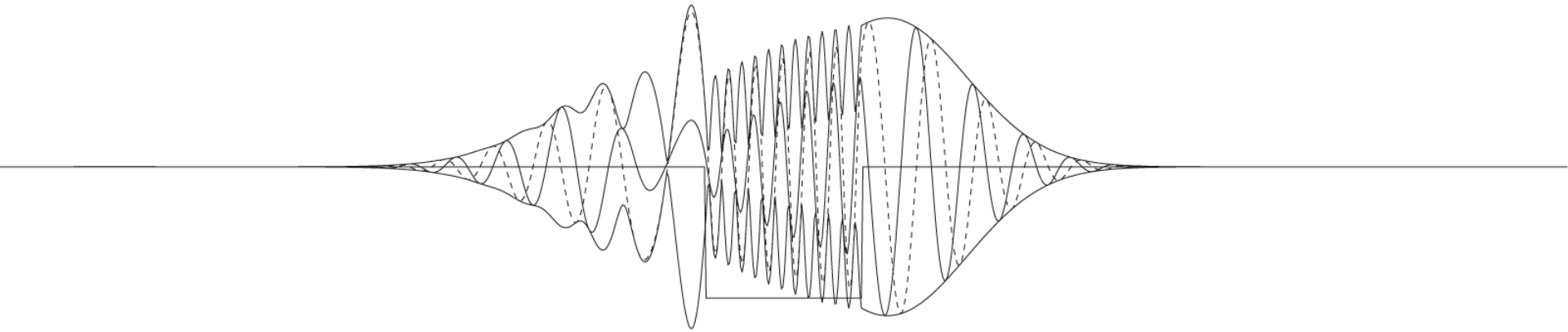
Wave packet scattering in one dimension

visualizations of transmission and reflection phenomena



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R	RESTRICTED
	SOME MATERIAL NOT SUITABLE FOR ALL AUDIENCES
CONTAINS COMPLEX MATHEMATICS, ABSTRACT PHYSICAL CONCEPTS, AND GRATUITOUS JARGON	

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	SUITABLE FOR INDIVIDUALS OF ALL AGES AND BACKGROUNDS
CONTAINS GRAPHIC SCENES OF QUANTUM PHENOMENA	

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AMERICAN JOURNAL of PHYSICS

Reflectionless eigenstates of the sech^2 potential

John Lekner[a)]
School of Chemical and Physical Sciences, Victoria University of Wellington, PO Box 600, Wellington, New Zealand

(Received 23 May 2007; accepted 28 August 2007)

The one-dimensional potential well $V(x)=-(\hbar^2\nu(\nu+1)/2ma^2)\,\mathrm{sech}^2(x/a)$ does not reflect waves of any energy when ν is a positive integer. We show that in this reflectionless case the solutions of Schrödinger's equation can be expressed in terms of elementary functions. Wave packets can be constructed from these energy eigenstates, and the propagation of such wave packets through the potential region can be studied analytically. We find that the group velocity of a particular packet can substantially exceed the group velocity of a free-space Gaussian packet. The bound states of the potential can also be expressed in terms of elementary functions when ν is an integer. The special properties of the integer ν potentials are associated with critical binding. © *2007 American Association of Physics Teachers.*

[DOI: 10.1119/1.2787015]

Visualization/conceptualization just plain weird

> **“Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, the do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen.”**

R.P. Feynman, *The Feynman Lectures on Physics Volume III*, p. 1-1, Basic Books (2010).

Visualization/conceptualization not without controversy

> **“In order to obtain a consistent account of atomic phenomena, it was necessary to renounce even more the use of pictures.”**

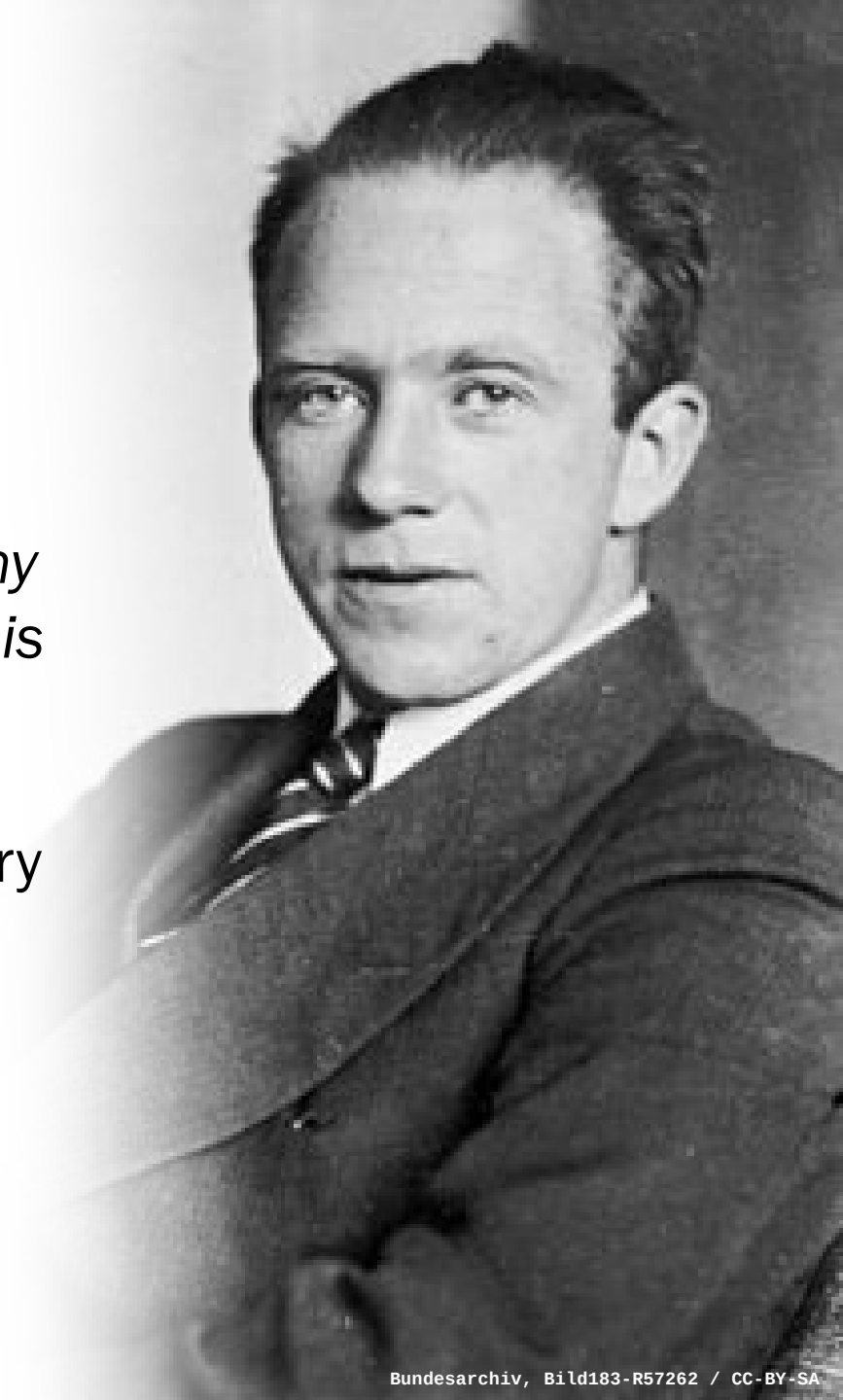
N. Bohr, *Atoms and Human Knowledge*, p. 87, Wiley (1958).

“The more I think of the physical part of the Schrödinger theory, the more detestable I find it.

What Schrödinger writes about visualization scarcely makes any sense, in other words, I think it is shit.

The greatest results of his theory is the calculation of matrix elements.”

