Abstract.

Basic concepts and principles of quantum mechanics are discussed. One-dimensional as well as two-dimensional simulations of gaussian wave packet's behaviour in short range potential field are performed; the pictures of which are meant to enhance intuitive understanding for beginners.

Contents

Chapter 1 Introduction

§ 1.1 Aim

§ 1.2 Synopsis

§ 1.3 Brief History of Early Quantum Theory

§1.1 Aim

The aim of this thesis is twofold. One is to introduce quantum mechanics to the mechanical engineering students. The other is to discuss the basic concepts and some important principles of quantum mechanics. The approach and style therefore are somewhat pedagogical. However, through and in-depth discussion of the subject-matter will not be undertaken. It is the author's opinion that engineering students need to have at least rudimentary knowledge of quantum mechanics, because it is the very background material that ossify the growth of transistor technology, lazer applications, nuclear engineering, material engineering, chemical engineering ----- the list is not exhausted. Even in our department, there is one subject on atomic reactor lectured by Professor Hirata, which requires the basic knowledge concerning chain reaction. It would be more interesting if we were given some exposure to quantum mechanics and nuclear physics, so as to appreciate the mechanism from the microscopic point of view better. While classical mechanics, electromagnetic theory, thermodynamics and fluid mechanics are included in the curriculum as obligatory subjects, with the objective that we become aware of what is going on inside a steam engine, a hydraulic pump and so on, it is bewildering that not even a subject on modern physics is included. Without the knowledge of classical physics, it is practically impossible to undertake a good portion of mechanical design. And, without the basic knowledge

of modern physics, it is hopeless to widen the scope and plough a new field for fundamental innovation and progress. No doubt Watt did not have any knowledge in thermodynamics, and Edison a total layman of electromagnetism. Yet in modern context where efficiency, optimization and compactness are highly valued, we could no longer afford to do trial-and-error with high technology. In this sense, it is required that each engineer knows the behaviour and properties of matter thoroughly, not only at the macroscopic level but also at the microscopic scale. Protein engineering, for example, deals with the molecular structure of protein, and it goes without saying that protein engineer is required to first understand, then apply the basic sciences of microscopic realm.

I was given the task to produce intuitive pictures of microscopic phenomenology. But the sad thing is we still do not have a sound theory to exactly describe how a microscopic particle move as we did for its classical counterpart. There are still open questions, both physical and philosophical, regarding the reality abumbrated by quantum mechanics. These unresolved, paradoxical problems, though very fundamental, and very difficult, do not seem to cast their dire sceptres over the development and applications of quantum mechanics, simply because physicists find that quantum mechanics's predictions tarry so well with experimental results, and that it is replete with possibilities for applications. In fact, solid state physics, plasma physics, particle physics, cosmology, quantum statistical physics, quantum optics and quantum electronics share a great part of their heritage in quantum mechanics. The far

reaching effects of quantum mechanics do not end here: It is the flower-bed that nurtures revolutionary ideas in the recent development of chemistry and biology.

What is the significance of quantum mechanics in mechanical engineering then? It is evident that as yet we still do not witness any direct application of quantum mechanics in mechanical engineering, and the likehood for one in the future is meagre. But I believe, as the technology advances still further, harnessing energy at the atomic, or subatomic level, be it nuclear fission, nuclear fusion or whatever, will become the main stream of generating power. It is necessary then to know how microscopic roam, as much as is necessary for conventional engineers to know what $PV = kT$ means.

§1.2 Synopsis

With the above consideration in mind, I shall endeavour illustrating some important ideas and concepts in quantum mechanics intuitively, by which I mean simulating time-evolutions of quantum mechanical system and displaying them in a visually appealing form. The hardware whereby these simulations are performed is a modest 16-bit personal computer. "C" language is used throughout for coding the algorithms

Brief historical accounts of the development of quantum mechanics is given in §1.3, followed by a general discussion of state functions and the duality of wave and particle. The rest of chapter 2 is devoted to explaining the prerequisites of understanding the simulation pictures. The approach undertaken will be largely in the Schrödinger picture. Wave aspects of particle are featured, for I believe it is easier to start the discourse of quantum mechanics from Schrödinger's point of view. As probabilistic interpretation of Schrödinger equation is adopted, concepts such as probability density function, expectation value are elucidated Chapter 3 is devoted to the explanation of fundamental principles of quantum mechanics. With this minimum exposure, we shall look into some simple quantum mechanical systems and their behaviour in a potential field, which forms the subject matter of simulation. In chapter 5, the nature of computer experiment is discussed. Chapter 6 gives brief outlines of the method of producing simulation

pictures. Some qualitative comments on the pictures are made. The whole work is summarised at the last chapter, together with some speculations on the possible candidates for same treatment.

§1.3 Brief History of Early Quantum History

Towards the end of 19th century, most of the physical observations were explicable within Newtonian mechanics and Maxwellian electromagnetism. In 1893, Wien studied the thermal radiation of blackbody and discovered a relation between the wave length of the maximum spectral radiancy λ_m and absolute temperature T, which is known as Wien's displacement law.

$$\lambda_m T = \text{constant}$$

He deduced from thermodynamical point of view that the energy denisty distribution ρ is related to frequency ν and absolute temperature T as

$$\rho(\nu, T) = \nu^3 f(\nu/T)$$

where he determined empirically $f(\nu/T)$ to be

$$f(\nu/T) = \frac{\alpha}{c^2} \exp(-\beta\nu/T)$$

Here, α and β were obtained from experiment data, c being the speed of light.

But $f(\nu/T)$ was at conflicts with experiment values when $\frac{\nu}{T}$ was getting small.

On the other hand, Rayleigh and Jeans did some calculations of the energy density of blackbody radiation using classical kinetic theory and found it to be

$$\rho(\nu)\,d\nu = \frac{8\pi\nu^2 kT}{c^3}\,d\nu$$

where k is Boltzmann constant.

However this expression did not predict realistic values when the frequency was large. Worst still, this expression is divergent because ν is second order.

Then, M. Planck was led to speculate the possibility of a violation of the law of equipartition of energy on which the theory was based. His revolutionary idea was to consider the radiation energy as discrete variable, instead of as the continuous variable of which classical theory is purporting. Furthermore, the energy could take on only certain discrete values, which were uniformly distributed. In 1900, "On the Theory of the Energy Distribution Law of the Normal Spectrum" was read to the German Physical Society. He succeeded in deriving the energy density distribution which explained remarkably well all experiment data!

$$\rho(\nu)\,d\nu = \frac{8\pi h}{c^3}\,\frac{1}{e^{\frac{h\nu}{kT}} - 1}\,\nu^3\,d\nu$$

Here $h = 6.625 \times 10^{-34}$ J·sec was named after him.

The idea that energy is discrete Einstein assumed to develop a theory for photoelectric effect. Energy content of a quantum is related to the its frequency ν by

$$E = h\nu$$

Einstein's photoelectric theory also scored highly in realistic predictions.

In 1913, Bohr postulated a quantization condition

$$\oint p_\theta \, d\theta = nh$$

when he sought to propose a model for hydrogen atom. He ruled that the angular momentum p_θ of orbiting electrons, after integration with respect to angle θ for a full cycle, must be a discrete multiple of Planck's constant. From this assumption, he was able to explain quantitatively the energy spectra of hydrogen atom.

Then, de Broglie in 1924 attempted to give physical meaning to Bohr's quantization condition. He conjectured that it was responsible for the duality of particle and wave, and he predicted that electrons must also possess wave properties. In 1925, Schrödinger wrote down an equation for de Broglie wave, which turned out to be a fundamental equation for all microscopic particles.

Chapter 2 Basic Concepts

§ 2.1 Particle and Wave

§ 2.2 State Function $\Psi(x,t)$

§ 2.3 Physical Quantities and Operators

§ 2.4 Schrödinger Equation

§ 2.1 Particle and Wave

In Newtonian as well as Einsteinian mechanics, the concept of particle is indispensable for rigorous formalism. It is also meaningful and intuitively favourable to idealise physical objects with particles, so as to simplify the description of myriad natural phenomena into aesthetically compact form. In Maxwellian theory, the concept of wave is integral to the mathematical construct, whereby all the electrical and magnetic properties of matter are described. Though we can not visualize electromagnetic radiation, it is not too difficult to imagine with the analogy of water wave one that extends spatially without limits and displays periodic characteristics all the time. Thus, particle and wave, as postulated in classical physics, are totally different concepts invented for different purposes; they are antonymous. Particle is understood as a point, while wave a field; they are completely incompatible. So there is no confusion.

However, this dichotomy breaks down at the microscopic level. In quantum mechanics, particle is no longer the well-meant particle, and wave is not really a wave. Indeed, both the particle and wave aspects have to be taken into account to explain the overwhelming experiment facts. The behaviour of matter at microscopic realm serves as a good illustration of how classical concepts, which are basically meant for macroscopic description, fail frequently in the task of acquiring unambiguous meanings. The first step towards understanding quantum mechanics is to discard away the classical

notions of particle and wave. As a prerequisite, one must not be too obsessed with strictly deterministic interpretation of equations of motion that are supposed to predict the behaviour of microscopic entities. If one insists that, since a celestial body orbits exactly on some mathematically charted route, a microscopic particle must also follow a well-defined locus, he will not be able to accept quantum mechanics as it is.

What then, is the equivalent of particle or wave ?

The answer to this equation is best answered by the following formulae.

$$E = \hbar\omega \qquad (1.a)$$

$$\mathbb{P} = \hbar\mathbb{k} \qquad (1.b)$$

They say that a "particle" with energy E and momentum $\mathbb{P}$ is not distinguishable from a wave with angular frequency ω and wave number $\mathbb{k}$. Conversely, a wave that propagates with angular frequency ω and wave number $\mathbb{k}$ is compatible to a particle with energy E and momentum $\mathbb{P}$. $\hbar$ is Planck's constant divided by 2π.

Notice that $\hbar = 1.0546 \times 10^{-34}$ Joule $\cdot$ s is very small and hence particle-wave duality fades away if E and $\mathbb{P}$ take on the typical macroscopic values. For instance, a macroscopic object travelling with momentum 1 kg m/s has, according to (1.b) wave-number of magnitude 1.0546×10^{34} m^{-1}. The wavelength is $\lambda = \frac{2\pi}{k} \sim 10^{-34}$ m, which is less than the typical

dimension of macroscopic object. Therefore no wave property is physically observable. In other words, particle is strictly particle.

In the case of electromagnetic radiation, the corpuscular character of light is concluded from Planck's studies on blackbodies' radiation and by Einstein's theory of photoelectric effects. Energy E is absorbed and radiated in discrete package $\hbar\omega$ called quantum, or photon. On the other hand, when homogeneous beam of electrons passes through parallel slits, it is diffracted in the manner of a monochromatic wave with de Broglie wavelength λ. These experimental facts are summarised into relations (1.a) and (1.b).

One must be reminded that particle and wave are no more than convenient names. It is misleading to think that quantum mechanical entities are wave-particles, or particle-waves. We are only borrowing intuitive ideas from classical physics to connotate the phenomenological properties of quantum mechanical entities, simply because they are very similar to the classical ones. The true nature of fundamental existence of photons, electrons and so on are still not within our intellectual grips, although there are many plausible theories to categorise the whole range of interactions among the so-called elementary particles.

§2.2 State Function $\Psi(x,t)$

A state function is a convenient mathematical representation of quantum-mechanical system, constructed in such a way that information on its state may be derived. By itself it has no physical substance; it is not the wavy path in which particle moves either. But its norm $\|\Psi(x,t)\|^2$ is proportional to the probability density function which details the mode of existence in space at a particular time. Here, quantum-mechanical system is understood as the physical entity analogous to that which is represented by the concept of particle in classical mechanics. It is written a priori as

$$\Psi(x,t) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int A(k,t)\cdot\exp[i(kx-\omega t)]\,d^3k \qquad (2.a)$$

$$A(k,t) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int \Psi(x,t)\cdot\exp[-i(kx-\omega t)]\,d^3x \qquad (2.b)$$

Note here that this pair of expressions is Fourier transform one another.

These two expressions are dual: if we want to know the state function with coordinates as variables, then we must gather all the components of different wave number k together and weigh them by their respective exponential phases. Conversely, if we wish to look at the state function with wave number k as variables, then we must take into consideration all the possible contributions from different localities weighed against their exponential phases. Idea to write state function thus comes from classical wave mechanics

where, according to Fourier theorem, the most general wave is written in the following form:

$$u(x,t) = \int A(k,t) \cos(kx - \omega t + \delta(k))\, d^3k$$

This is nothing but a superposition of waves with all sorts of wave numbers but same angular frequency. (See Appendix A)

A wave function $\frac{\pi}{2}$ radians out of phase is:

$$v(x,t) = \int A(k,t) \sin(kx - \omega t + \delta(k))\, d^3k$$

In quantum mechanics, we postulate that the state function is a generalization of real-valued wave functions, just as the set of complex numbers is a generalization of the set of real numbers. Thus we put $\psi(x,t)$ as

$$\psi(x,t) \equiv u(x,t) + iv(x,t)$$

How shall we construe (2a),(2b) so that physically intelligible meanings are obtainable?

Since $\psi(x,t)$ is generally a complex function, we shall consider its norm $\|\psi(x,t)\|^2 = \psi^*\psi$, which is real. In physics, as in other sciences, it is evident that we are measuring physical quantities which are all real numbers. To begin with, we postulate that the probability to find a quantum-mechanical system in the infinitesimal volume dV at time t is proportional to

$$\|\psi(x,t)\|^2 d^3x = \|A(k,t)\|^2 d^3k$$

One must not be misled to think that $\Psi(x,t)$ predicts the trajectory of an individual quantum mechanical system. In practice, there is no such thing as a quantum mechanical system. When we do experiments, we always prepare an ensemble of homogeneous quantum mechanical systems, for example, a steady beam of electrons. It is because of the huge number of these quantum mechanical systems that we are prompted to interprete it probabilistically. With these hundreds and thousands of coherent electrons, we obtain interference patterns and so on. And by measuring their relative intensities, we learn that electrons tend to pin themselves on certain spots more than the other. And this tendency is put into the probability language. Since it is more convenient to tell the story of an electron which is representative of the ensemble, we prefer to talk about the probability density of an electron, rather than the diffraction pattern of the ensemble. This will save us the trouble of considering the number of electrons in the beam.

