$ .

*Mathematica* knows about Hermite polynomials, and so it is easy to construct a function for harmonic oscillator wavefunctions. Here is the *Mathematica* function for the wavefunction with  $j$  loops.

$$\psi[j\_ , \rho\_ ] := \frac{1}{\sqrt{2^{j-1} (j-1)! \sqrt{\pi}}} \text{HermiteH}[j-1, \rho] e^{-\rho^2/2}$$

These wavefunctions are normalized to 1; for example,

$$\int_{-\infty}^{\infty} \psi[6, \rho]^2 d\rho$$

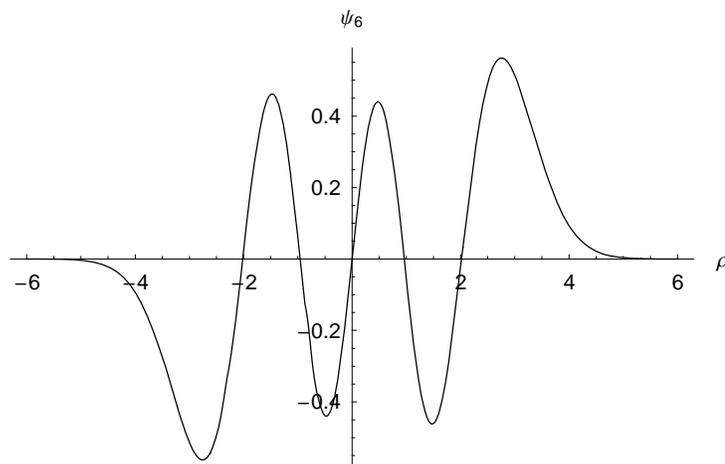
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They are also orthogonal, as must be so since they are eigenfunctions of the harmonic oscillator Hamiltonian operator which is hermitian; for example

$$\int_{-\infty}^{\infty} \psi[6, \rho] \psi[3, \rho] d\rho$$

0

Here is a plot of  $\psi_6(\rho)$ .



Analytic harmonic oscillator wavefunction  $\psi_6(\rho)$ . The function is normalized to 1. Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$

This is the same as the function that we obtained earlier using Numerov integration, to within the accuracy of the numerical implementation.

## ■ Quantal harmonic motion

To treat harmonic *motion* quantum mechanically, we need to construct wavepackets. A general expression for a wavepacket is

$$\Psi(\rho) = N \sum_j g_j \psi_j(\rho),$$

in terms of relative weights  $g_j$  and the normalization constant

$$N = 1 / \sqrt{\sum_j g_j^2}.$$

For example, a packet composed of waves with 1, 2 and 3 loops, with relative weights 25%, 50% and 25% is

$$\Psi(\rho) = \frac{1}{\sqrt{0.25^2 + 0.5^2 + 0.25^2}} (0.25 \psi_1(\rho) + 0.5 \psi_2(\rho) + 0.25 \psi_3(\rho))$$

Use of the orthonormality of the component waves, that is, that  $\int \psi_j(\rho) \psi_k(\rho) d\rho = \delta_{jk}$ , to confirm that this wavepacket is normalized, that is, that  $\int |\Psi(\rho)|^2 d\rho = 1$ .

Let's use *Mathematica* to construct and plot harmonic oscillator wavepacket probability densities. First, we can define the list of weights  $g_j$ . For the example above, this is

$$\mathbf{g} = \{0.25, 0.50, 0.25\};$$

Next, we can construct a list of wavefunctions. For the example above, this is

$$\mathbf{f} = \psi[\#, \rho] \& /@ \{1, 2, 3\}$$

$$\left\{ \frac{e^{-\frac{\rho^2}{2}}}{\pi^{1/4}}, \frac{\sqrt{2} e^{-\frac{\rho^2}{2}} \rho}{\pi^{1/4}}, \frac{e^{-\frac{\rho^2}{2}} (-2 + 4 \rho^2)}{2 \sqrt{2} \pi^{1/4}} \right\}$$