Werner Heisenberg in a letter to Wolfgang Pauli (June 8, 1926)

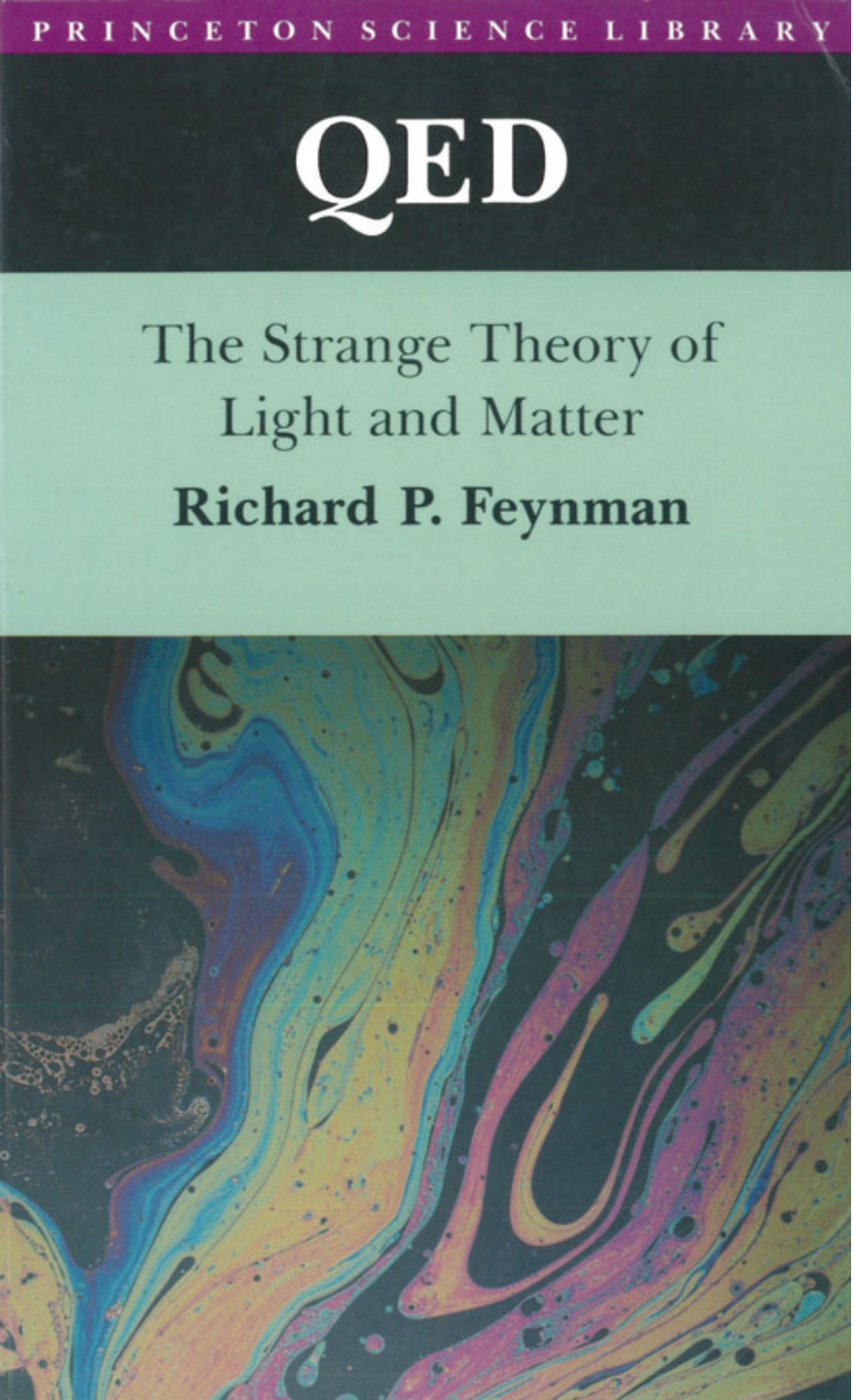


Bundesarchiv, Bild183-R57262 / CC-BY-SA

Visualization/conceptualization not without controversy

> “It is important to keep in mind that the wave packets in the ensemble are not intended to correspond to the individual neutrons in the beam. If this were so then each neutron in the beam would be in a pure state. In fact, each neutron is in a mixed state that is represented by the ensemble of wave packets…*there is clearly not a one-to-one correspondence between the neutrons and the wave packets*.”

-neutron optics expert



Phasors

$$\psi = \psi_{re} + i\,\psi_{im}$$

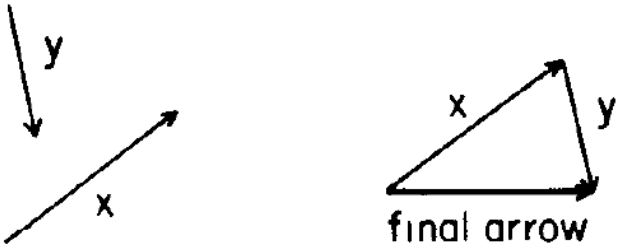


FIGURE 8 *Arrows that represent each possible way an event could happen are drawn and then combined ("added") in the following manner Attach the head of one arrow to the tail of another—without changing the direction of either one—and draw a "final arrow" from the tail of the first arrow to the head of the last one*

Solving the Schrodinger Equation

Finite-difference time-domain method

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VOLUME 35, NUMBER 3 MARCH 1967

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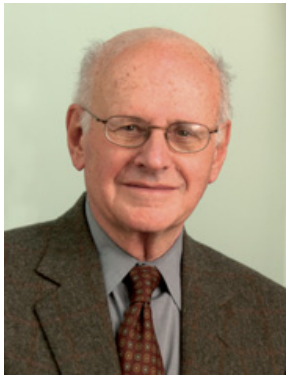
On the visualization of a wave packet *propagating* in a crystal



“Quite aside from their pedagogical value these films are visually very beautiful, easily on par with visual displays occasionally shown in museums of modern art.

The propagation of a wave packet in a crystal proves to have the elegance and grace of the best ballet.”

Kurt Gottfried, Am. J. Phys. **46**, 315 (1978).

Launching wavepackets at a barrier

a numerical “experiment”

Analytical

“Experimental”

Launching wavepackets at a barrier

a numerical "experiment"

Analytical

"Experimental"

$$r(k_o) = 1 - \int_{-\infty}^{\infty} dk\, T(k)\, P(k; k_o)$$

$$P(k; k_o) = |\varphi(k, 0; k_o)|^2$$

$$\varphi(k, t = 0; k_o) = \left(\frac{\sigma_x^2}{\pi}\right)^{\frac{1}{4}} e^{-\frac{1}{2}\sigma_x^2 (k - k_o)^2}$$

Launching wavepackets at a barrier

a numerical "experiment"

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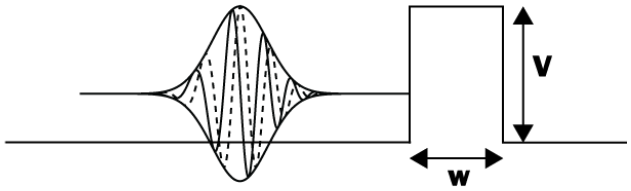
"Experimental"



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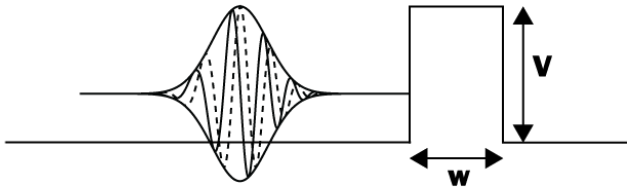


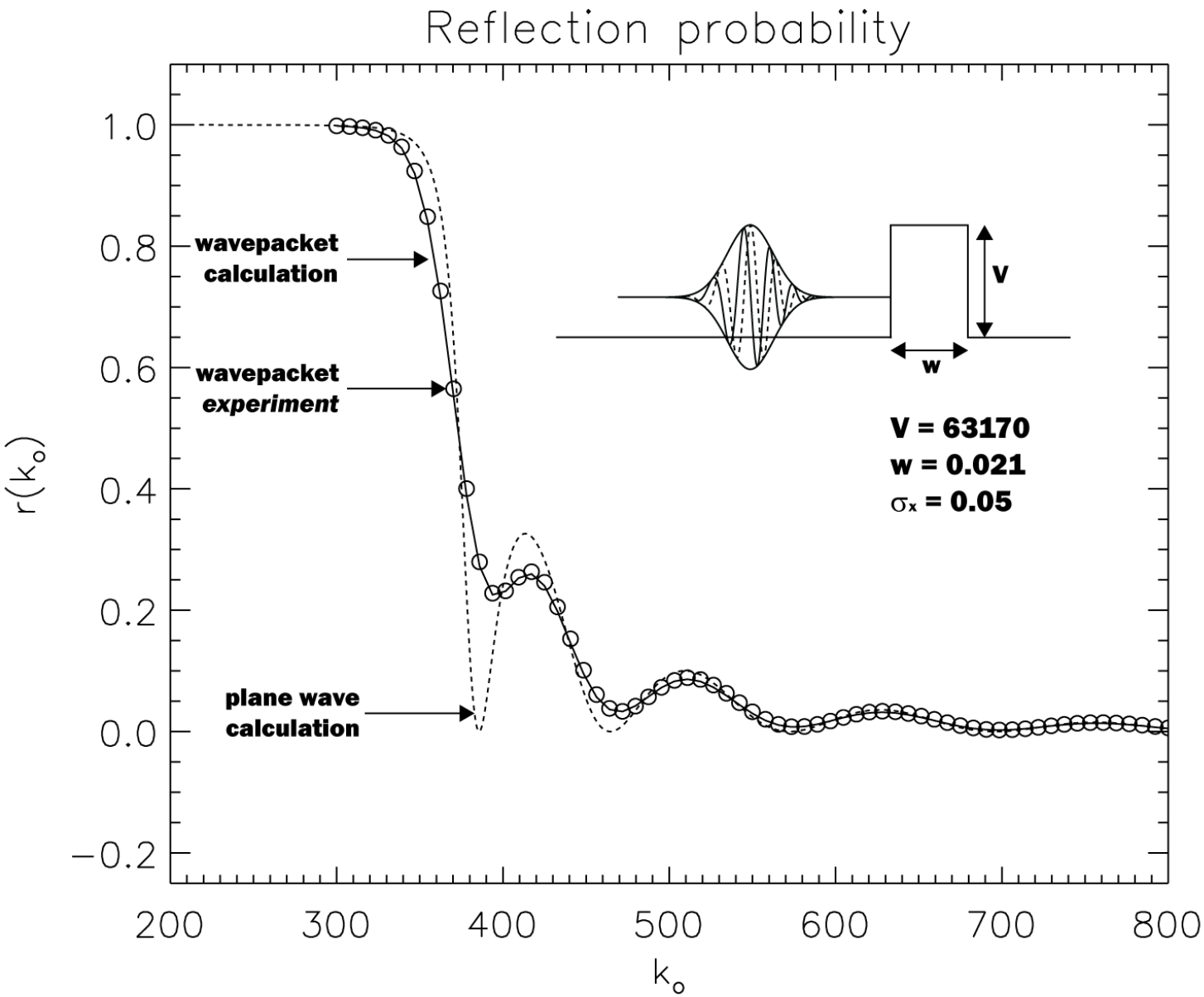
Launch wavepackets with different k_o

Wait until the reflected wavepacket is far enough away from the barrier so that it is no longer interacting with it