We say that a state function is normalised if

$$\int \| \Psi(x,t) \|^2 d^3x = 1 \qquad (3)$$

is satisfied. The meaning of this postulate is clear: the probability of finding an quantum mechanical system represented by a state function in the whole space under study is equal to one. In other words, the quantum mechanical system is out there somewhere, we can definitely find it.

Mathematically, for (3) to be valid, $\Psi(x,t)$

must vanish rapidly as $\|x\| \longrightarrow \infty$. Otherwise the integral is divergent. State function therefore must be square integrable.

We may interpret the mathematical statement if $\|x\| \longrightarrow \infty$ then $\psi(x) \longrightarrow 0$ as all quantum mechanical system exists within our Universe.

§2.3 Physical Quantities and Operators

It is a postulate of quantum mechanics that physically observable quantities are to be represented by operators which serve as mathematical tools for grinding physical quantities out of a state function. We operat on the wavefunction with a suitable operator followed by some other mathematical procedures, and we get predictions about the physically observable quantities. Here, we need to know the exact structure of an operator. More often than not, they are designed in such a way that the whole problem is reduced to solving the eigenvalue problem

$$\hat{A}\,\bar{\Psi}_\lambda = a_\lambda \bar{\Psi}_\lambda$$

$\hat{A}$ is operator, and a its eigenvalue which corresponds to the physically observable quantities. This is the well known problem in linear algebra. The state functions will be called eigenfunctions. Take note that although state functions may be a complex function, the eigenvalues, for them to be observable, must be real numbers. This requirement imposes that operator $\hat{A}$ must be Hermitian

$$\hat{A}^+ = A$$

The motivation to introduce operators into the framework may be seen in the following discussion.

Since we consider $\| A(\mathbb{k},t) \|^2 d^3\mathbb{P}$ to be the probability for a quantum mechanical system to move with momentum $\mathbb{k}$, we may write the expectation value as follows

$$\langle p_z \rangle = \int p_z \, A^*(\mathbb{k},t) \, A(\mathbb{k},t) \, d^3\mathbb{k}$$

$$= \frac{1}{(2\pi)^{\frac{3}{2}}} \int \int p_z \, A^*(\mathbb{k},t) \, \Psi \exp[-i(\mathbb{k}\mathbb{x} - \omega t)] \, d^3\mathbb{x} \, d^3\mathbb{k}$$

Partial integration with respect to z yields

$$-\frac{1}{i k_z} \psi(\mathbb{x},t) \exp[-i(\mathbb{k}\mathbb{x} - \omega t)] \Big|_{-\infty}^{+\infty}$$

$$+ \int \frac{1}{i k_z} \frac{\partial \Psi}{\partial z} \exp[-i(\mathbb{k}\mathbb{x} - \omega t)] \, dz$$

Since $\psi(\mathbb{x},t) = 0$ at $+\infty$ and $-\infty$, the first term is equal to 0. Because $p_z = \hbar k_z$, we have

$$\langle p_z \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \int \int A^* \left(\frac{\hbar}{i}\right) \frac{\partial \psi}{\partial z} \exp(-i(\mathbb{k}\mathbb{x} - \omega t)) \, d^3\mathbb{x} \, d^3\mathbb{k}$$

From (2.2.1a),

$$\psi^*(\mathbb{x},t) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int A^*(\mathbb{k},t) \exp(-i(\mathbb{k}\mathbb{x} - \omega t)) \, d^3\mathbb{k}$$

Finally we get

$$\langle p_z \rangle = \int \psi^* \left(\frac{\hbar}{i}\right) \frac{\partial \psi}{\partial z} \, d^3\mathbb{x}$$

To simplify the calculation of the expectation value of p_z, we may put formally

$$\hat{P}_z \equiv \frac{\hbar}{i}\frac{\partial}{\partial z} \tag{4}$$

Then,

$$\langle P_z \rangle = \int \Psi^* \hat{P}_z \Psi \, d^3x$$

This is a smarter way to calculate. We generalize it to other components and write them conveniently as

$$\hat{\mathbb{P}} = \frac{\hbar}{i}\nabla$$

In the same manner, we may define the angular momentum operator and energy operator respectively as

$$\mathbb{L} = \mathbb{r} \wedge \mathbb{P} \longrightarrow \hat{\mathbb{L}} = \frac{\hbar}{i}\mathbb{r} \wedge \nabla$$

$$E = \frac{P^2}{2m} + U(r) \longrightarrow \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(r)$$

§2.4 Schrödinger Equation

The equation of motion of a state function with mass m in a potential field $U(\vec{r})$ is given by Schrödinger.

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + U(\vec{x})\Psi \quad (5)$$

This is a fundamental equation in quantum mechanics. All the state functions' temporal behaviour is described by it.

Now, consider a quantum mechanical system with a known initial state $\Psi(\vec{x}, 0)$. Suppose that the energy of the quantum mechanical is conservative, ie the Hamiltonian does not increase or increase. We may integrate formally to obtain the state function at time $t > 0$

$$\Psi(\vec{x}, t) = e^{-\frac{i}{\hbar}\hat{H}t}\Psi(\vec{x}, 0)$$

Here, we call $e^{-\frac{i}{\hbar}\hat{H}t}$ an evolution operator. It makes an old state evolve into a new state.

Chapter 3 Basic Principles.

§3.1 The Principle of Superposition

§3.2 Correspondence Principle.

§3.3 Uncertainty Principle

§3.1 The Principle of Superposition

In classical mechanics, the principle of superposition is assumed a priori so that interference phenomena are explicable. In quantum mechanics, with same motive, the state functions are also assumed to be linear. Suppose a quantum mechanical system can take on two states, ψ_1 and ψ_2. Then it can also take on the states

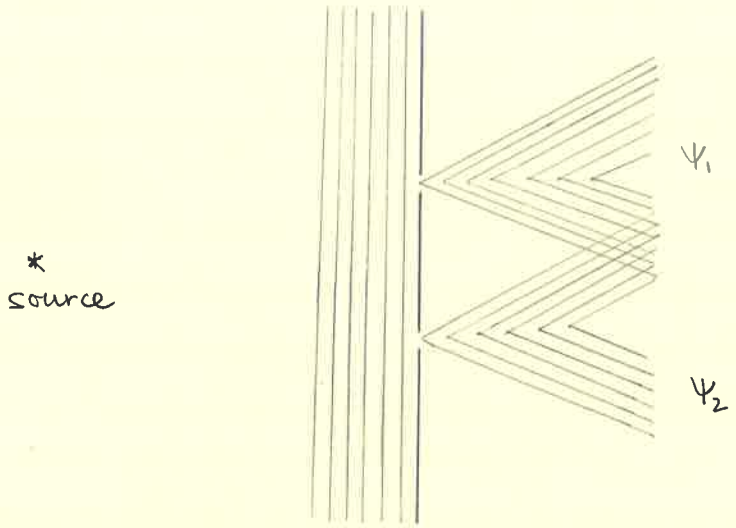
$$\psi = a_1\psi_1 + a_2\psi_2 \qquad (1)$$

where a_1 and a_2 are arbitrary complex numbers which serve as weights to indicate that ψ looks more like ψ_1 if $|a_1| > |a_2|$, and vice versa.

This principle, though gets its idea from classical mechanics, has no parallel in Newtonian mechanics. With this principle in store, the diffraction pattern of electrons can be explained easily.

In the homogeneous beam — double slits experiment, we may make use of superposition principle to denote the quantum mechanical system after it has passed the slits by (1) Equivalently, its dual partner can also be written as

$$A = a_1A_1 + a_2A_2 \qquad (2)$$



It must be stressed here that by homogeneous, we mean the state function of source is known. In other words, we have purposed to prepare a pure state function in the beginning. In this case, we create a simple relationship between a_1 and a_2

$$|a_1|^2 + |a_2|^2 = 1$$

This must not be mistaken with a statistical mixture of states: we do not know the state of a quantum mechanical system; all we know is the statistical frequencies to find the system in various possible pure states In other words, the ensemble is not homogeneous; it has

$$\Psi_{\omega_i}(\mathbf{x},t) = \int A(\mathbf{k},t)\exp[i(\mathbf{k}\mathbf{x} - \omega_i t)]\, d^3\mathbf{k}$$

$$\omega_i \neq \omega_j \qquad (i \neq j)$$

mixed together. In this case, we can not write a state

function for π, because we do not have exact information on which state the system is in. An example of statistical mixture is an unpolarised light source. The polarization vectors have different directions. And we do not know which direction is π pointing at

§3.2 Correspondence Principle

Let's start from Schrödinger equation (5) of §2.4

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right) \psi^* \qquad (3)$$

We shall take $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})$ to be time conservative and $V(\mathbf{r})$ a real function.

The complex conjugate is

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) \right) \psi^* \qquad (4)$$

The expectation value of x coordinate is

$$\langle x \rangle = \int \psi^* x \psi \, d^3x \qquad \text{then}$$

$$\frac{d}{dt}\langle x \rangle = \int \frac{d\psi^*}{dt} x\psi + \psi^* x \frac{d\psi}{dt} \, d^3x$$

$$= -\frac{i\hbar}{2m} \int \nabla^2\psi^* \cdot x\psi - \psi^* x \nabla^2 \psi \, d^3x$$

$$= \int \nabla\psi^* \, x\psi - \psi^* x \nabla\psi \, d^2x$$

$$+ \frac{i\hbar}{2m} \int \nabla\psi^* \cdot \nabla(x\psi) - \nabla(\psi^* x)\nabla\psi \, d^3x$$

We have carried out partial integration. When $|x| \to \infty$, $\psi \to 0$, $\nabla\psi \to 0$, therefore the surface integral vanishes. Because $\nabla x = (1,0,0)$, we obtain

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int \frac{\partial\psi^*}{\partial x}\psi - \psi^*\frac{\partial\psi}{\partial x}\, d^3x$$

Now $$\int \psi^*\frac{\partial\psi}{\partial x}\, d^3x = \int \psi^*\psi\, d^2x - \int \frac{\partial\psi^*}{\partial x}\psi\, d^3x$$

$$= -\int \frac{\partial\psi^*}{\partial x}\psi\, d^3x$$

$$\therefore \quad \frac{d}{dt}\langle x\rangle = \frac{i\hbar}{m}\int \frac{\partial\psi^*}{\partial x}\psi d^3x \qquad (5)$$

We shall differentiate with respect to time t again.

$$m\frac{d^2}{dt^2}\langle x\rangle = i\hbar\int \frac{\partial^2\psi}{\partial x\partial t}\psi + \frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial t}\, d^3x \qquad (6)$$

Substitute in (3) and (4) into (6), and simplify,

$$m\frac{d^2}{dt^2}\langle x\rangle = \int \frac{\hbar^2}{2m}\{\nabla^2\frac{\partial\psi^*}{\partial x}\cdot\psi - \frac{\partial\psi^*}{\partial x}\cdot\nabla^2\psi\} - \frac{\partial V}{\partial x}\psi^*\psi\, d^3x$$

$$= \int \frac{\hbar^2}{2m}\nabla\cdot\{\nabla\frac{\partial\psi^*}{\partial x}\cdot\psi - \frac{\partial\psi^*}{\partial x}\cdot\nabla\psi\} - \frac{\partial V}{\partial x}\psi^*\psi\, d^3x$$

Since $\int \nabla\cdot\{\nabla\frac{\partial\psi^*}{\partial x}\cdot\psi - \frac{\partial\psi^*}{\partial x}\nabla\psi\}\, d^3x$ upon partial integration is a surface integral which vanishes, finally we have

$$m\frac{d^2}{dt^2}\langle x\rangle = -\int \psi^*\frac{\partial V}{\partial x}\psi\, d^3x$$

$$= -\langle\frac{\partial V}{\partial x}\rangle = \langle F_x\rangle \qquad (7)$$

This is nothing but Newton's second law!

From (5) and (4) of §2.3,

$$m \frac{d}{dt}\langle x \rangle = \langle p_x \rangle \qquad (8)$$

This is none other than the definition of momentum in classical mechanics !

Equation (7) and (8) are the expressions of Ehrenfest's theorem.

Thus, we see that the expectation values of quantum mechanical system corresponds to the respective physical quantities of classical particle.

It can also be proved that Schrödinger equation is invariant under Galilei transformation. When $\rho = \psi^* \psi$ is interpreted as the probability density function, Schrödinger equation is also invariant under time reversal.

These properties are inherently important for crediting Schrödinger equation as an extension of Newton second law.

§3.3 Uncertainty Principle.