The normalization factor,

$$\frac{1}{\sqrt{0.25^2 + 0.5^2 + 0.25^2}},$$

evaluates to

$$\mathbf{norm} = \frac{1}{\sqrt{\mathbf{g} \cdot \mathbf{g}}}$$

$$1.63299$$

The sum of the products of the functions times their weights,

$$g_1 \psi_1(\rho) + g_2 \psi_2(\rho) + g_3 \psi_3(\rho),$$

is

**g.f**

$$0.187781 e^{-\frac{\rho^2}{2}} + 0.531126 e^{-\frac{\rho^2}{2}} \rho + 0.0663907 e^{-\frac{\rho^2}{2}} (-2 + 4 \rho^2)$$

Putting everything together, the normalized wavepacket is

**packet = norm g.f**

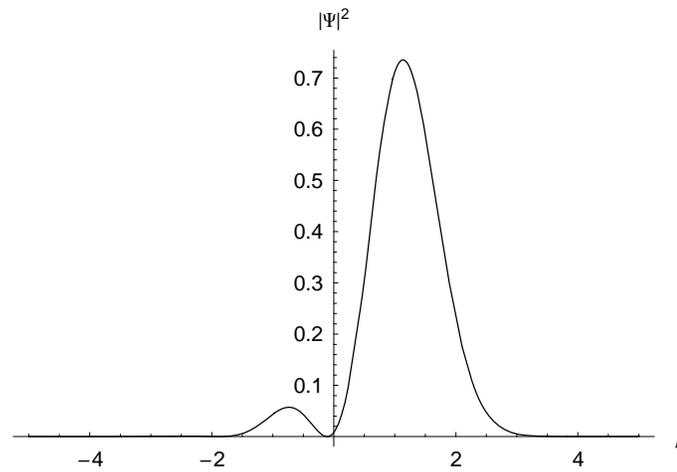
$$1.63299 \left( 0.187781 e^{-\frac{\rho^2}{2}} + 0.531126 e^{-\frac{\rho^2}{2}} \rho + 0.0663907 e^{-\frac{\rho^2}{2}} (-2 + 4 \rho^2) \right)$$

We can check that this packet is normalized, as

$$\int_{-\infty}^{\infty} \text{packet}^2 d\rho$$

1.

Here is what the probability density (the square of the wavepacket) looks like.



Probability density  $|\Psi(\rho)|^2$  of a three component harmonic oscillator wavepacket  $\Psi(\rho)$ . The probability density is normalized to 1. Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$

The packet is localized near the right classical turning point. If we were to add more waves to the packet, the width of the localized region would become smaller, in accordance with the Heisenberg indeterminacy relation.

The next thing we need to do is to make the wavepacket move. To do this we need only to insert the time dependent phase factors,

$$e^{-iE_j t/\hbar} = e^{-i \frac{\hbar\omega}{2} (2j-1) t/\hbar} = e^{-i \omega(j-\frac{1}{2}) t},$$

to the components of the packet. For our example packet, the list of these phase factors is

$$\text{phase} = e^{-i \omega (\# - \frac{1}{2}) t} \ \& \ /@ \ \{1, 2, 3\}$$

$$\{ e^{-\frac{1}{2} i t \omega}, e^{-\frac{3}{2} i t \omega}, e^{-\frac{5}{2} i t \omega} \}$$

The list of functions times their phase factors is

**f phase**

$$\left\{ \frac{e^{-\frac{\rho^2}{2} - \frac{i t \omega}{2}}}{\pi^{1/4}}, \frac{\sqrt{2} e^{-\frac{\rho^2}{2} - \frac{3 i t \omega}{2}} \rho}{\pi^{1/4}}, \frac{e^{-\frac{\rho^2}{2} - \frac{5 i t \omega}{2}} (-2 + 4 \rho^2)}{2 \sqrt{2} \pi^{1/4}} \right\}$$

The sum of the products of the functions times their phase factors and their weights, and multiplied by the normalization factor,

$$\frac{1}{\sqrt{\sum_j g_j^2}} \left( g_1 \psi_1(\rho) e^{-i \omega(1-\frac{1}{2})t} + g_2 \psi_2(\rho) e^{-i \omega(2-\frac{1}{2})t} + g_3 \psi_3(\rho) e^{-i \omega(3-\frac{1}{2})t} \right),$$