"Measure" the amount reflected (integrated probability density)

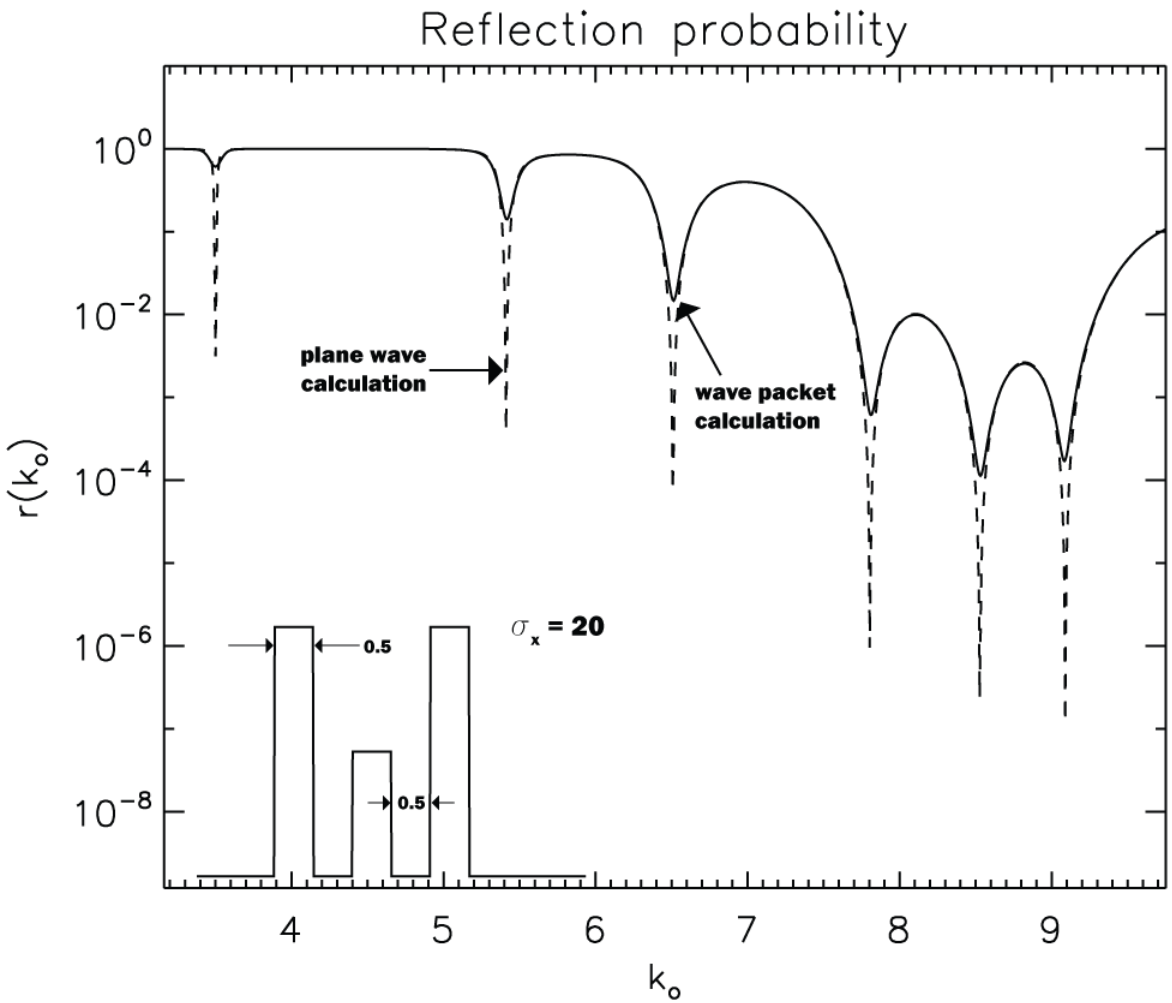
Launching wavepackets at a barrier

a numerical "experiment"