To make the discussion simple, we shall consider the 1-dimensional state function.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int A(k,t) \exp[i(kx - \omega t)]\, dk$$

Same arguments apply to 3-dimensional case.
At time $t = 0$, we write simply

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int A(k) \exp(ikx)\, dk. \qquad (1)$$

The Fourier transform is

$$A(k) = \frac{1}{\sqrt{2\pi}} \int \Psi(x) \exp(-ikx)\, dx \qquad (2)$$

As we have shown A and Ψ are symmetric. Furthermore, if Ψ is normalised, we get the famous Parseval formula

$$\int \Psi^*(x) \Psi(x)\, dx = \int A^*(k) A(k)\, dk = 1$$

Up to now, we are only reviewing what was discussed earlier

We are interested in the variances of locality and momentum. Therefore we consider the following quantities

$$\langle \delta x \rangle^2 = \langle (x - \langle x \rangle)^2 \rangle$$

$$\langle \delta k \rangle^2 = \langle (k - \langle k \rangle)^2 \rangle$$

For the time being, let us set up a coordinates system such that $\langle x \rangle = \langle k \rangle = 0$. To calculate $\langle k^2 \rangle$, all we have to do is but repeating the same procedures in section 2.5 twice.

$$\langle k^2 \rangle = \int \psi^*(x) \left(-\frac{\partial^2}{\partial x^2} \right) \psi(x)\, dx = \int \frac{\partial A^*}{\partial x} \cdot \frac{\partial A}{\partial x}\, dx$$

$\langle x \rangle$ and $\langle x^2 \rangle$ are calculated dually. We have

$$\langle x \rangle = \int A^*(k)\, i \frac{\partial}{\partial k} A(k)\, dk$$

$$\langle x^2 \rangle = \int \psi^*(x) \left(-\frac{\partial^2}{\partial x^2} \right) \psi(x)\, dx$$

Furthermore, we can do one more time partial integration for $\langle x^2 \rangle$ and $\langle k^2 \rangle$.

$$\langle x^2 \rangle = \int \frac{\partial A^*}{\partial k} \frac{\partial A}{\partial k}\, dk$$

$$\langle k^2 \rangle = \int \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x}\, dx$$

We will not integrate these expressions directly. Instead let

$$\Delta \equiv \left| \frac{x}{2\langle x^2 \rangle} \psi(x) + \frac{\partial \psi}{\partial x} \right|^2 \geq 0 \qquad (3)$$

$$\Delta = \frac{x^2}{4\langle x^2 \rangle^2} \psi\psi^* + \frac{x}{2\langle x^2 \rangle} \left(\psi \frac{\partial \psi^*}{\partial x} + \psi^* \frac{\partial \psi}{\partial x} \right) + \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x}$$

$$= \frac{1}{4} \left(\frac{x}{\langle x^2 \rangle} \right)^2 \psi\psi^* + \frac{1}{2} \cdot \frac{\partial}{\partial x} \left(\frac{x}{\langle x^2 \rangle} \psi\psi^* \right) - \frac{1}{2} \frac{1}{\langle x^2 \rangle} \cdot \psi\psi^*$$

$$+ \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x}$$

$$= \frac{1}{4}\frac{1}{\langle x^2\rangle^2}(x^2 - 2\langle x^2\rangle)\psi\psi^* + \frac{1}{2}\frac{\partial}{\partial x}\cdot\left(\frac{x}{\langle x^2\rangle}\psi\psi^*\right)$$

$$+ \frac{\partial\psi}{\partial x}\frac{\partial\psi^*}{\partial x}$$

Integrate Δ, and make use of expressions

$$\int \Delta(x)\,dx = -\frac{1}{4\langle x^2\rangle} + \langle k^2\rangle$$

Since $\Delta(x) \geq 0$, we have

$$\langle k^2\rangle\langle x^2\rangle \geq \frac{1}{4}$$

After a translation of coordinates,

$$\langle \delta k\rangle^2\langle \delta x\rangle^2 \geq \frac{1}{4}$$

Define

$$\Delta k \equiv \sqrt{\langle \delta k\rangle^2}$$

$$\Delta x \equiv \sqrt{\langle \delta x\rangle^2}$$

$$\Delta p \equiv \sqrt{\langle \delta p\rangle^2}$$

We have

$$\Delta k\,\Delta x \geq \frac{1}{2}$$

therefore

$$\Delta p\,\Delta x \geq \frac{\hbar}{2} \qquad (4)$$

This is the well known Heisenberg uncertainty relations. It says that if we can locate a quantum mechanical

system within an uncertainty Δx, then uncertainty in its momentum must be equal or greater than $\frac{\hbar}{2\Delta x}$. If we know the location of quantum mechanical system very well, so that Δx is arbitrarily small, then Δp tends to infinity! Therefore, in principle, we can not know precisely the location and momentum at the same instance.

This is a consequence that is at odds with the strictly deterministic picture of classical mechanics where knowing a particle's location does not have anything to do with knowing its momentum. In other words, one is allowed to measure x and p with uncertainties Δx and Δp as small as one desires. But here, as we have seen, even in theory, it is impossible to know x and p accurately at the same time.

(4) is derived from the assumption of state functions (1) and (2), and the adoption of a philosophy which tolerates probabilistic statements about the existence of matter. As long as we stick to these postulates, whose introduction as discussed earlier is motivated by the dualism of particle and wave, we must be content with uncertainty principle.

In fact, a careful look at the definition of state function (1) reveals that $\Psi(x)$ is integrated with respect to all the wave numbers k. Therefore there is no way to tell exactly which momentum is associated to the state function $\Psi(x)$. Same things can be said about $A(k)$

Though (4) forbids us to know x and p accurately at the same time, it has many interesting

applications.

Chapter 4 Scattering by Short Range Potential

§ 4.1 Gaussian Wave Packet

§ 4.2 Bound State and Unbound State

§ 4.3 Transmission Coefficient and Reflection Coefficient

§ 4.4 Tunnel Effect and Resonance Scattering

§ 4.5 Cross Section

§4.1 Gaussian Wave Packet

As we have learned, $\psi(x)$ determines the spatial likelihood for a quantum mechanical system to be found. And $A(k)$ determines the likelihood for it to be found travelling with momentum $p = \hbar k$. We also learn that $\Delta x \Delta p \geq \frac{\hbar}{2}$. We are interested to know which type of $\psi(x,t)$ satisfies $\Delta x \Delta p = \frac{\hbar}{2}$. ie one that begets minimum uncertainties. To do so, we set (3) of chapter 3

$$D = 0$$

ie $$\frac{\partial \psi}{\partial x} = -\frac{x}{2\langle x^2 \rangle}\psi$$

then $$\psi(x) = \sqrt[4]{\frac{2a}{\pi}}\exp(-ax^2) \qquad (1a)$$

where $$a = \frac{1}{4\langle x^2 \rangle}$$

Let's see how does $A(k)$ look like

$$A(k) = \frac{1}{\sqrt{2\pi}} \cdot \sqrt[4]{\frac{2a}{\pi}} \int \exp[-ax^2 - ikx]\, dx$$

$$= \frac{1}{\sqrt{2\pi}} \cdot \sqrt[4]{\frac{2a}{\pi}} \int \exp\left[-a\left(x + \frac{ik}{2a}\right)^2\right] dx \cdot e^{-\frac{k^2}{4a}}$$

$$x + \frac{ik}{2a} \longrightarrow y$$

$$\therefore \quad A(k) = \frac{1}{\sqrt{2\pi}} \sqrt[4]{\frac{2a}{\pi}} \int \exp(-ay^2)\, dy\; e^{-\frac{k^2}{4a}}$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt[4]{\frac{2a}{\pi}} \sqrt{\frac{\pi}{a}}\, e^{-\frac{k^2}{4a}} = \frac{1}{\sqrt[4]{4\pi a}}\, e^{-\frac{k^2}{4a}} \qquad (1b)$$

$A(k)$ is also gaussian! If state function

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int A(k)\, e^{i(kx-\omega t)}\, dk \qquad (2)$$

with $A(k)$ given by (1b), it is named gaussian wave packet.

Consider now a gaussian wave packet moving in a free field. The evolution operator is then $\exp\left(i\frac{\hbar t}{2m}\frac{\partial^2}{\partial x^2}\right)$. Initially, we rewrite (1a) by putting $\sigma_0 = \sqrt{\langle x^2\rangle}$

$$\Psi(x,0) = \frac{1}{\sqrt[4]{4\pi}\sqrt{\sigma_0}}\, e^{-\frac{x^2}{4\sigma_0^2}}$$

We shall employ the following formulae for calculations

$$\frac{\partial^2}{\partial x^2}\frac{e^{-\frac{x^2}{4s^2}}}{s} = \frac{\partial}{\partial(s^2)}\frac{e^{-\frac{x^2}{4s^2}}}{s}$$

$$\exp\left(\frac{i\hbar^2 t}{2m}\right) = \sum_{k=0} \frac{1}{k!}\left(\frac{i\hbar t}{2m}\right)^k \frac{\partial^{2k}}{\partial x^{2k}}$$

$$\therefore \exp\left(\alpha\frac{\partial}{\partial(s^2)}\right) f(s^2) = \sum \frac{\alpha^k}{k!}\frac{\partial^k}{\partial(s^2)^k} f(s^2) = f(s^2+\alpha)$$

$|\alpha| \ll 1$

These formulae speak for themselves. We now operate on $\Psi(x,0)$ the evolution operator

$$\Psi(x,t) = \exp\left(\frac{i\hbar t}{2m}\frac{\partial^2}{\partial x^2}\right) \frac{1}{(2\pi)^{\frac{1}{4}}\sigma_0^{\frac{1}{2}}}\, e^{-\frac{x^2}{4\sigma_0^2}}$$

$$= \frac{\sigma_0^{\frac{1}{2}}}{(2\pi)^{\frac{1}{4}}} \exp\left(\frac{i\hbar t}{2m}\frac{\partial^2}{\partial x^2}\right) \frac{e^{-\frac{x^2}{4\sigma_0^2}}}{\sigma_0}$$

$$= \frac{\sigma_0^{\frac{1}{2}}}{(2\pi)^{\frac{1}{4}}} \exp\left(\frac{i\hbar t}{2m}\frac{\partial}{\partial(s^2)}\right) \frac{e^{-\frac{x^2}{4\sigma_0^2}}}{\sigma_0}$$

$$= \frac{\sigma_0^{\frac{1}{2}}}{(2\pi)^{\frac{1}{4}}} \frac{1}{(\sigma_0^2 + i\hbar t/2m)^{\frac{1}{2}}} \exp\left[-\frac{x^2}{4(\sigma_0^2 + i\hbar t/2m)}\right]$$

This is none other than the explicit expression of (2)

Probability density function is then

$$\rho = \Psi^* \Psi$$

$$= \frac{1}{(2\pi)^{\frac{1}{2}}} \frac{\sigma_0}{(\sigma_0^4 + \hbar^2 t^2/4m^2)^{\frac{1}{2}}} \exp\left(-\frac{\sigma_0^2 x^2}{2(\sigma_0^4 + \hbar^2 t^2/4m^2)}\right)$$

$$= \frac{1}{(2\pi)^{\frac{1}{2}}} \frac{1}{(\sigma_0^2 + \hbar^2 t^2/4m^2\sigma_0^2)^{\frac{1}{2}}} \exp\left(-\frac{x^2}{2(\sigma_0^2 + \hbar^2 t^2/4m^2\sigma_0^2)}\right)$$

$$= \frac{1}{(2\pi)^{\frac{1}{2}}\sigma} \exp\left(-\frac{x^2}{2\sigma}\right)$$

where $\sigma^2 = \sigma_0^2 \left(1 + \frac{\hbar^2 t^2}{4m^2\sigma_0^4}\right)$

Initially $\rho_0 = \Psi_0^* \Psi_0 = \frac{1}{(2\pi)^{\frac{1}{2}}\sigma_0} \exp\left(-\frac{x^2}{2\sigma_0}\right)$

Therefore we see that the probability density function spreads out as t evolves. How shall we account for this phenomenon?

From Ehrenfest's theorem (7) (8) of § 3.2

$$m\frac{d^2}{dt^2}\langle x\rangle = \frac{d}{dt} m \frac{d}{dt}\langle x\rangle = \frac{d}{dt}\langle p\rangle = 0$$

Since the gaussian wave packet is moving in a free region. Therefore we know that the average momentum does not change. This is self-evident intuitively ——— asmuch as external force is not exerted upon π, its momentum changes not

From (2) π is easy to see that its Fourier transform is

$$A(k,t) = A(k)\, e^{-i\omega t}$$

$$= \frac{1}{\sqrt[4]{2\pi a}} e^{-\frac{k^2}{4a} - i\omega t}$$

We see also that the width of $A(k,t)$ does not change too. In other words, its momentum dispersion $\hbar\Delta k$ is a constant when the gaussian wave packet is free. The velocity of the wave packet is known therefore within

$$\Delta v \approx \frac{\Delta p}{m} = \frac{\hbar \Delta k}{m} = \frac{\hbar\sqrt{a}}{m}$$

This is responsible for the spreading of wave packet! Because as time ticks on,

$$\Delta x \approx \Delta v \cdot t$$

Thus, we conclude that because of uncertainty principle, the width of a wave packet spreads as it evolves

§4.2 Bound State and Unbound State

At a certain fixed time, if a state function $\psi(x)$ satisfies the following conditions, it is said to be in bound state.

i) $\psi(x)$ is square integrable:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx < \infty$$

and ii) It is an eigenfunction of time dependent Schrödinger equation.

$$\hat{H}\psi(x) = E\psi(x)$$

where $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

and E is an eigenvalue

We may rewrite Schrödinger equation and the imposed boundary conditions as

$$\begin{cases} \frac{d}{dx}\left(\frac{\hbar^2}{2m}\frac{d}{dx}\psi(x)\right) - V(x)\psi(x) + E\psi(x) = 0 \\ \lim_{x \to \pm\infty} \psi(x) = 0 \end{cases}$$

This is the well known Sturm-Liouville eigenvalue problem (See Appendix B). It is known that

a) eigenvalue E is real and takes on discrete values which are countable infinite in number.

b) the eigenfunctions $\psi_n(x)$ form an orthonormal system.

$$\int \psi_n^*(x)\,\psi_m(x)\,dx = \delta_{nm}$$

On the other hand, an unbound state corresponds to those state functions which do not satisfy (i) and (ii) simultaneously. Because we have defined a state function to vanish at $x = \pm\infty$, and that after normalization

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\,dx = 1$$

, so as to make probabilistic interpretation possible, we conclude that an unbound state does not satisfy condition (ii), ie. it does not satisfy time-independent Schrödinger equation. Therefore it can not be stationary.

The energy spectrum of unbound state, contrary to the bound state's, is continuous. This is self-evident

§4.3 Transmission Coefficient and Reflection Coefficient

Though an unbound state function does not satisfy time-independent Schrödinger equation, we may represent it as a superposition of non-square-integrable exponentials $e^{\pm ikx}$. This is justifiable because from the very beginning we have introduced (2.a) which is a continuous superposition of exponentials $e^{\pm ikx}$ with $A(k)$ as weight.

This being the reason, it is still worthwhile to consider the 'components' $e^{\pm ikx}$.

Apparently $e^{\pm ikx}$ satisfy

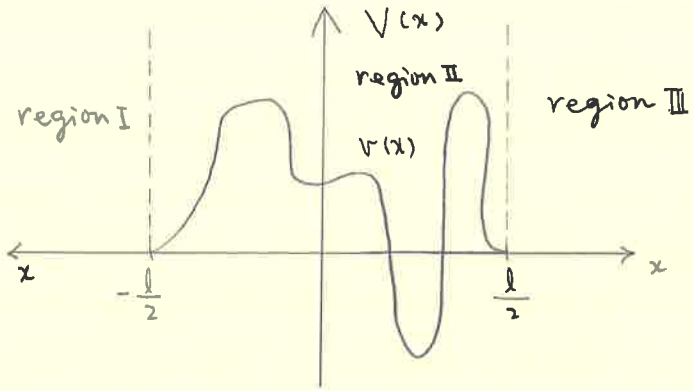
$$\left\{ \frac{d^2}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)] \right\} \psi(x) = 0 \qquad (2)$$

For the sake of simplicity, take $V(x)$ to be

$$V(x) = \begin{cases} v(x) & |x| \leq \frac{1}{2} \\ 0 & |x| \geq \frac{1}{2} \end{cases}$$

where $v(x)$ is any arbitrary function.