is

```
packetWithTime = norm g . (f phase)
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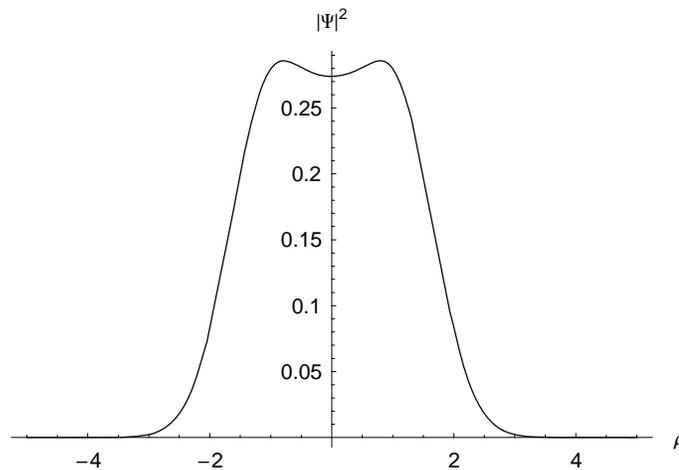
$$1.63299 \left( 0.187781 e^{-\frac{\rho^2}{2} - \frac{i t \omega}{2}} + 0.531126 e^{-\frac{\rho^2}{2} - \frac{3 i t \omega}{2}} \rho + 0.0663907 e^{-\frac{\rho^2}{2} - \frac{5 i t \omega}{2}} (-2 + 4 \rho^2) \right)$$

▮ Show that this wavepacket is normalized to 1, for every value of time,  $t$ .

At  $t = 0$  the time-dependent wavepacket,  $\Psi(\rho, 0)$ , is identical to the time independent wavepacket,  $\Psi(\rho)$ , and so gives the same probability density.

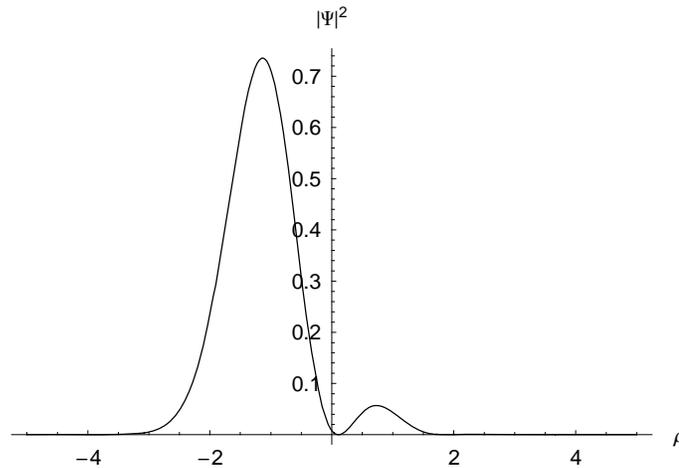
▮ Verify that this statement is correct.

Here is what the probability density (the square of the wavepacket) looks like at time  $t = 0.25/\nu$ , one quarter of the way through one oscillation period.



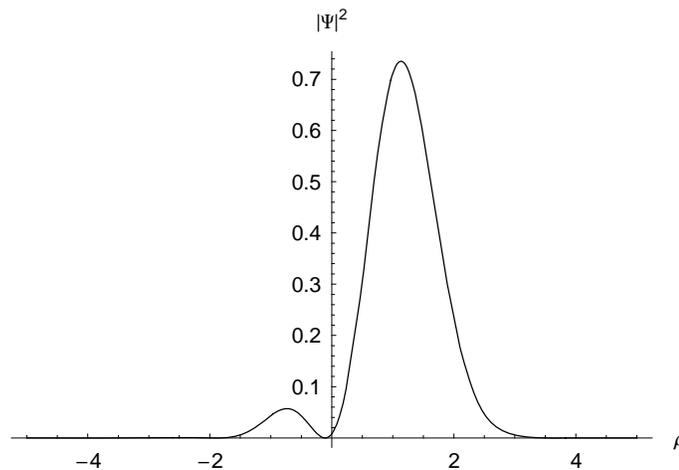
Probability density  $|\Psi(\rho, t)|^2$  of a three component harmonic oscillator wavepacket  $\Psi(\rho, t)$  at time  $t = 0.25/\nu$ . The probability density is normalized to 1. Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$

Here is what the probability density looks like at time  $t = 0.5/\nu$ , half way through one oscillation period.



Probability density  $|\Psi(\rho, t)|^2$  of a three component harmonic oscillator wavepacket  $\Psi(\rho, t)$  at time  $t = 0.5/\nu$ . The probability density is normalized to 1. Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$

Finally, here is what the probability density looks like at time  $t = 2\pi/\omega = 1/\nu$ , after one oscillation period.



Probability density  $|\Psi(\rho, t)|^2$  of a three component harmonic oscillator wavepacket  $\Psi(\rho, t)$  at time  $t = 1/\nu$ . The probability density is normalized to 1. Displacement  $\rho$  from equilibrium is in units  $\sqrt{\hbar/m\omega}$

The packet has returned to its original form and location at  $t = 1/\nu$ .

## ■ Energy of wavepackets: expectation values

The energy of a wave packet is defined to be

$$\langle H \rangle = \int_{-\infty}^{\infty} \Psi^*(\rho, t) H \Psi(\rho, t) d\rho.$$

The notation  $\langle \dots \rangle$  denotes "average" or "expectation" and such an expression is known as the average value of the *expectation value* of the physical quantity corresponding to the operator that appears between the brackets. For example, the expectation value of position would be

$$\langle \rho \rangle = \int_{-\infty}^{\infty} \Psi^*(\rho, t) \rho \Psi(\rho, t) d\rho.$$