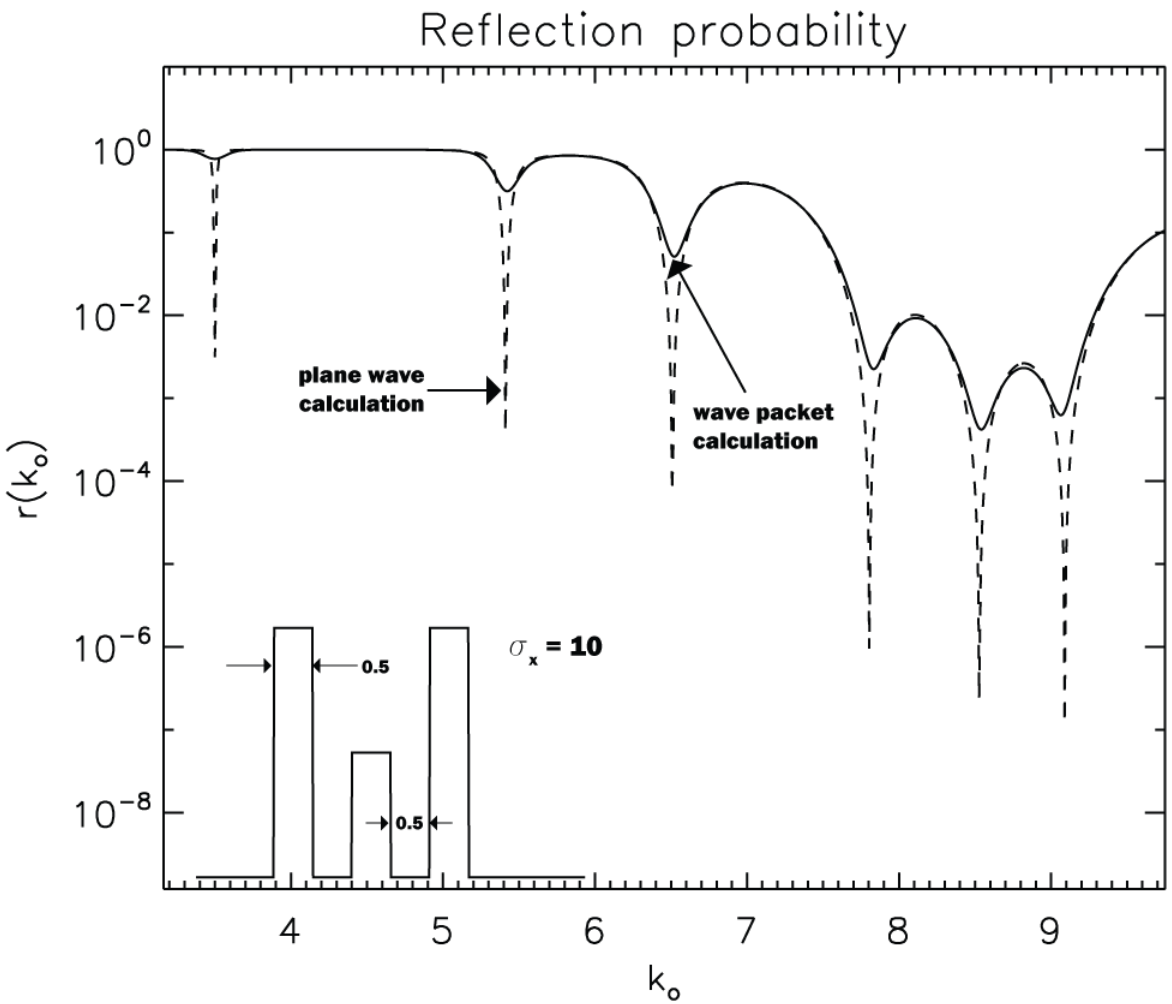
Launching wavepackets at a structure

wavepacket width effects



Launching wavepackets at a structure

wavepacket width effects



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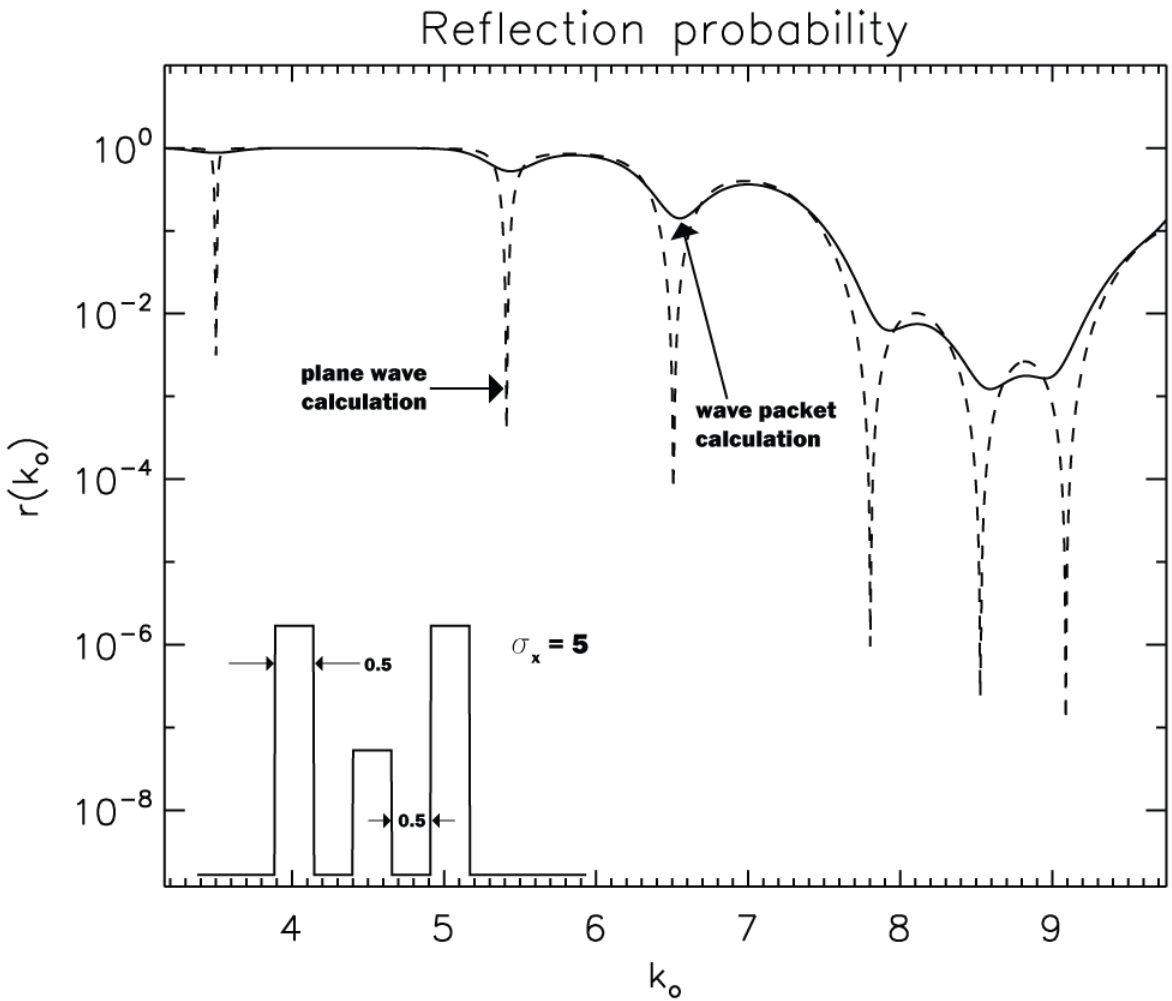
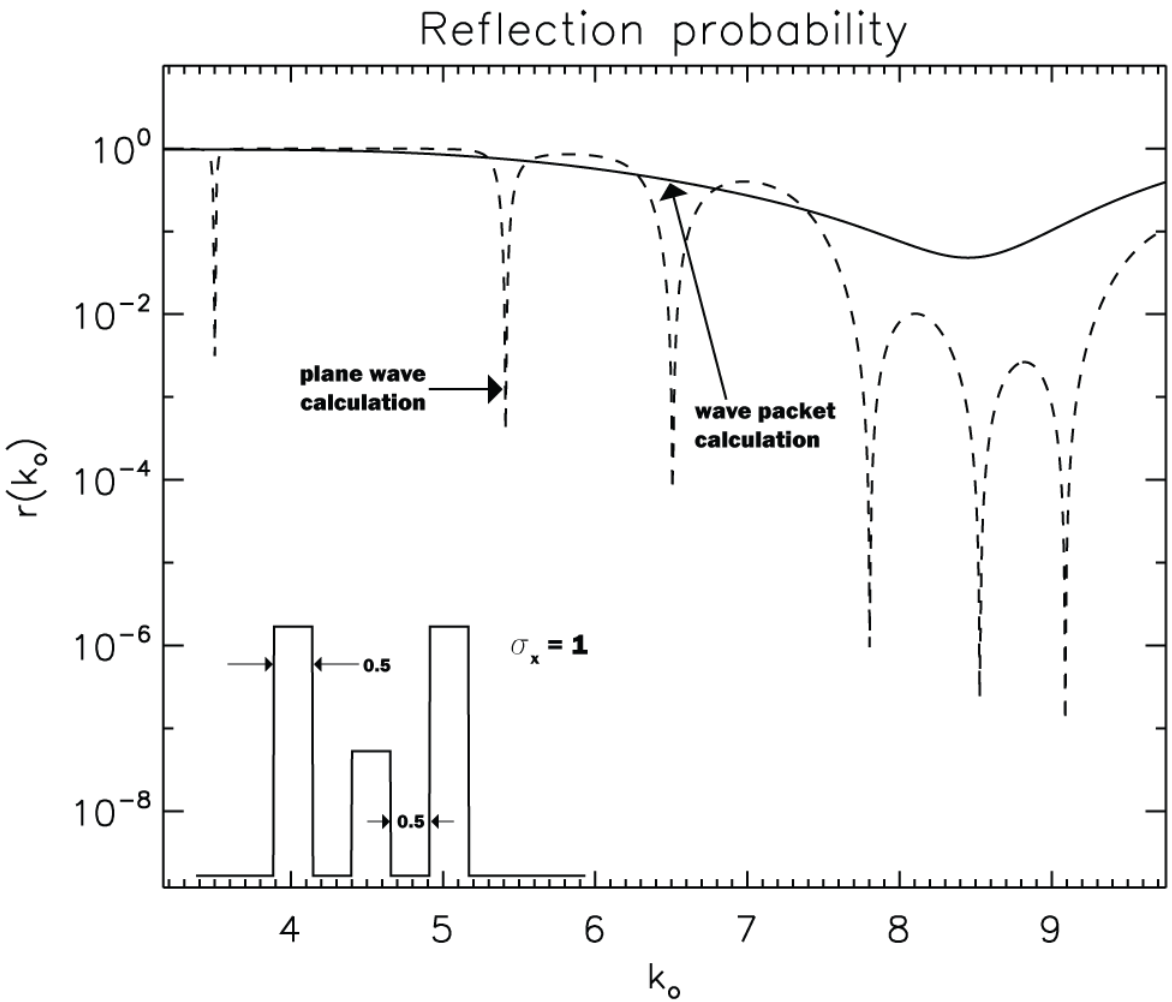
wavepacket width effects