Consider the plane wave components $e^{\pm i(kx-\omega t)}$ of a state function interacting with the potential $V(x)$.



Here $e^{\pm ikx}$ satisfy (2) with

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{when} \quad |x| > \frac{l}{2}$$

The most general solution of * for a given value of E is a linear superposition of e^{ikx} and e^{-ikx}.

$$\begin{cases} \text{at region I} & \varphi_k(x) = Ae^{ikx} + Be^{-ikx} \\ \text{at region III} & \varphi_k(x) = Ce^{ikx} + De^{-ikx} \end{cases}$$

where A, B, C, D are arbitrary complex numbers.

Specifically, we shall consider plane wave $e^{i(kx-\omega t)}$ approaching the potential from the left. Since the complex conjugate is $e^{-i(kx+\omega t)}$, which represents a wave travelling in the negative x direction, D must be equal to zero. The general solution becomes

$$\begin{cases} \text{at region I} & \varphi_k(x) = Ae^{ikx} + Be^{-ikx} \\ \text{at region III} & \varphi_k(x) = Ce^{ikx} \end{cases}$$

In this context, we define $T \equiv \left|\frac{B}{A}\right|^2$ and $R = \left|\frac{C}{A}\right|^2$

as reflection coefficient and transmission coefficient respectively. Here, we witness again the strife between classical mechanics and quantum mechanics. According to the classical theory, a particle approaching a potential will pass through its sphere of influence if its total energy E is greater than the maximum value of $V(x)$, and will be reflected back if E is less than the maximum value of $V(x)$. However, in the case we have just discussed, a quantum mechanical system, whatever its total energy, has in general a finite probability of passing through the barrier, and a finite probability of being reflected from it.

The reflection coefficient and transmission coefficient are generally a function of wave number k and the explicit form of potential $V(x)$. By the law of conservation of matter

$$T + R = 1$$

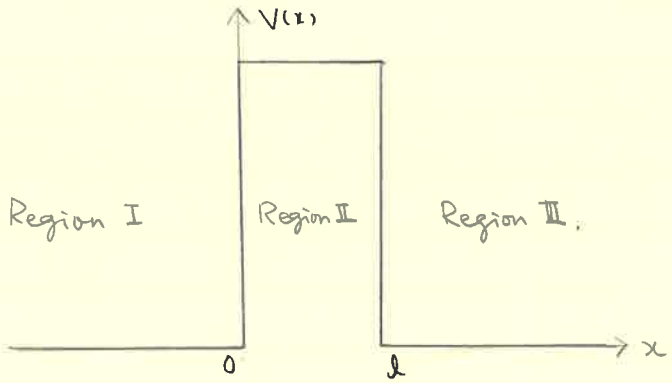
§4.4 Tunnel Effect and Resonance Scattering

In this section, we shall discuss one simple case which serve to illustrate two important phenomena in quantum mechanics.

First, consider the potential to be

$$V(x) = \begin{cases} +V_0 & \text{when } 0 \leq x \leq l \\ 0 & \text{otherwise} \end{cases}$$

This is the simplest potential among the potential barriers



We may consider 2 cases: $E > V_0$ and $E < V_0$. We shall consider the case $E > V_0$ first. It is easy to write down the general solutions to * for region I, II and III with the notations

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

Region I	$\varphi_I(x) = A_1 e^{ik_1 x} + A_1' e^{-ik_1 x}$	3a
Region II	$\varphi_{II}(x) = A_2 e^{ik_2 x} + A_2' e^{-ik_2 x}$	3b
Region III	$\varphi_{III}(x) = A_3 e^{ik_1 x} + A_3' e^{-ik_1 x}$	3c

Again, let us assume that the quantum mechanical system approaches the potential from the left. Therefore $A_3' = 0$.

We require that at $x = 0$ and $x = l$, $\varphi(x)$ be smooth. (These conditions are termed matching conditions)

ie.

$$\varphi_I(0) = \varphi_{II}(0)$$

$$\frac{d\varphi_I}{dx}\Big|_{x=0} = \frac{d\varphi_{II}}{dx}\Big|_{x=0}$$

$$\varphi_{II}(l) = \varphi_{III}(l)$$

$$\frac{d\varphi_{II}}{dx}\Big|_{x=l} = \frac{d\varphi_{III}}{dx}\Big|_{x=l}$$

These conditions will help us find an expression for transmission coefficient and reflection coefficient each.

$\therefore$

$$\begin{cases} A_1 + A_1' = A_2 + A_2' \\ ikA_1 - ik_1 A_1' = ik_2 A_2 - ik_2 A_2' \\ A_2 e^{ik_2 l} + A_2' e^{-ik_2 l} = A_3 e^{ik_1 l} \\ k_2 (A_2 e^{ik_2 l} - A_2' e^{-ik_2 l}) = A_3 k_1 e^{ik_1 l} \end{cases}$$

From these expressions,

$$A_1 = \left[\cos k_2 l - i \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin k_2 l \right] e^{ik_1 l} A_3$$

$$A_1' = i \frac{k_2^2 - k_1^2}{2k_1 k_2} \sin k_2 l \, e^{ik_1 l} A_3$$

From these we are able to calculate R and T

$$R = \left| \frac{A_1'}{A_1} \right|^2 = \frac{(k_1^2 - k_2^2)^2 \sin^2 k_2 l}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2 k_2 l}$$

$$T = \left| \frac{A_3}{A_1} \right|^2 = \frac{4k_1^2 k_2^2}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2 k_2 l}$$

It is easy to see that $R + T = 1$

Substitute in k_1 and k_2, we have

$$T = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2 [\sqrt{2m(E - V_0)}\, l / \hbar]}$$

When $T = 1$, we say that resonance occurs. It can be easily seen that the condition for it to take place is

$$k_2 l = n\pi \quad , \; n \text{ is any integer}$$

When this condition is satisfied, the probability for the state function to transmit through the potential barrier is 100%.

Next, we shall consider the case when $E < V_0$

Set

$$\rho_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad \text{in this case}$$

and replace (3b) by

Region II $\quad \psi_{II}(x) = A_2 e^{\rho_2 x} + A_2' e^{-\rho_2 x}$

We shall not repeat the arguments about matching conditions for this case. Simply we replace k_2 by $-i\rho_2$, We then have

$$T = \left|\frac{A_3}{A_1}\right|^2 = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2[\sqrt{2m(V_0 - E)}\, l/\hbar]}$$

$$R = 1 - T$$

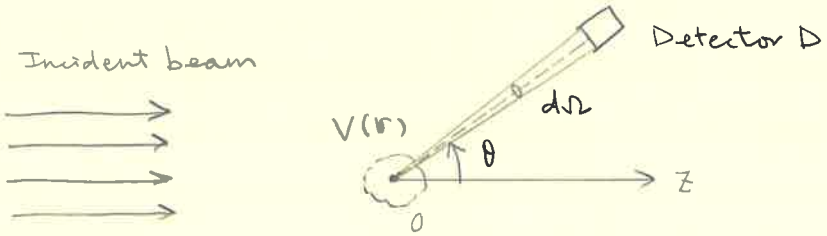
When $\rho_2 l \gg 1$, we see that,

$$T \simeq \frac{16E(V_0 - E)}{V_0^2} e^{-2\rho_2 l}$$

ie. even if the energy of the particle is less than the potential barrier, the quantum mechanical has a non-zero probability of crossing the potential barrier. If $l \lesssim 1/\rho_2$, T is considerably larger, and the quantum mechanical system has a greater chance of crossing the potential barrier, resulting in the so-called "tunnel effect". Josephson effect, the α-decay of certain nuclei, etc are attributable to this effect. In transistors, the tunnel diode is a direct application of this effect.

§ 4.5 Cross Section

Cross section is an important concept in subatomic physics where collisions between incident beams and targets are being examined and studied.



Consider an incoming beam parallel to z-axis, with a flux of particles F_i. A potential $V(r)$ centered at origin 0 scatters the incident beam. Far from the sphere of influence of potential, a detector D measures the number dn of quantum mechanical systems scattered per unit time into the solid angle $d\Omega$, centered around the direction defined by the polar angles θ and φ.

dn is obviously proportional to $d\Omega$ and to the incident flux F_i

$$dn \propto F_i \, d\Omega$$

We shall define $\sigma(\theta, \varphi)$ to be the coefficient of proportionality between dn and $F_i \, d\Omega$

$$dn = F_i \, \sigma(\theta, \varphi) \, d\Omega$$

The dimension of dn and F_i are, respectively, T^{-1} and $(L^2 T)^{-1}$. $\sigma(\theta, \varphi)$ therefore has the dimensions of a

surface. It is called the differential scattering cross section in the direction (θ, φ).

The total scattering cross section σ is defined by the formula

$$\sigma = \int \sigma(\theta, \varphi)\, d\Omega.$$

Intuitively, this may be understood as the part of surface area of the potential's sphere of influence which interacts with the incident beam.

Chapter 5 Computational Physics.

§ 5.1 Introduction

§ 5.2 Computer Experiment

§ 5.3 Merits and Perspective

§5.1 Introduction

The progress in micro-electronics and computer technology has rendered it feasible for physicists to perform the so-called computer experiments. Using high performance hardwares, physicists are able to simulate complicated physical systems with discrete algebraic models, thus carry out numerical experiments, which are either too costly, technologically unfeasible, or physically impossible to perform in the orthodox way. These years, "physics with computer" ——— Computational Physics flourishes extravagantly, and in no time is recognised by the physicists' community as the "third physics" It is a new methodology of studying physics besides the orthodox experimental physics and theoretical physics. While theoretical physics plays the role of synthesizing systematically and speculating certain aspects of Nature into theories, and experimental physics that of extracting ordered information from the laboratory set up of physical systems under the controlled conditions, in computational physics, complicated equations are solved numerically, behaviour of physical systems simulated, models examined and perturbation calculations done with required precision. In one sense, it serves to bridge the gap between theoretical physics and experimental physics.

One of the pioneer works in computational physics, which has ever become a classic, was done in 1950's, when Fermi, Pasta and Ulam (See [Fe65]) chose the problem of energy partition of a nonlinear system as the subject matter for computer experiment. Despite their expectations

that introducing nonlinearity into lattice would cause the mutually independent modes of oscillation to correlate each other and thus result in an energy flow among them, and eventually energy partition would be obtainable, results from the calculations (performed on the Los Almos Computer MANIAC I) showed that even with an anharmonic lattice, energy partition does not take place to a large extent among normal modes of lattice oscillation —— a discovery par excellence.

Zabusky (See [Za69]) then took on the task of explaining the negative results from Fermi, Pasta and Ulam's experiment. He performed numerical experiments which he credited as a "new form of asymptotic or perturbation analysis", and went on to create movies on the dynamically invariant behaviour of solitons, knowing very well "the power to communicate unbiased information in a credible manner is much beyond the power of words, graphs and, often times, equations." He thus proposed to use computer positively in studying the laws of Nature —— the synergetic approach, accordingly is to be highly regarded as a efficient analytical methodology.

Today, nearly all branches of physics capitalise on the calculating power of computer to attempt solving difficult equations. Research works with computers lead to the development of new theories and applications. Perhaps, the representative of all these is K. G. Wilson's lattice gauge theory which employs Monte Carlo's method to inquire the

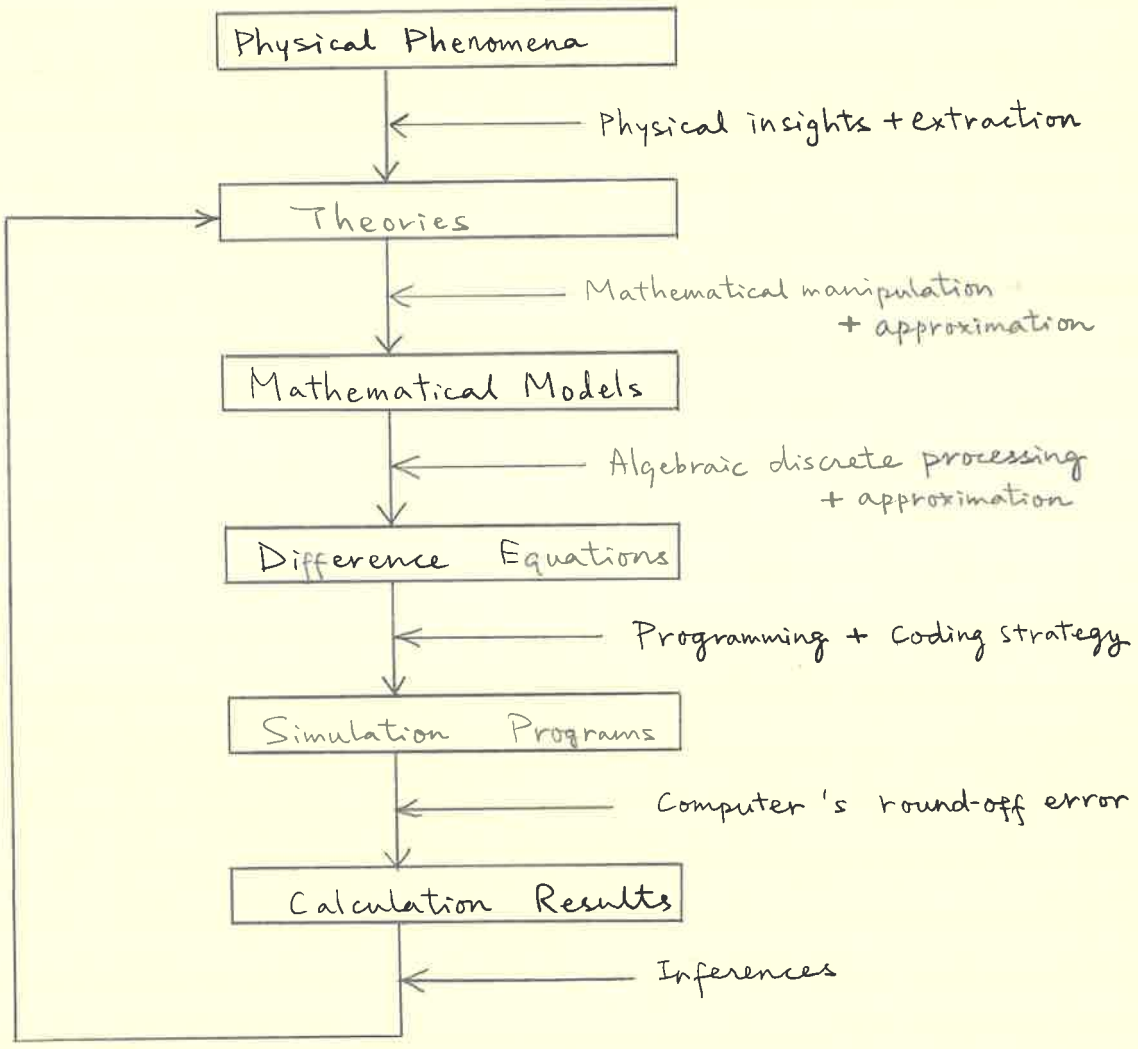
asymptotic behaviour of quark fields.

