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Motion of a wave packet

Ronald Lovett
Washington University in St. Louis

The Motion of a Wave Packet

References

Principles of Modern Physics, R. B. Leighton, Chapter 4 (Phys QC173 L48).
Molecular Quantum Mechanics, P. W. Atkins, 3rd Edition, Appendix 3 (Chem QD462 A84).

A wave packet

A free particle in one dimension with momentum $p = \hbar k$ has a time-evolving state function

$$\psi_k(x,t) = e^{ikx - ik^2\hbar t/2m}.$$

A superposition of such waves with a Gaussian distribution on k (centered a $k = k_0$ with width σ^{-1}) gives a state

$$\psi(x,t) = \frac{\sigma}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, e^{-\frac{1}{2}\sigma^2(k-k_0)^2 + ikx - \frac{ik^2\hbar t}{2m}}$$

$$= \frac{1}{\sqrt{1 + i\hbar t/m\sigma^2}} \exp\left\{\frac{-x^2/2\sigma^2 + ik_0x - i\hbar k_0^2 t/2m}{1 + i\hbar t/m\sigma^2}\right\} \tag{1}$$

The state (1) is called a *wave packet*, for, although it is a superposition of plane waves, (1) $\Rightarrow$

$$|\psi(x,t)|^2 = \frac{1}{\sqrt{1 + \hbar^2 t^2/m^2\sigma^4}} \exp\left\{-\frac{(x - \hbar k_0 t/m)^2}{\sigma^2(1 + \hbar^2 t^2/m^2\sigma^4)}\right\}. \tag{2}$$

The probability distribution on x is localized in space. In fact, the distribution (2) on x is Gaussian with center

$$x = \frac{\hbar k_0}{m} t, \tag{3}$$

and width

$$\sigma_x^2 = \frac{1}{2}\sigma^2\left(1 + \frac{\hbar^2 t^2}{m^2\sigma^4}\right). \tag{4}$$

For times

$$t \ll m\sigma^2/\hbar$$

this wave packet does not appear to spread spatially. It moves like a classical particle. The dispersion of the energy about the classical energy $\hbar^2 k_0^2/2m$ is negligible if

$$k_0\sigma \ll 1.$$

Problem Set #4

1. Show that the sum of $2N+1$ terms

$$S_N(x) = \frac{1}{L}\sum_{n=-N}^{N} e^{2\pi i n x/L} = \frac{1}{L}\frac{\sin\left[\pi(2N+1)x/L\right]}{\sin\left[\pi x/L\right]} \tag{1}$$

can be evaluated easily. (The sum is over a *geometrical series*.) Show that $S_N(x+L) = S_N(x)$ for all x and

$$\int_0^L dx\, S_N(x) = 1 \tag{2}$$

for all N. Make plots of $S_N(x)$ for different N to show that $S_N(x)$ becomes increasingly peaked at $x = 0$ as $N \to \infty$. What is $S_N(0)$ and what is the smallest x_0 for which $S_N(x_0) = 0$?

Look up the text-book definition of the *Dirac δ-function*. It is reasonable that, when $S_N(x)$ appears in an integral, the rapid oscillation present as $N \to \infty$ makes $S_N(x)$ behave as zero for $x \neq 0$. That is,

$$S_N(x) \underset{N\to\infty}{\longrightarrow} S(x) = \sum_{k=-\infty}^{\infty} \delta(x - kL). \tag{3}$$

2. Use the set of wave vectors (atomic units)

$$\ell_n = 25 + 0.2n, \qquad n = -5, -4\ldots, +5, \tag{4}$$

to form a wave packet

$$\psi(x,0) = \sum_{n=-5}^{5} e^{i\ell_n(x+8)}. \tag{5}$$

What will the period of $|\psi(x,0)|^2$ be? Where will the wave packet be located at $t = 0$? If the width is the distance between the surrounding zeros of $|\psi(x,0)|^2$, what will this be? What is $\psi(x,t)$ if $\psi(x,0)$ has the value given in (5)? How rapidly will the wave packet move, and in what direction? How much will the packet spread in 1 atomic time unit? Make an animated presentation of the time evolution of $|\psi(x,t)|^2$ in $0 \le t \le 1$ using 40 plots.

> Generation of the data for the plots symbolically requires an intolerably long time. Since numerical processing is much quicker than symbolic processing, the data generation can be sped up by introducing numbers at an early stage. Let xs=Table[0.25*i,{i,-40,60}] give a discrete set of the x-values, ls=Table[25+0.2n, {n,-5,5}] give the ℓ_n values which will be summed over,
> and ones = Table[1, {n,-5,5}] be a list with all elements = 1. Then, if 'psi' is the wave function, a formal (symbolic) expression for the wave function in terms of ℓ, x and t, then "Psi[x,t]=(psi/.$\ell \to$ ls).ones" will give the result of summing over all the ℓ's. Psi[xs,t] will then be a list of numerical values of Psi[x,t] at the corresponding x's and prob =Abs[Psi[xs,t]]^2 will give a list of probability values at the corresponding x's, i.e., a discrete representation for $|\psi(x,t)|^2$ which can be plotted with ListPlot[$\cdots$,PlotJoined->True].

3. The energy of the wave packet realized in problem 2 is a little above $V = 300$. Consider bouncing this wave packet off the potential (i.e., the wave packet moves from $x < 0$ to $x > 0$)

$$V(x) = \begin{cases} 0, & x \leq 0, \\ -V, & x > 0, \end{cases}$$

with $V = 1000$. Form a wave packet out of the energy eigenstates of this problem that describes the scattering off this potential discontinuity of the wave packet introduced in problem 2. Make an animated presentation of $|\psi(x,t)|^2$ as a function of time to show the dynamics of a collision of this wave packet with a potential discontinuity.