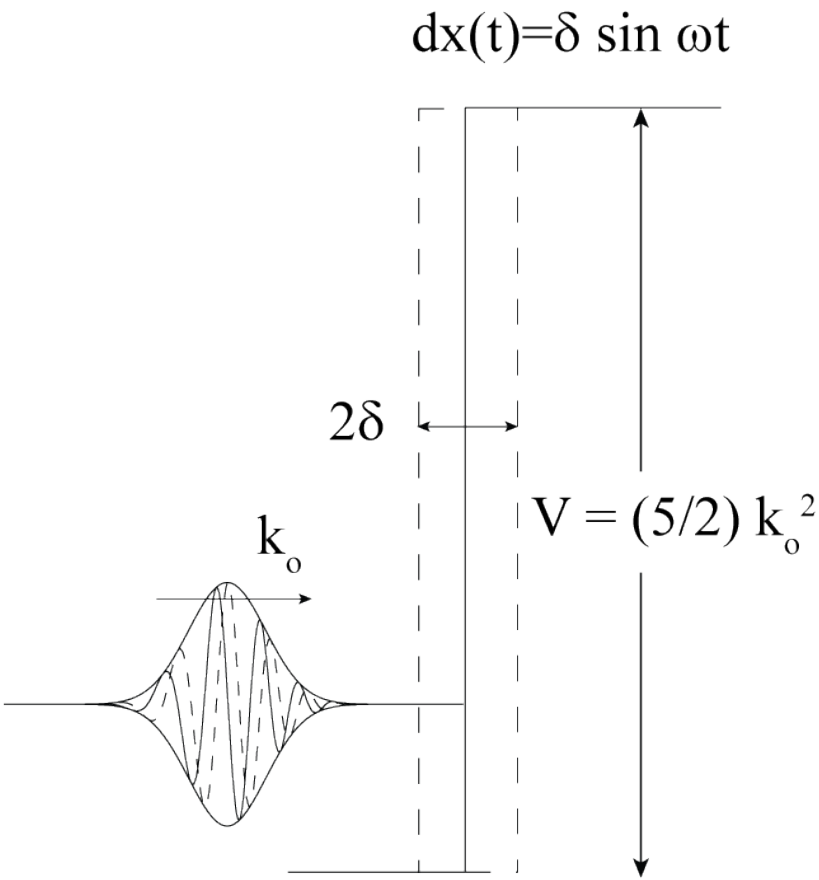
Launching wavepackets at a structure

wavepacket width effects



Reflection from an oscillating barrier

multi-phonon exchange



$$E_n = E_o + n\hbar\omega$$

reflected wavepacket energies

wavepacket's nominal energy

wall oscillator energy levels

$$k_n = -\sqrt{2E_n}$$

reflected wavevector transfer

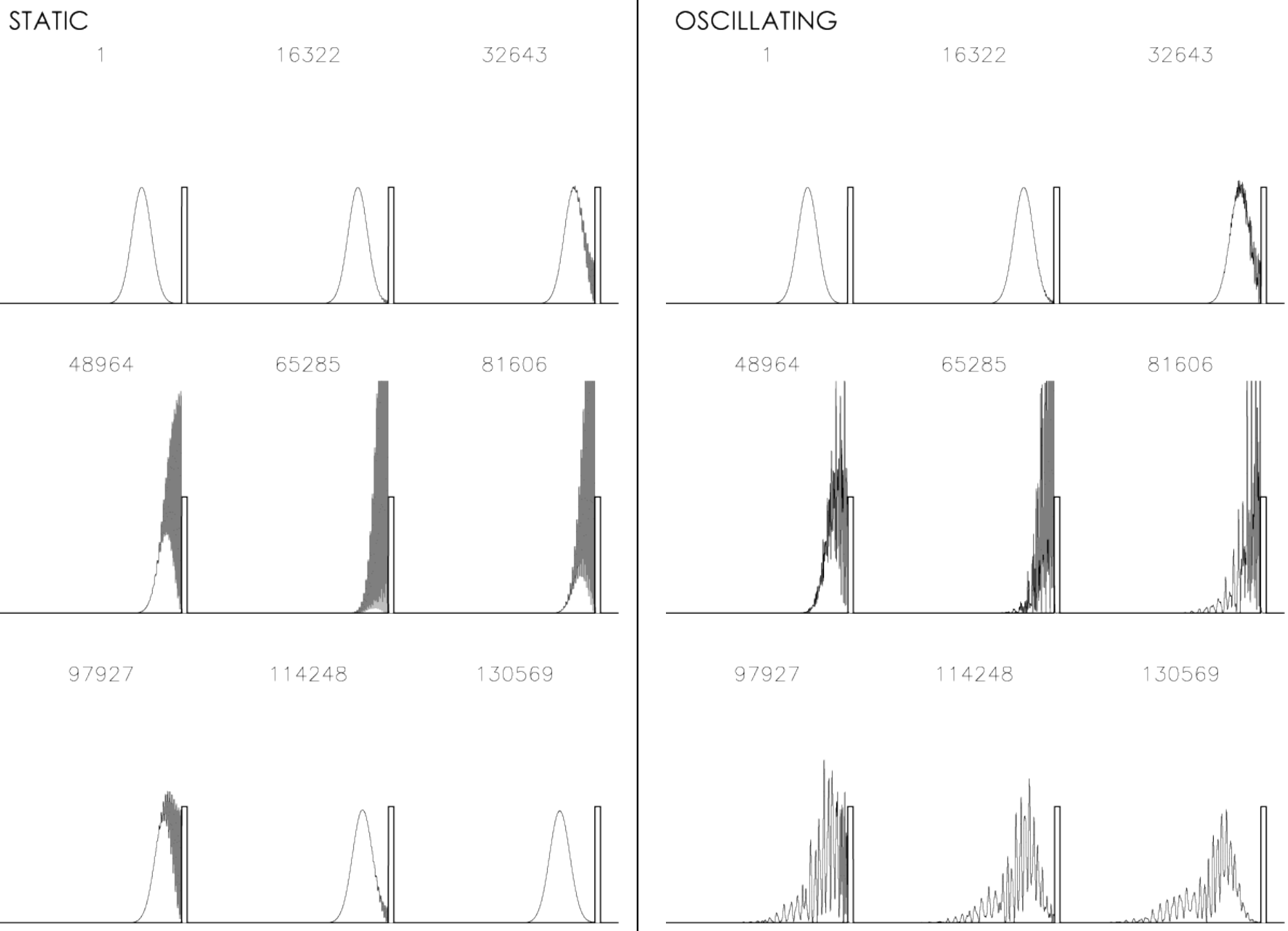
Matter waves at a vibrating surface: Transition from quantum-mechanical to classical behavior, J. Felber, R. Gahler, C. Rausch, and R. Golub, PRA **53**, 319 (1996).

Reflection from a stationary barrier

reminder: what does it look like?