In fact, this synergetic approach is by no means limited to physics. The ab initio calculation of electronic configuration of molecule, the use of digital picture processing technique in ascertaining the conformal structure of protein, the finite element method for analyzing the stress distribution of a structure of complicated geometry, are only some typical examples of how computer can be of extreme importance. Even in pure mathematics, some ingenious employments of computer to solve problems may spark yet another revolution of ideas.

A comprehensive collection of various fields of computational physics is found in [Su84]

§5.2 Computer Experiment

The flow chart of a computer experiment is given in next page. It must be stressed here that the type of algorithms that one chooses to convert a set of continuous mathematical models into difference equat-tons must be in coherence with the physical aspects under study. This is a golden rule that must be observed strictly, and must be top in priority list. The type of approximation and symmetry conditions aimed at reducing the burden of computation should not bring about any appreciable corruption of the generalities of the problem. At the same time, a computer experimentalists must also work out a strategy to resolve the calculation volumes, so as to obtain optimization in terms of calculation time, memory storage, precision and calculation cost. He must know very well the capabilities and limits of his computer. It is obvious he must make sure that the algorithms are stable. Consistent checks of calculation results should be done assi-duously in the lights of various conservative and invariant properties of the physical systems. These checks will enhance credibility to the calculation results. Whenever possible, the same problem is worth the effort to be solved by another numerical technique of the same order of the accuracy. Stabilization method, predictor-corrector method, component-by-component method etc are available. (See [Ma82]), yet it is still not clear which scheme



Synergetic Approach

works best for a particular problem. Another incentive of course is to compare the subtle differences between the calculation results yielded from different schemes These results from solving equations with different numerical techniques will be different to within, say second order in time step. One must ensure that it is physically significant to consider the case under study to that order.

Basically, there are three categories of computer experiments (See [HE81] for details):

(i) Simulations designed to predict accurately the workings of complex devices in order to allow many variations to be evaluated before expensive technology is employed in constructing the optimal choice

(ii) calculations made to obtain information not readily accessible to laboratory experiments.

(iii) simulations aimed at establishing certain aspects of a theory.

The requirements of precision, time factor and other hardware related problems are different in different categories. One ought to think of effective means of input and output of the programming environment. More often than not, graphical presentation of calculated results is desirable, for it is far more effective to communicate in graphics, rather than sheer tabulation of figures.

§ 5.3 Merits and Perspectives.

What are the merits of a computer experiment ? What is the justification for compromising rigorous solutions with approximate numerics ? Indeed, there are still many orthodox physicists who tend to regard computer experiments as some kinds of fashionable indulgence. Nobel physicist Liftshitz put it more candidly : Computers are spoiling physicists.

But I think, in view of the following merits, this methodology must be continued and further developed as a powerful analytical tool.

(i) We can be as precise as we desire about the assumptions and controlled parameters. Experimental physics does not in practice able to provide absolutely precise and unambiguous controlled environment.

(ii) Readjustments of parameters are easy and effortless.

(iii) It is feasible to construct macroscopic pictures ; dynamical evolutions can be followed step-by-step.

(iv) Some experiments which are not realizable due to technical constraints, even natural constraints can be done easily by computer.

(v) plausibility of a theory can be examined

(vi) Computer experiments may be heuristic as in the Fermi Pasta and Ulam case.

(vii) economy of costs and efforts

(viii) General nonlinear equations are solvable

Furthermore, remarkable advancement in supercomputers, computing techniques, and information processing methods make it more attractive to do computer experiments. With parallel processors and concurrent programming techniques, the time of calculation is shortened, thus enabling even more complicated, and higher dimension calculations to be done reasonably.

To conclude, it must be emphasized that computer experiments should go hand-in-hand with the theoretical and experimental studies. The ultimate justification of all calculations lies at the mercy of Nature.

Chapter 6 Comments

§ 6.1 Method

§ 6.2 Programming Environment

§ 6.3 One-dimensional Simulation Pictures

§ 6.4 Two-dimensional Simulation Pictures

§ 6.1 Methods

It was Goldberg, Schey and Schwarz who began the pioneer work (See [GSS67]). They discussed in details methods of solving Schrödinger equation numerically. And it was Galbraith, Ching and Abraham who used partial-wave analysis to discuss two dimensional scattering events (See [GYA83])

To solve Schrödinger equation numerically, one starts from an initial condition and evolution operator (See § 2.4) This is our mathematical model

$$\Psi(x,t) = \exp\left(-\frac{i}{\hbar} t \hat{H}\right) \Psi(x,0) \qquad (1)$$

where

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(x)$$

We shall choose a convenient unit so that

$$\hbar = 1 \qquad m = \frac{1}{2}$$

The initial state function is gaussian wave packet

$$\Psi(x,0) = e^{-\frac{|x-x_0|^2}{2\sigma_0^2}} e^{i k_0 x}$$

with initial position x_0 and average momentum k_0

The next step will be writing a difference scheme for (1). We want the following things in the difference scheme :

a) that it is unconditionally stable

b) that it keeps the normalization constant

c) that the scale of calculation is within the capability of 16-bit personal computer.

To satisfy these conditions, I used

(i) an implicit scheme which is unconditionally stable

(ii) Padé approximation to (1) which maintains unitarity of (1)

ie, we replace $\exp(-it\hat{H})$ by

$$\frac{1 - \frac{i}{2}t\hat{H}}{1 + \frac{i}{2}t\hat{H}}$$

(iii) Thomas tridiagonal Alogorithm to solve simultaneous linear equations. The merits of this method as compared to Gauss elimination method are mentioned by [HE.8] Parameters are chosen in such a way that the entire scattering event occurs within the square $[0,1] \times [0,1]$. At the edges, we impose boundary conditions

$$\Psi(x,t) = 0$$

§6.2 Programming Environment

MS-DOS Optimizing C is used because

(i) Floating point operations with 8087 processor is supported. The calculation time is shortened considerably

(ii) Many convenient functions are available in the library c86b2n

(iii) Access of RAM boards is possible

The main unsatisfactory aspect of Optimizing C is the long compiling time. This can be overcome by installing VRAM.

It must be remarked that Optimizing C does not check the following:

(i) overflow

(ii) overshooting the subscript range of array

(iii) division by zero

Therefore it is the programmer's responsibility to ensure that these faults be amended.

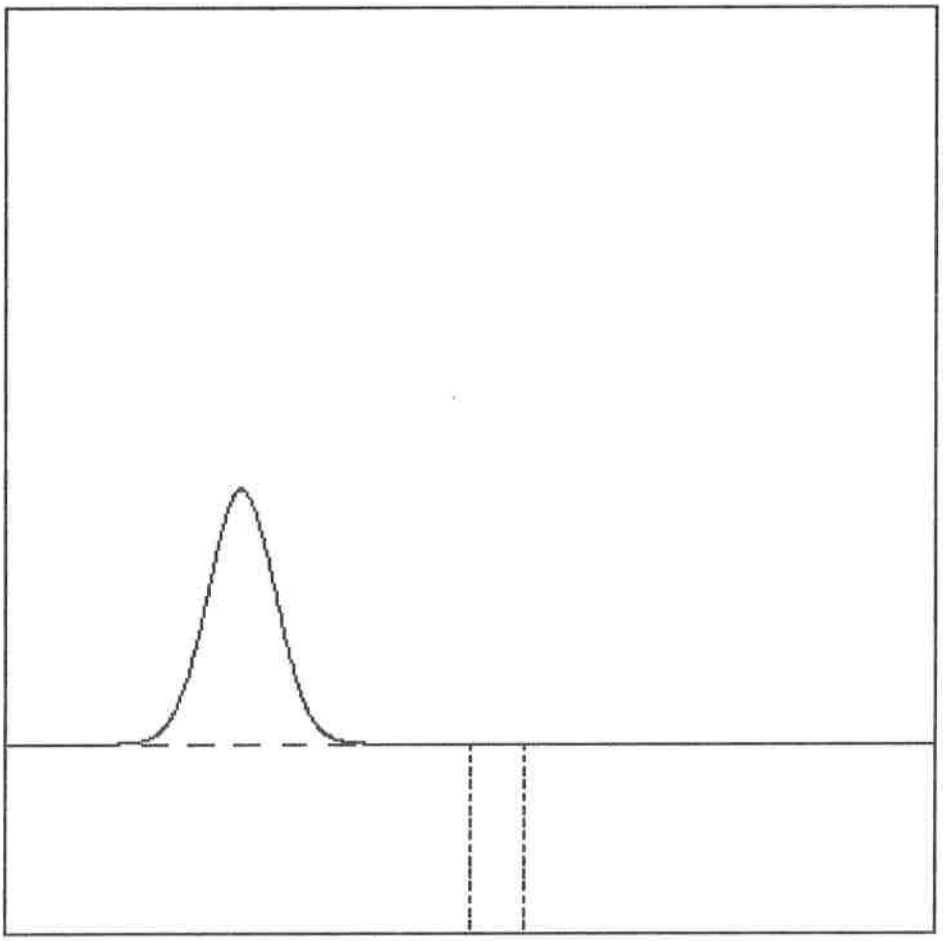
§ 6.3 One-dimensional Simulation Pictures

Simulation results of a gaussian wave packet scattering from a square well are presented in A series and B series. The average energy of A series's wave packet is one half the well depth, and that of B series is equal to the well depth.

Comparison between A series and B series shows that the wave packet seems to linger longer in the well when its average energy is equal to the well depth. This is because the probability of bound state components being formed is greater. As we can see, a small fraction of wave packet is reflected.

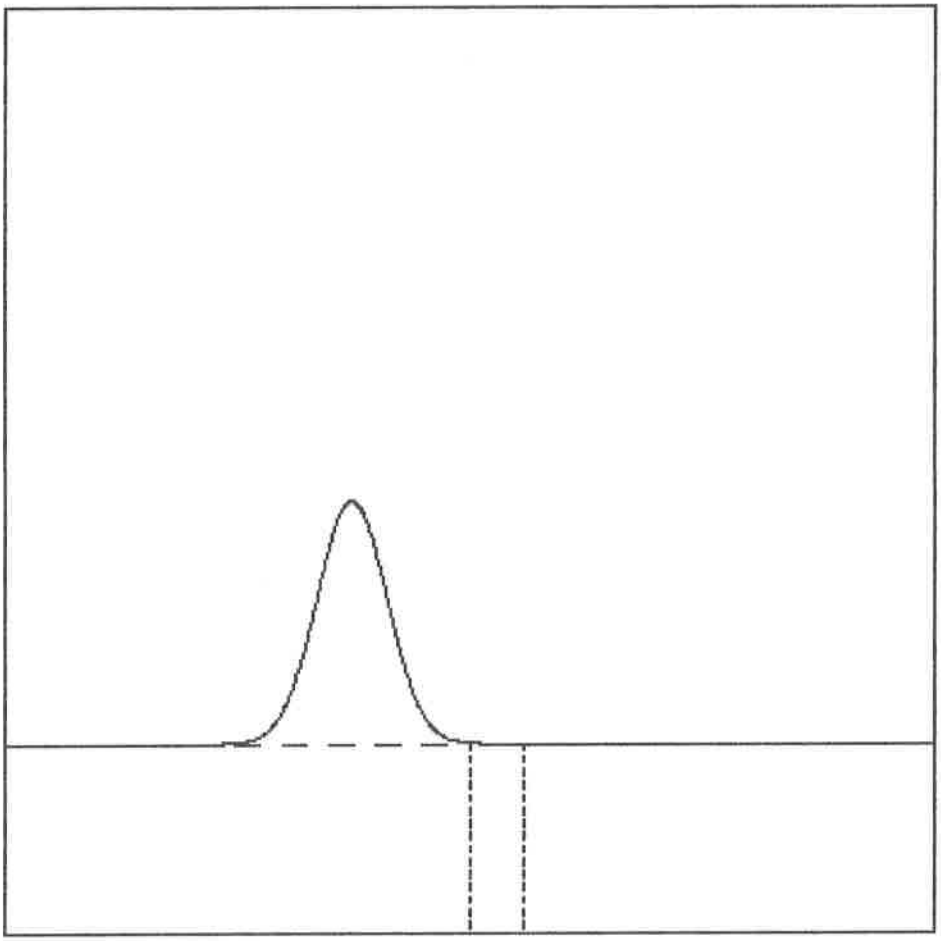
Simulation results of a gaussian wave packet scattering from a square barrier are presented in C series and D series. The average energy of C series's wave packet is one half the barrier height, and that of D series is equal to the barrier height. In D series, it is worth noting that resonance occurs. A part of the wave packet is trapped inside the potential barrier for quite a long time. We can observe that it bounces to- and-fro within the potential.