Since the operator for position is just "multiply by position," we can rearrange this expression as

$$\langle \rho \rangle = \int_{-\infty}^{\infty} \rho \left| \Psi(\rho, t) \right|^2 d\rho.$$

In this form the average value of the position is seen to be just the average of all possible positions, weighted by the probability that the particle is at each position. It is this interpretation that led of the name average value or expectation value. If the operator is more complicated than "multiply by", then we cannot rearrange things in this way, but we still interpret the expression in the same way.

Show that the expression for the expectation value of the squared momentum, in dimensionless units, is  $\langle p^2 \rangle = - \int \Psi^*(\rho, t) \partial^2 / \partial \rho^2 \Psi(\rho, t) d\rho$ .

Taking account of the orthonormality of the harmonic oscillator wavefunctions,

$$\int_{-\infty}^{\infty} \psi_j(\rho) \psi_k(\rho) d\rho = \delta_{jk},$$

it is not too difficult to show that

$$\langle H \rangle = \frac{1}{\sum_j g_j^2} \sum_k g_k^2 E_k,$$

an average of the component energies, each weighted by its relative contribution to the probability density.

Show that this expression is correct for any wavepacket composed of orthonormal components  $\psi_k(\rho)$ .

Why do you suppose this expression is independent of time?

Here is a *Mathematica* function that takes as input a list of component wavefunctions (in terms of the number of loops of each component) and a list of the corresponding weights, and computes the dimensionless energy expectation value of the packet.

$$\epsilon\text{Avg}[\text{j\_List}, \text{g\_List}] := \frac{1}{\text{g.g}} \text{g}^2 \cdot ((2 \# - 1) \& /@ \text{j})$$

For example, the average energy of a wavepacket consisting of an equal mixture of the one-loop and two-loop wavefunctions is

$$\epsilon\text{Avg}[\{1, 2\}, \{1, 1\}]$$

2

This is what we expect, since  $\psi_1$  has energy  $\epsilon_1 = 1$  and  $\psi_2$  has energy  $\epsilon_2 = 3$ . A packet composed of 10%  $\psi_1$  and 90%  $\psi_2$  has instead the average energy

$$2.97561$$

This is very close to  $\epsilon_2$ , as we would expect, since the packet is most  $\psi_2$ .

## ■ Wavepacket machine

Collecting everything together, a general time-dependent harmonic oscillator wavepacket is

$$\Psi(\rho, t) = \frac{1}{\sqrt{\sum_k g_k^2}} \sum_j g_j \psi_j(\rho) e^{-i \omega(j-\frac{1}{2})t}.$$