Reflection from an oscillating barrier

what does it look like?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32643
48964
65285
81606
97927
114248
130569
OSCILLATING
1
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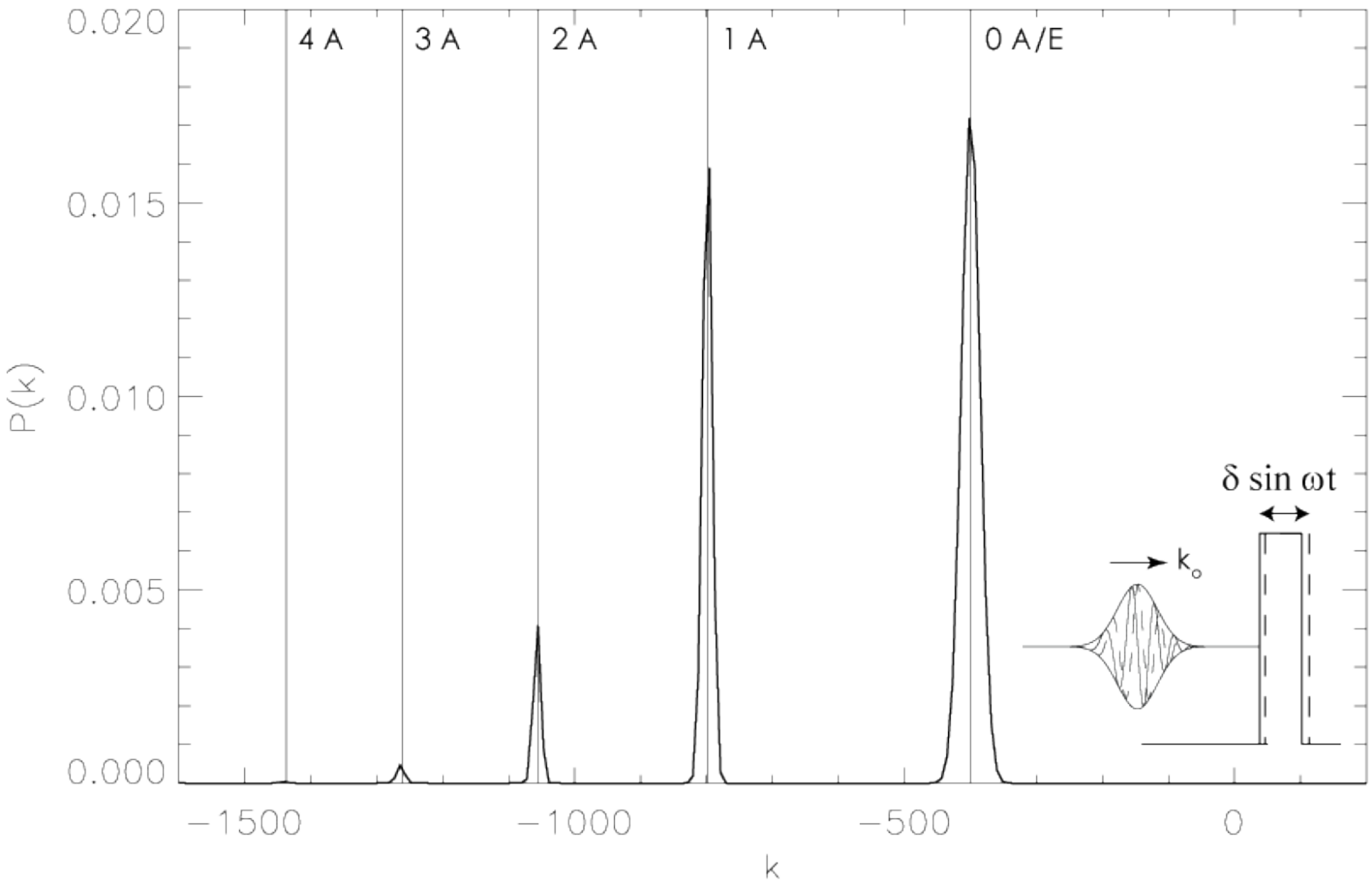
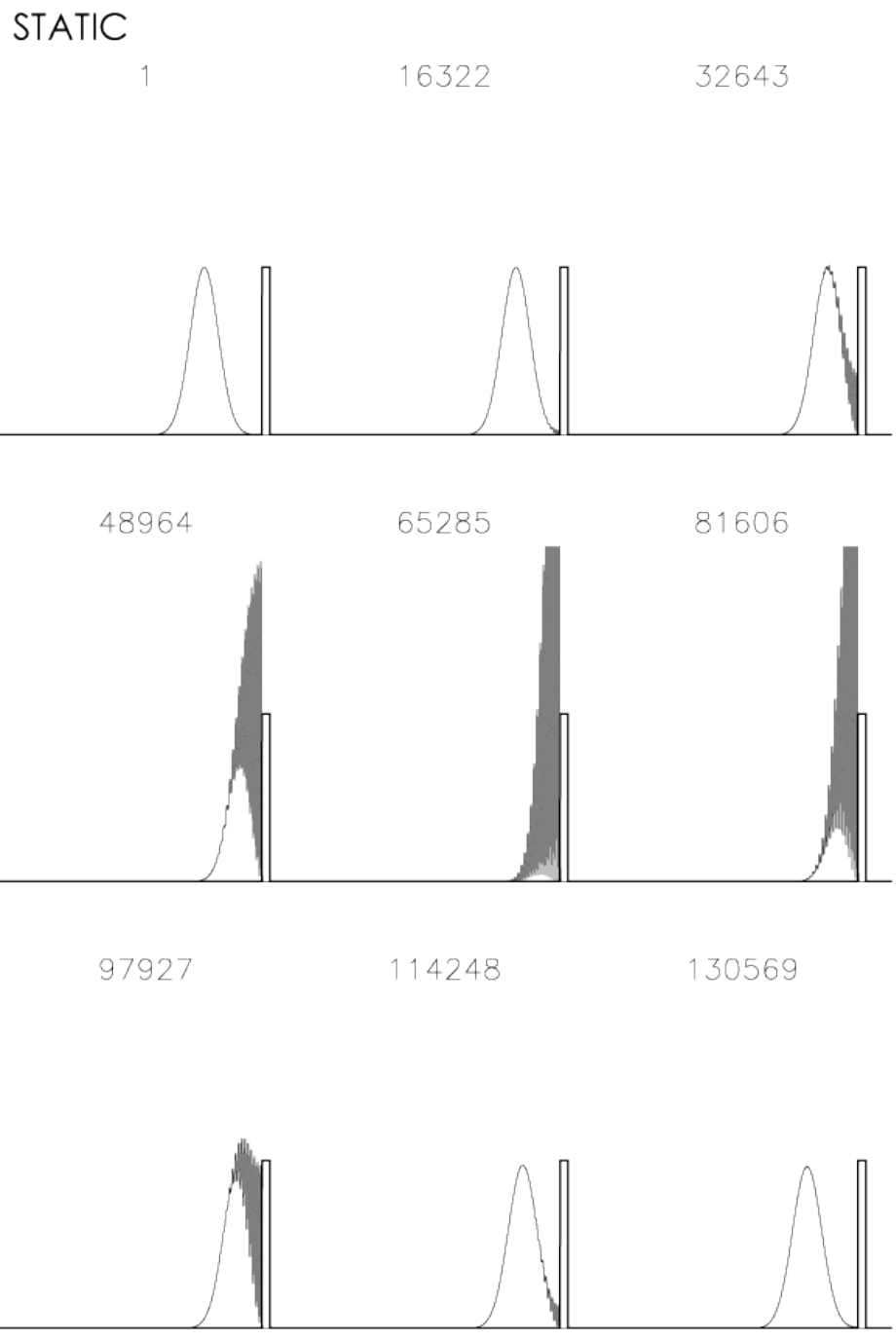
Reflection from an oscillating barrier

momentum distribution: $k_o^2/2 < \omega$



$$k_o = 400 \Rightarrow k_n = -400, -798, -1054, -1261, -1437, \ldots$$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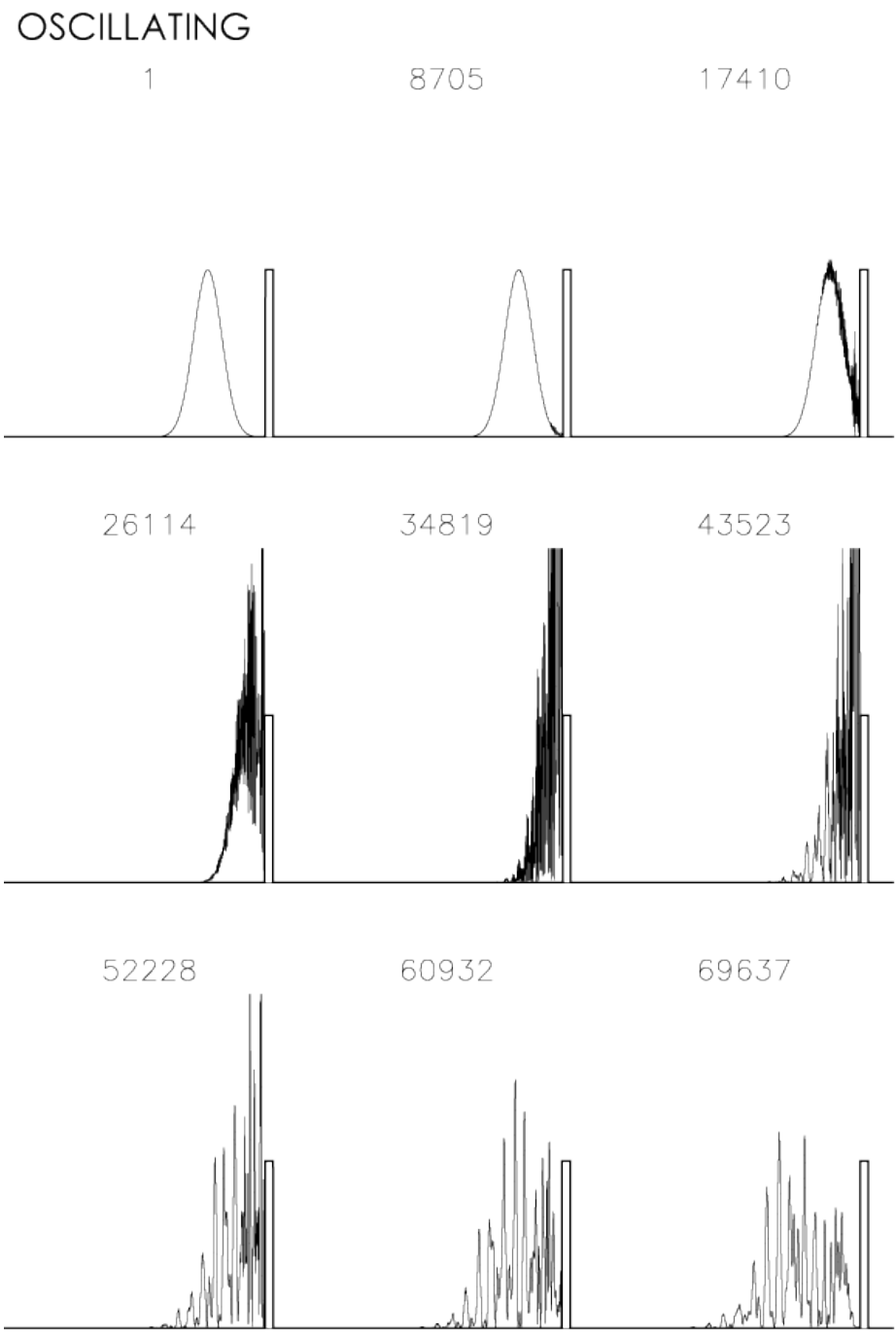
OSCILLATING
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26114
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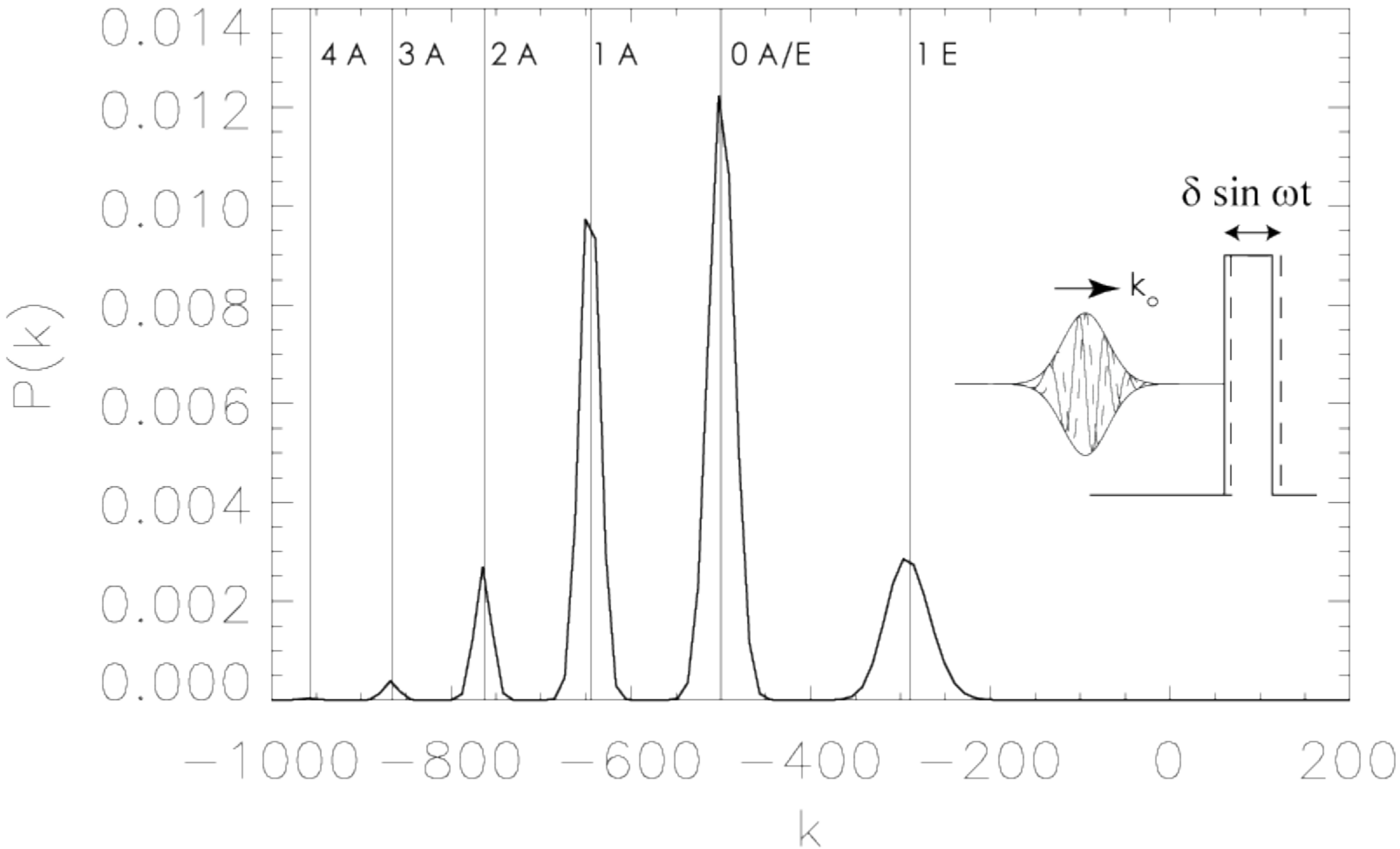
52228
60932
69637