$t = 0$



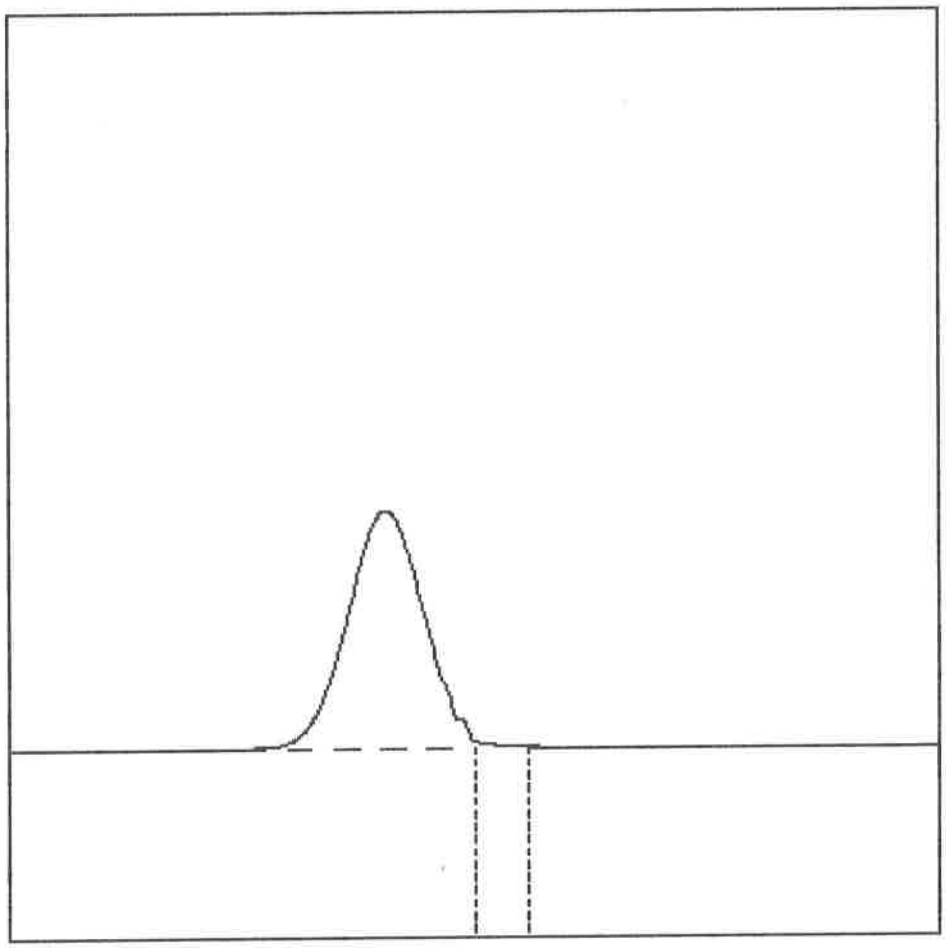
Initial position of series A and B

$t = 200$



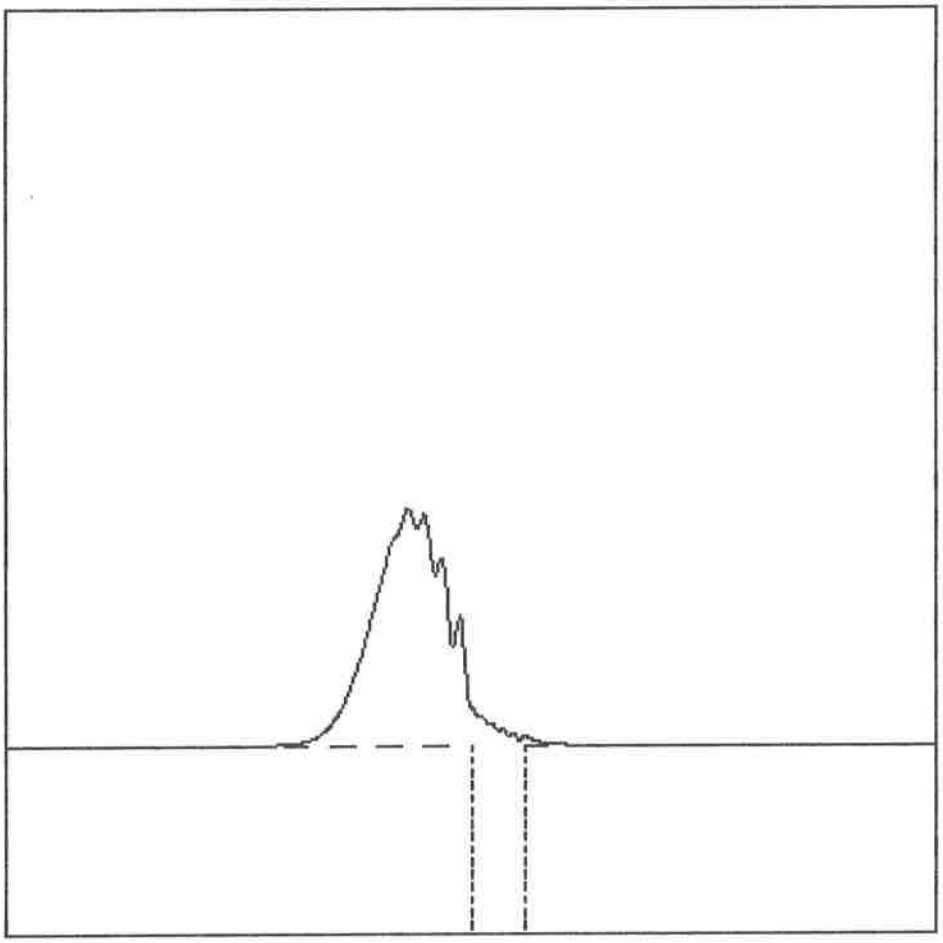
A Simulation results of a gaussian wave packet scattering from a square well. The average energy is one half the well depth.