| Show that this expression is normalized to 1 for all values of  $t$ .

| Show that  $|\Psi(\rho, t)|^2$  oscillates with period  $1/\nu$ .

Here is a *Mathematica* function that makes a wavepacket, for a specified choice of component wavefunctions,  $\psi_j$ , and weights,  $g_j$ .

$$\text{HOPacket}[\mathbf{j\_List}, \mathbf{g\_List}] := \frac{1}{\sqrt{\mathbf{g} \cdot \mathbf{g}}} \mathbf{g} \cdot (\psi[\#, \rho] e^{-i (\# - \frac{1}{2}) 2\pi t} \& /@ \mathbf{j})$$

In this function, time is measured in dimensionless units of the oscillation period,  $2\pi/\omega = 1/\nu$ ; this means that  $t = 1$  corresponds to elapsed time  $1/\nu = 2\pi\sqrt{m/k}$ . As example of this function, here is the two-component wavepacket composed of equal contributions of one-loop and two-loop components.

$$\frac{e^{-3i\pi t - \frac{\rho^2}{2}} (e^{2i\pi t} + \sqrt{2} \rho)}{\sqrt{2} \pi^{1/4}}$$

| Verify that this expression is correct, by constructing the wavepacket by hand.

Now that we have a tool to construct harmonic oscillator wavepackets, let's explore the properties of different packets.

## ■ Gaussian wavepacket

We can construct wavepackets of essentially arbitrary shape by appropriate choice of weights  $g_j$ . Experimentally, this amounts to appropriate excitation of the oscillator into a coherent superposition of wavefunctions  $\psi_j(\rho)$ . (Coherent means there is a definite phase relation between the components of the packet.) One common superposition results in a Gaussian distribution of weights. The Gaussian distribution centered at  $\mu$  and with mean squared deviation (variance)  $\sigma$  is

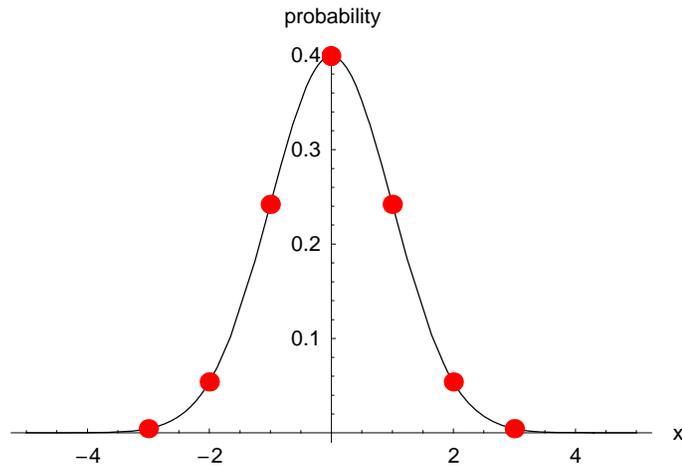
$$\text{gauss}[\sigma, \mathbf{x}, \mu] := \frac{1}{\sqrt{2\pi}\sigma} e^{-(\mathbf{x}-\mu)^2/(2\sigma^2)}$$

The Gaussian distribution is normalized to 1; for example

$$\int_{-\infty}^{\infty} \text{gauss}[1, \mathbf{x}, 0] d\mathbf{x}$$

1

Here is the Gaussian distribution centered about 0 with mean squared deviation 1 (the so-called *normal density function*).



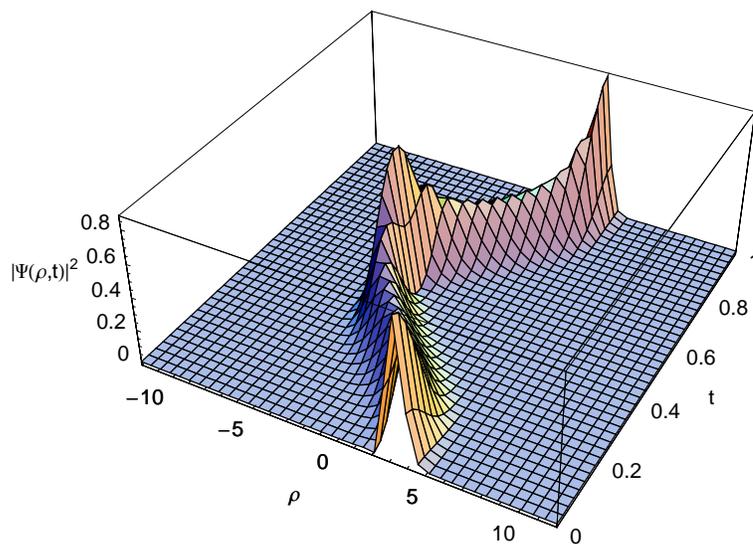
Gaussian probability distribution with mean 0 and variance 1. The filled circles marked values of the distribution at 7 equally spaced values of  $x$  centered on the mean.

We can select weights  $g_j$  that approximate this Gaussian distribution by evaluating the distribution at a range of points centered about the mean. For example, here is a set of thirteen such weights chosen to span the distribution.