Reflection from an oscillating barrier

momentum distribution: $k_o^2/2 > \omega$



$$k_o = 750 \Rightarrow k_n = -294, -750, -1019, -1231, -1411, -1571, -1716, \ldots$$

BACKUP

Solving the Schrodinger Equation

Finite-difference time-domain method

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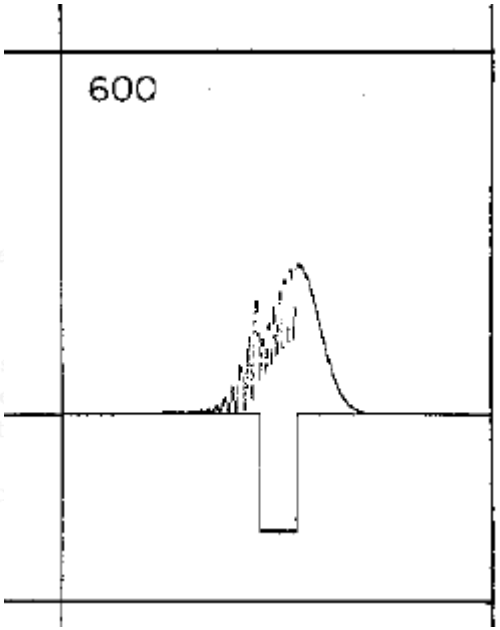
Finite-difference time-domain method

“The reader will note occasional breaks or discontinuities at various points in some of these pictures. This effect is due to an evidently inherent malfunction of the equipment involved in rendering the machine calculations into graphical form. At the present time there appears to be no simple way to avoid this problem…This situation emphasizes the fact that the use of computers to illustrate time development in physical systems by motion pictures is still in a preliminary, if no longer rudimentary, stage.”



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Implicit integrator

Stable

Unitary

Solving the Schrodinger Equation

Finite-difference time-domain method

A fast explicit algorithm for the time-dependent Schrödinger equation

P. B. Visscher

Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama 35487-0324

(Received 9 November 1990; accepted 1 May 1991)

An explicit algorithm for the time-stepping solution of the Schrödinger equation is described, which is second-order accurate in time. It is a staggered-time algorithm, in which the real and imaginary parts of the wave function are defined at alternate times. The method combines the speed and simplicity of explicit methods with the accuracy and stability of second-order implicit methods. Because of this simplicity and speed, the algorithm is well suited for pedagogical applications on personal computers, as well as for computation-intensive research applications.

P.B. Visscher, Computers in Physics, **5**, 596 (1991)

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Absorbing boundary conditions

T. Shibata, PRB, **43**, 6760 (1991)

PHYSICAL REVIEW B VOLUME 43, NUMBER 8 15 MARCH 1991-I

Absorbing boundary conditions for the finite-difference time-domain calculation of the one-dimensional Schrödinger equation

Tsugumichi Shibata
NTT LSI Laboratories, 3-1 Morinosato Wakamiya, Atsugi 243-01, Japan
(Received 30 August 1990)

The absorbing boundary conditions for the finite-difference calculation of the time-dependent one-dimensional Schrödinger equation are presented. These are the local boundary conditions that approximate the one-way wave equation of a wave function. The conditions minimize undesirable reflections at the artificial boundaries of the area of computation, thus enabling us to limit the computation area efficiently. The calculations of the transmission coefficient of multibarrier tunneling show the validity of the method.

Absorbing boundary conditions

T. Shibata, PRB, **43**, 6760 (1991)

$$\Psi(x,t) = e^{-i(\omega t - kx)}$$

$$i\hbar \frac{\partial}{\partial t}\Psi(x,t) = \left[-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial^2 x} + U(x) \right]\Psi(x,t)$$

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$$\hbar^2 k^2 = 2m^*(\hbar\omega - U)$$