$t = 250$



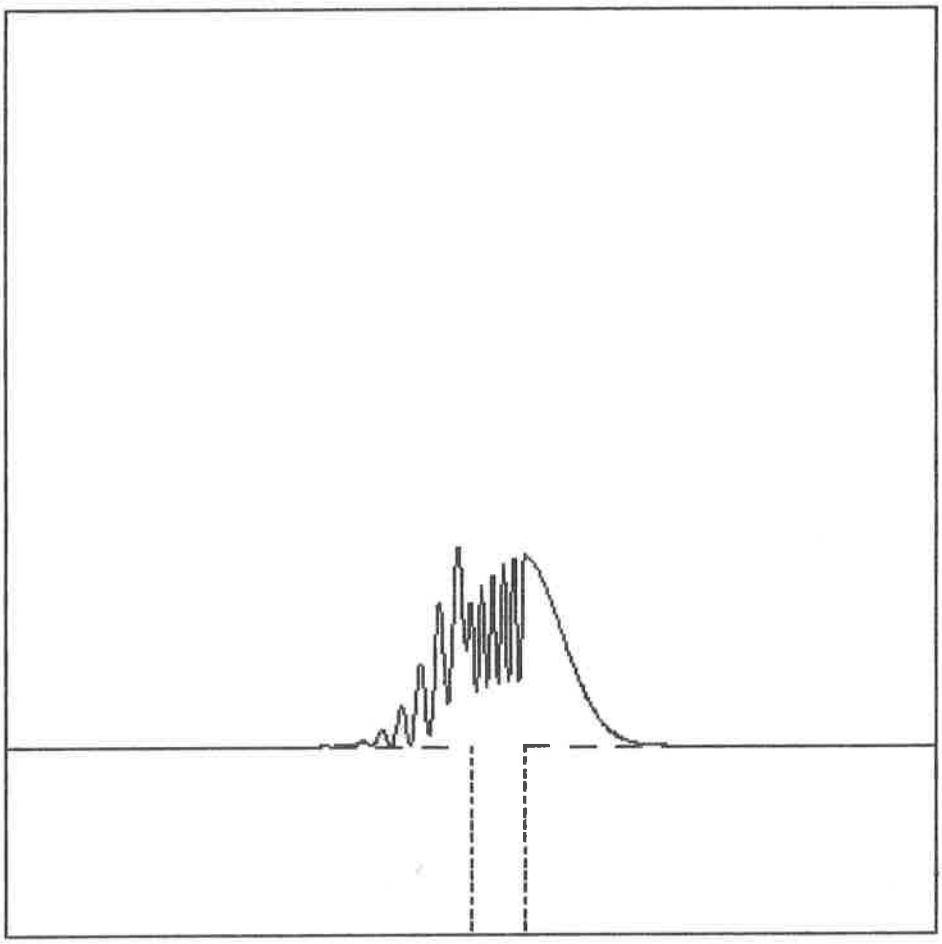
A

$t = 300$



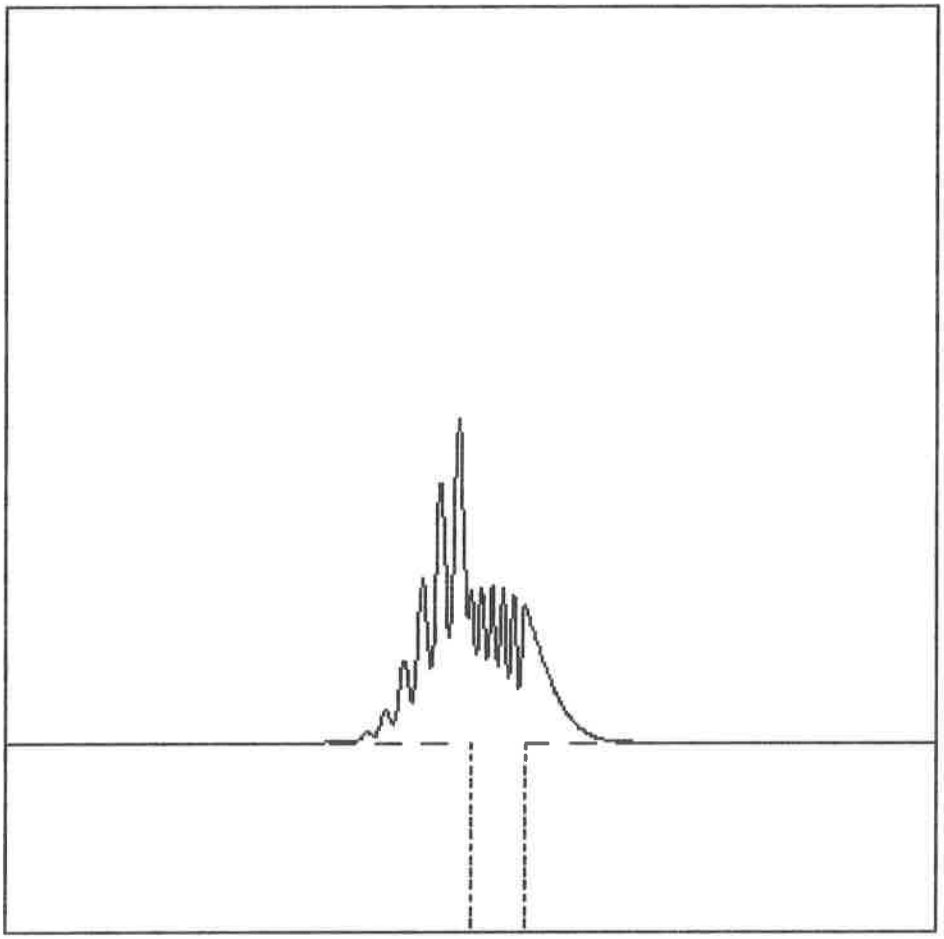
A

t = 400



A

t = 450

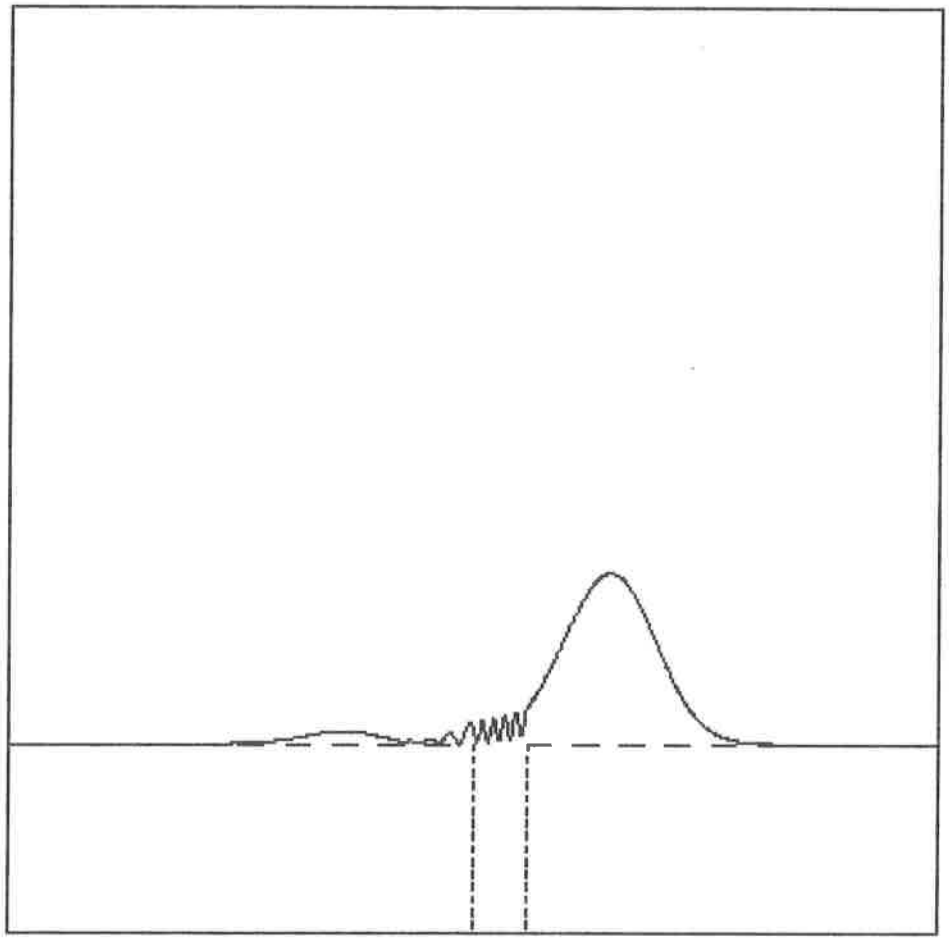


A

t = 550

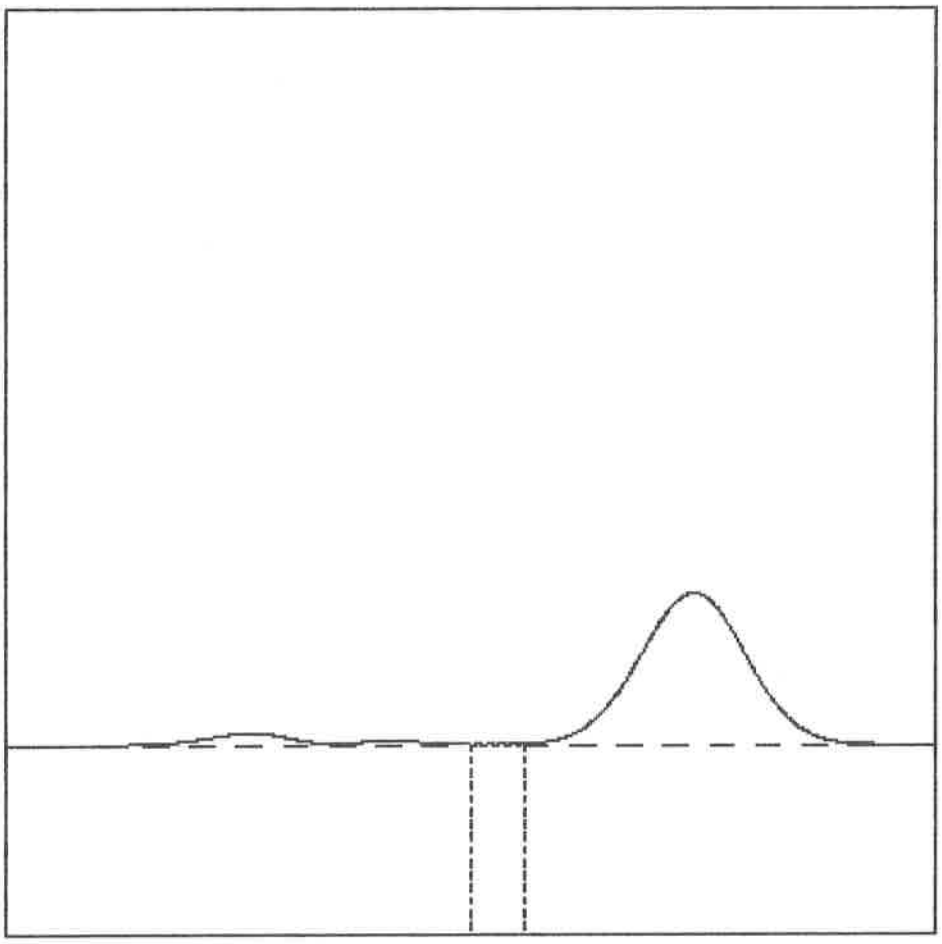
A

t = 600



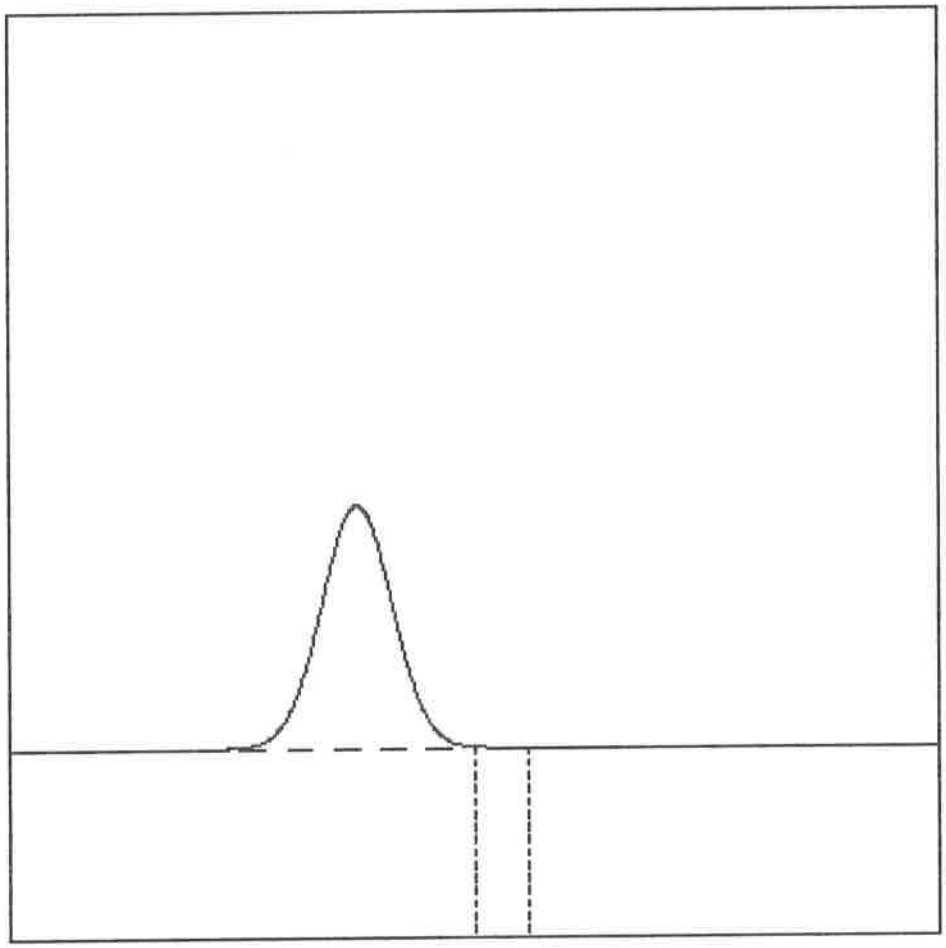
A

t = 750



A

$t = 200$

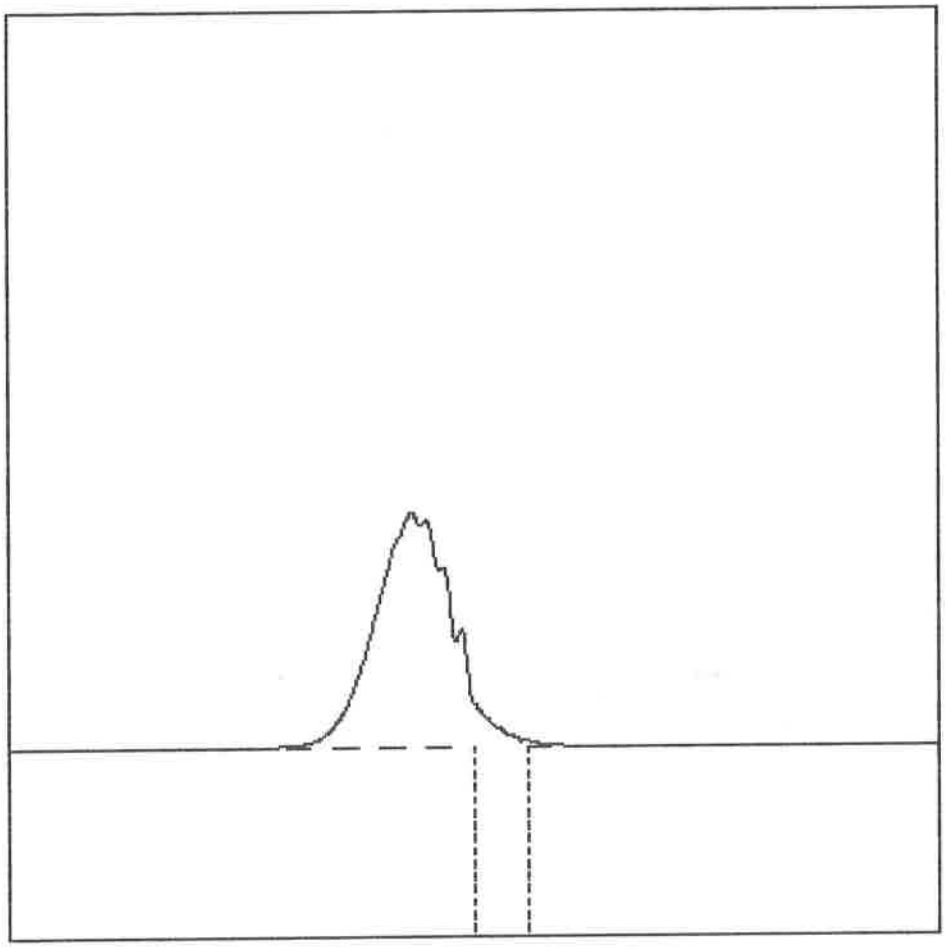


B Simulation results of a gaussian wave packet scattering from a square well. The average energy is equal to the well depth.