```
g = gauss[1, #, 0] & /@Range[-3, 3, 1] // N // sE2
{0.0044, 0.054, 0.24, 0.4, 0.24, 0.054, 0.0044}
```

These weights are indicated as the filled circles on the plot of the Gaussian distribution above.

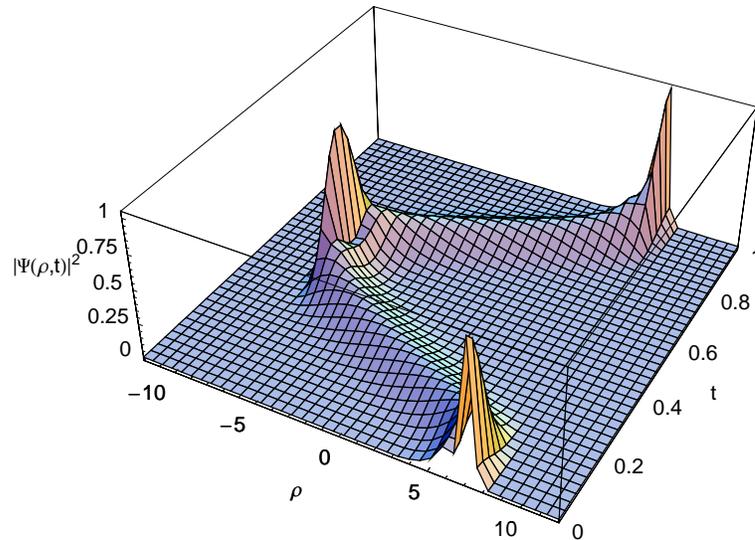
Here is a plot of a Gaussian wavepacket consisting of the first 13 harmonic oscillator wavefunctions  $\psi_j(\rho)$ , throughout one cycle of oscillation.



Harmonic oscillator Gaussian wavepacket probability density throughout one cycle of oscillation. The packet is composed of the first 13 wavefunctions  $\psi_j(\rho)$ .

Show that the dimensionless energy expectation value of this wavepacket is  $\langle H \rangle = 13$ .  
 Could you have predicted this result without doing a detailed calculation?

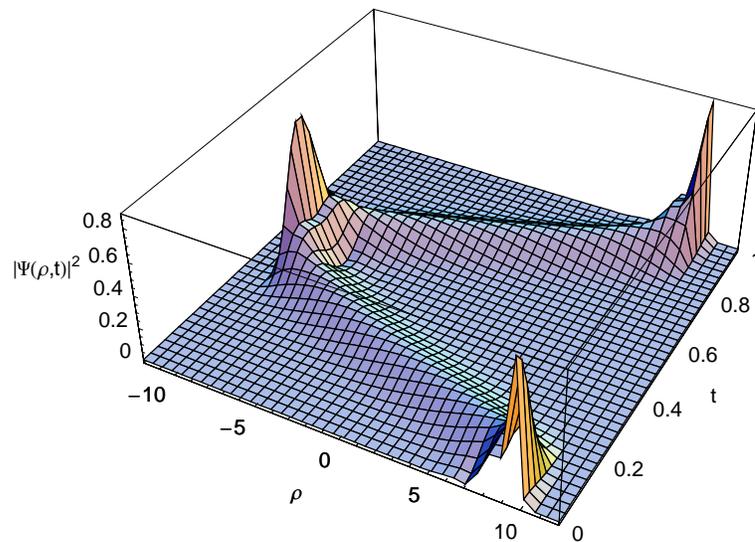
Here is a plot of a Gaussian wavepacket consisting of 13 harmonic oscillator wavefunctions  $\psi_j(\rho)$  centered about  $j = 27$ , throughout one cycle of oscillation.



Harmonic oscillator Gaussian wavepacket probability density throughout one cycle of oscillation. The packet is composed of 13 wavefunctions  $\psi_j(\rho)$  centered at  $j = 27$ .

Show that the dimensionless energy expectation value of this wavepacket is  $\langle H \rangle = 53$ .

Here is a plot of a Gaussian wavepacket consisting of 13 harmonic oscillator wavefunctions  $\psi_j(\rho)$  centered about  $j = 47$ , throughout one cycle of oscillation.