$$\hbar k = \pm[2m^*(\hbar\omega - U)]^{1/2}$$

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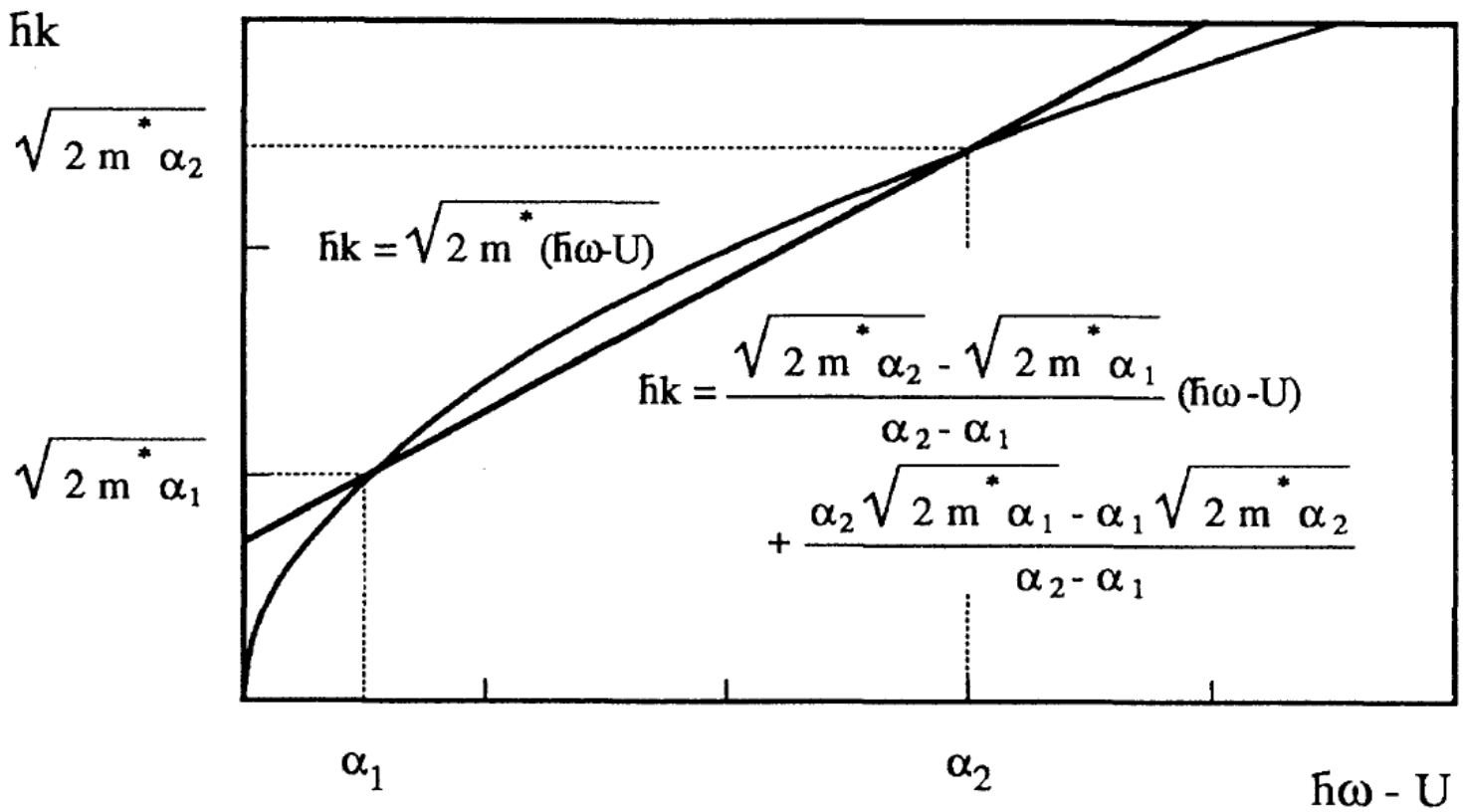
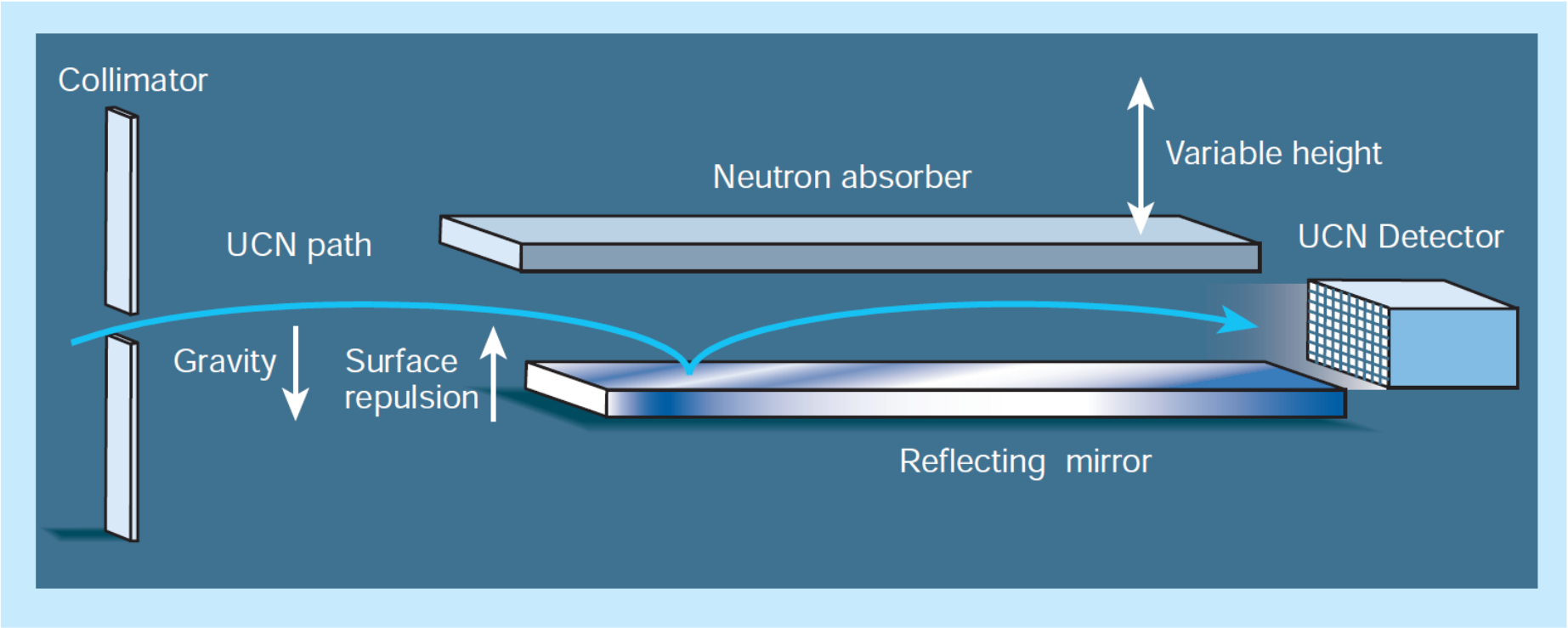


Quantum bouncer realized with neutrons

Nesvizhevsky et. al., *Quantum states of neutrons in Earth's gravitational field*, Nature **415**, 297 (2002).



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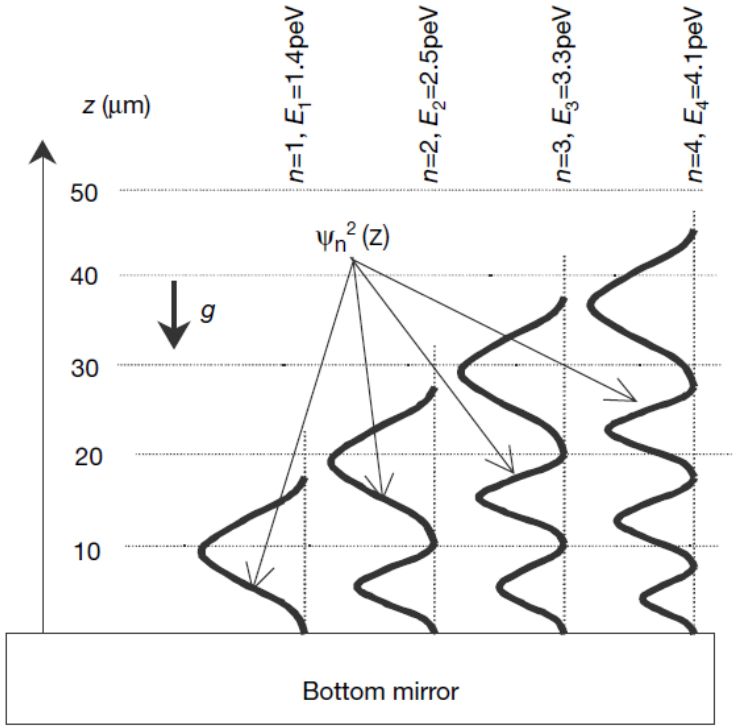
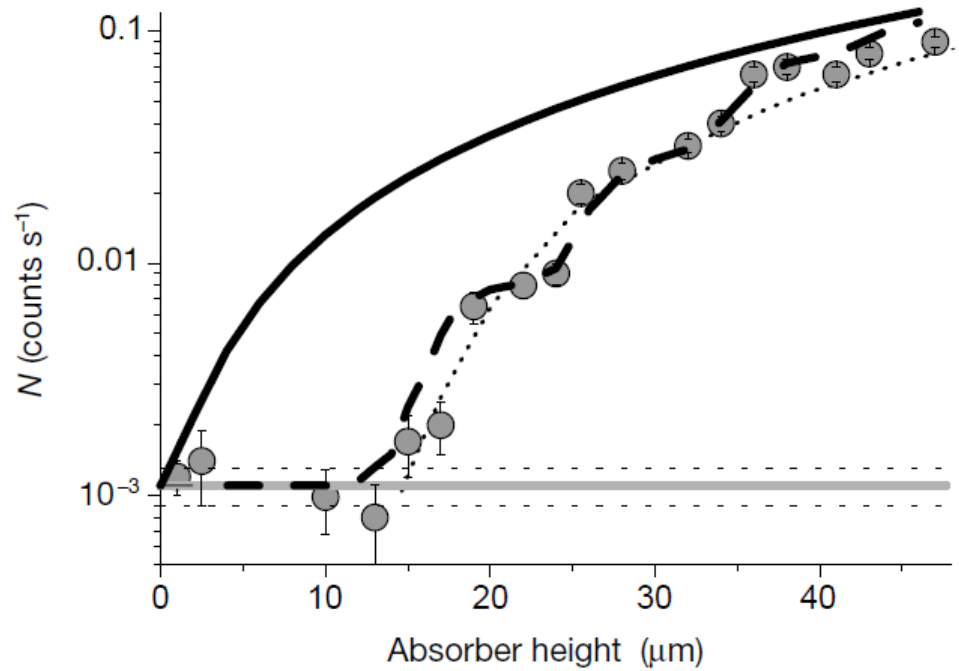


$v_n = 1.7$ cm/s

$h = 14.7$ μm