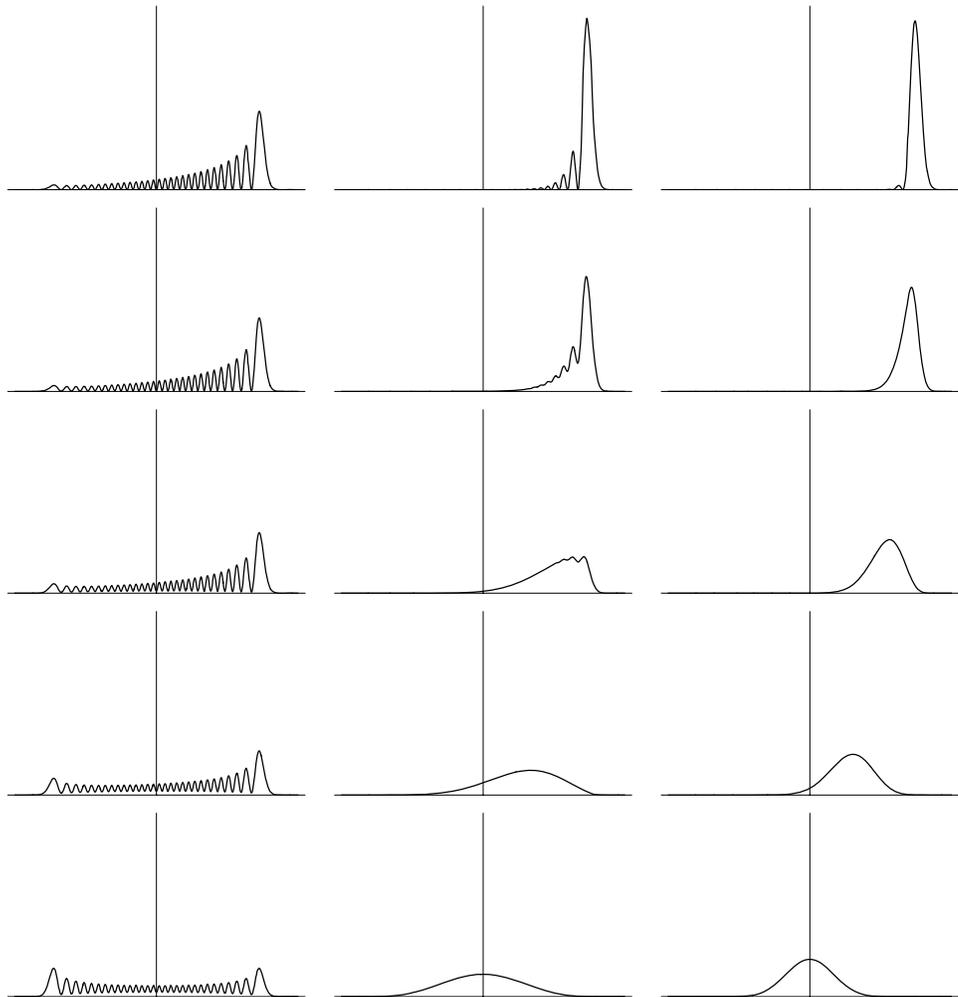
Harmonic oscillator Gaussian wavepacket probability density throughout one cycle of oscillation. The packet is composed of 13 wavefunctions  $\psi_j(\rho)$  centered at  $j = 47$ .

Show that the dimensionless energy expectation value of this wavepacket is  $\langle H \rangle = 93$ .

These three Gaussian harmonic oscillator wavepackets all have the same number of adjacent components, but the center component is successively higher. Use the surface plots of the probability densities to see what difference this corresponds to physically.

## ■ Localization of harmonic motion

We have seen that adding more components to a wavepacket localizes the probability density to a smaller region of space. We can illustrate this by constructing Gaussian packets centered at the same  $\psi_j$ , but with differing numbers of adjacent components. Here are the packets consisting of 5, 13 and 21 components, for times corresponding to the first quarter of the period,  $1/\nu$ .



Harmonic oscillator Gaussian wavepacket probability densities throughout one quarter cycle of oscillation. The packets are each centered about  $j = 30$ ; the left column is the 5-component packet, the middle column is the 13-component packet, and the right column is the 21-component packet.

The 5-component packet is poorly localized, the 13-component packet is fairly localized, and the 21-component packet is highly localized.