$t = 250$

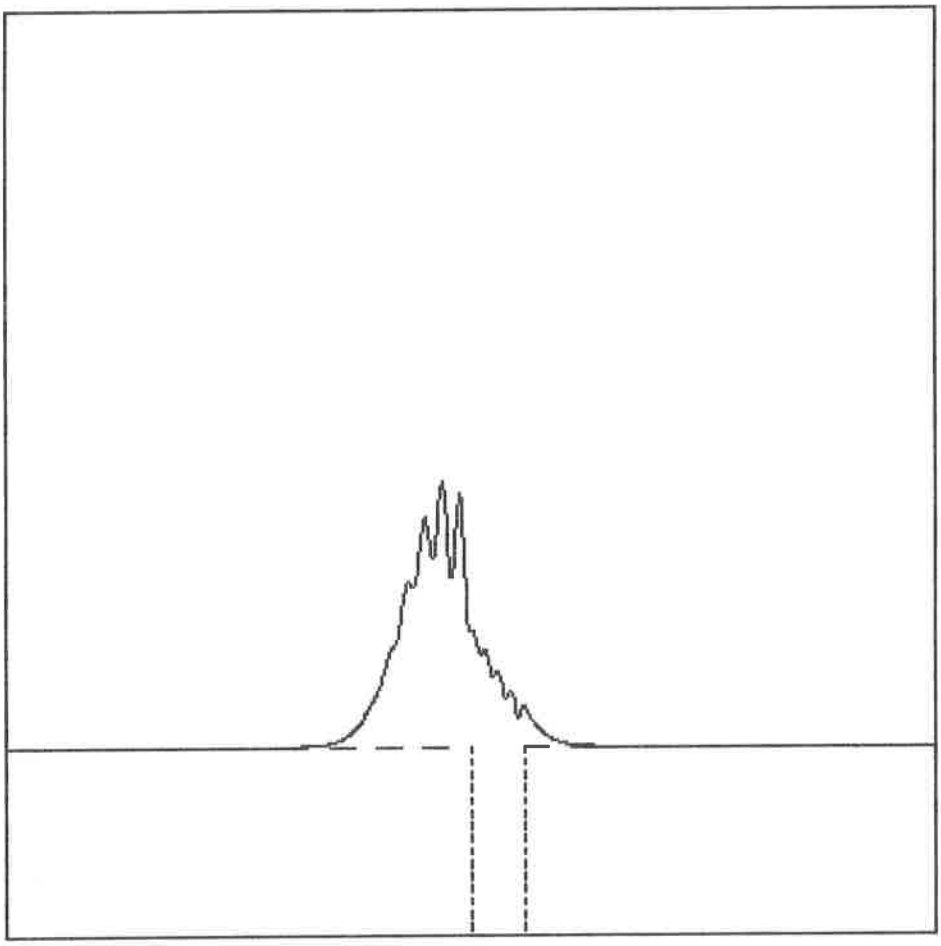
B

$t = 300$



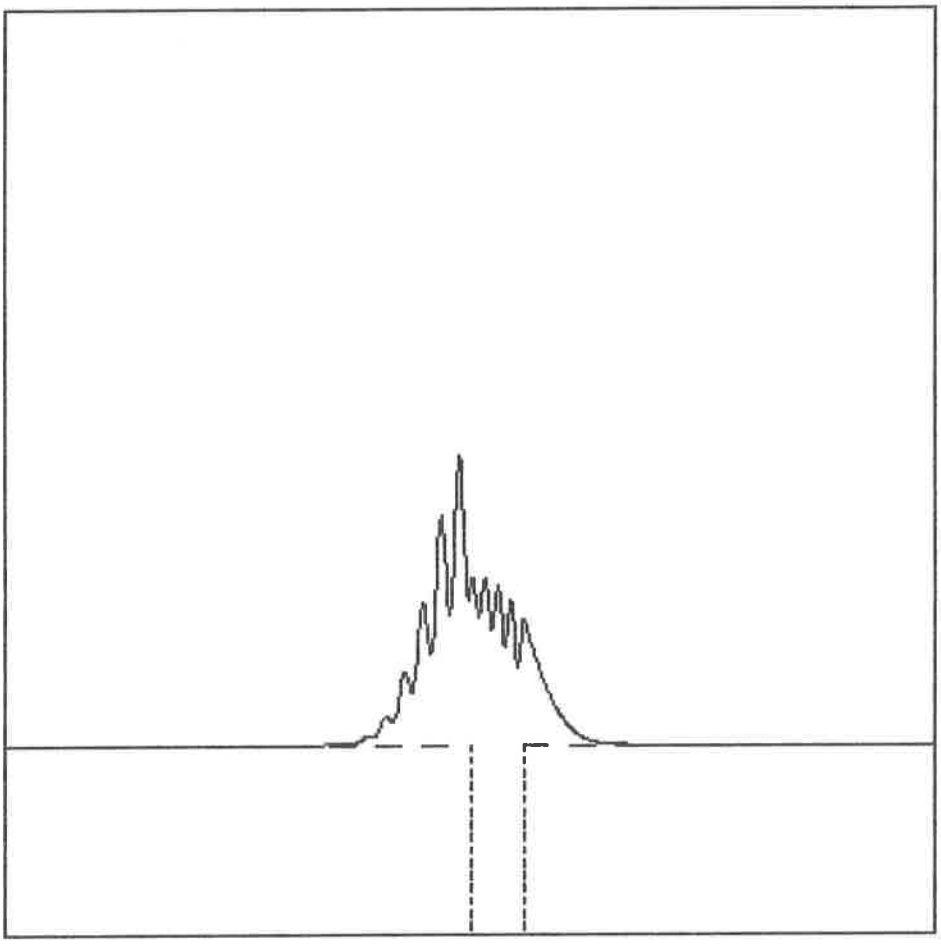
B

$t = 350$



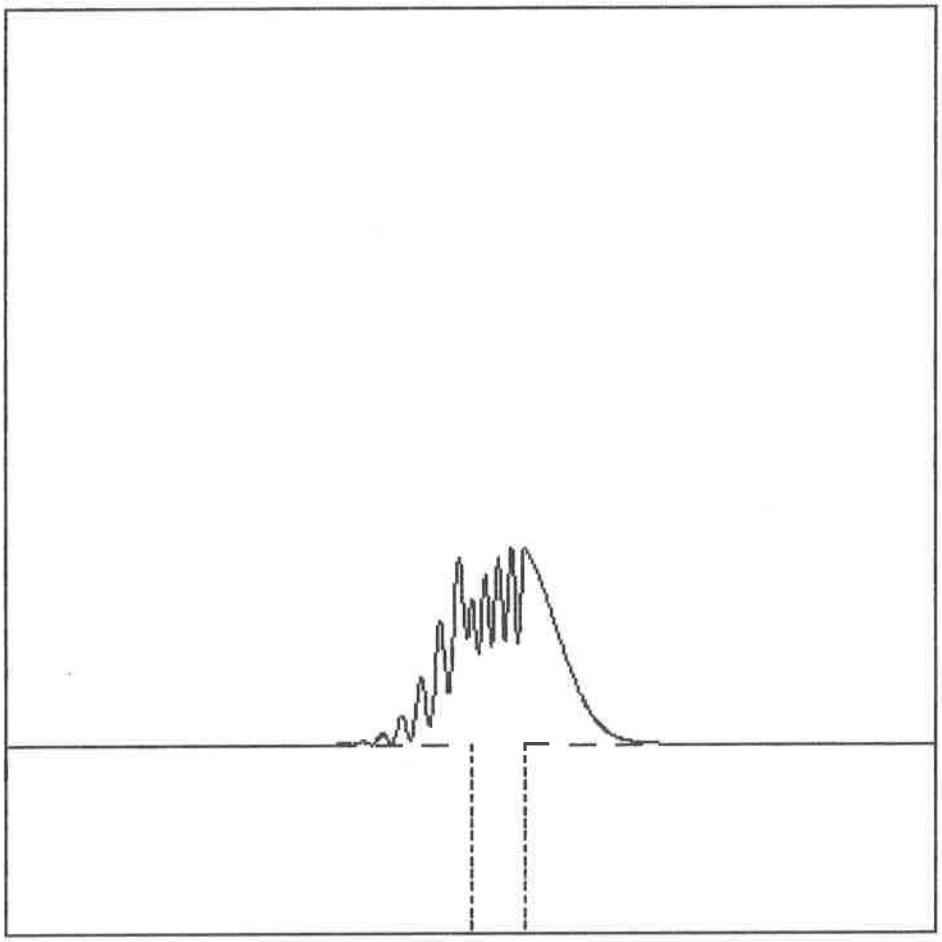
B

$t = 400$



B

t = 450

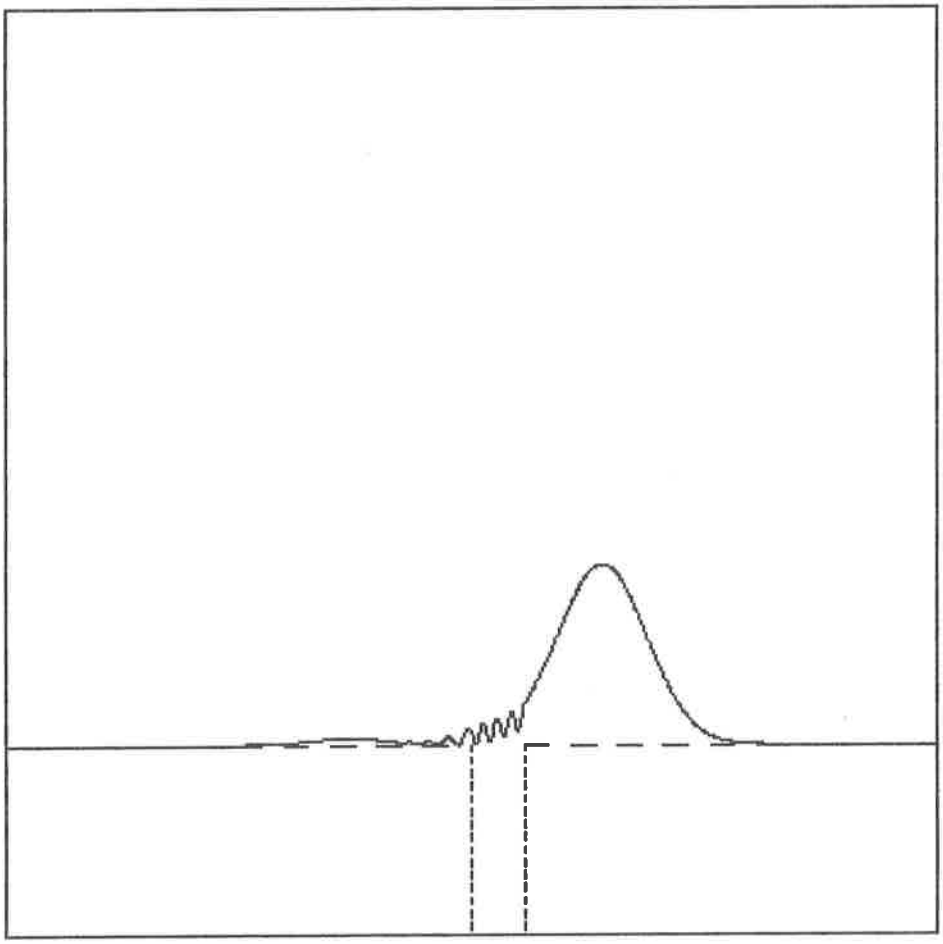


B

$t = 550$

B

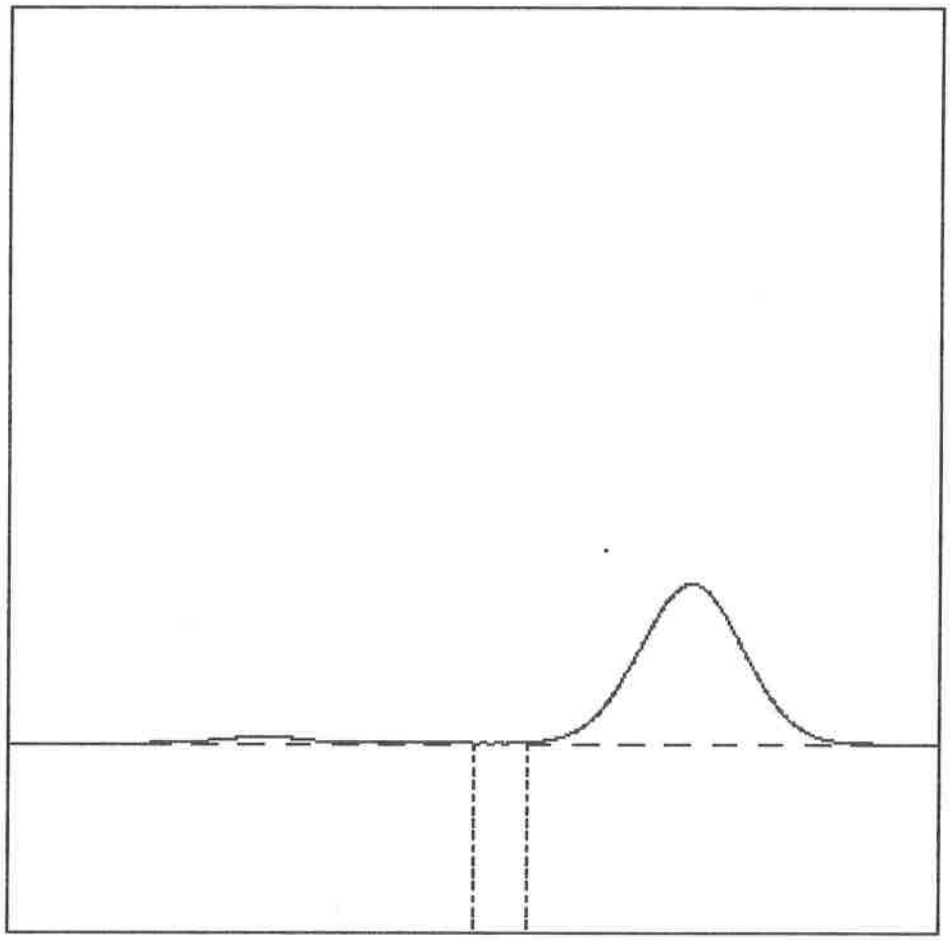
$t = 600$



B

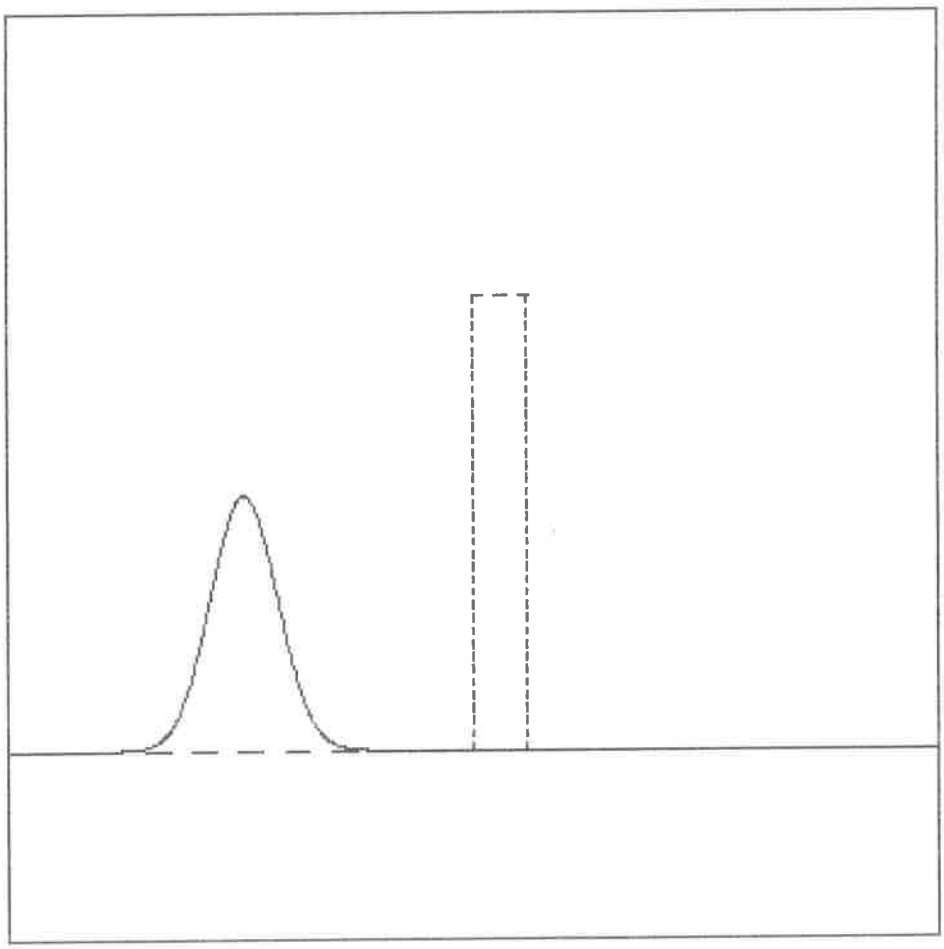
M

t = 750



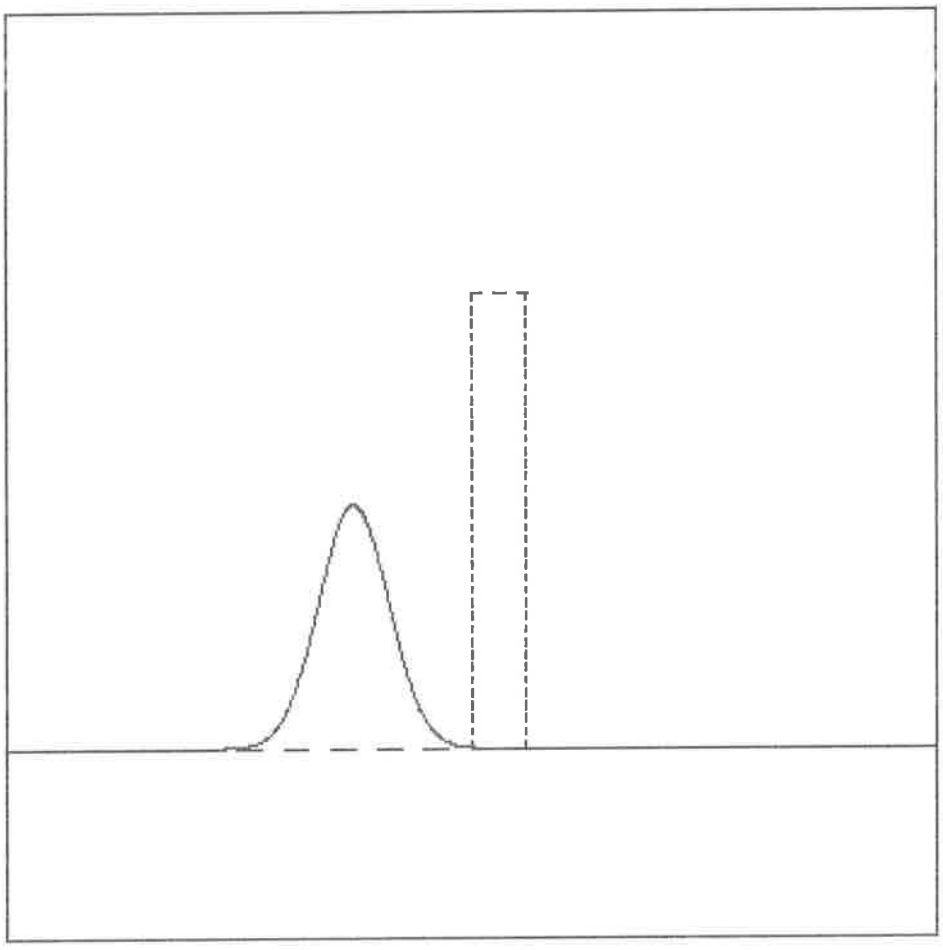
B

$t = 0$



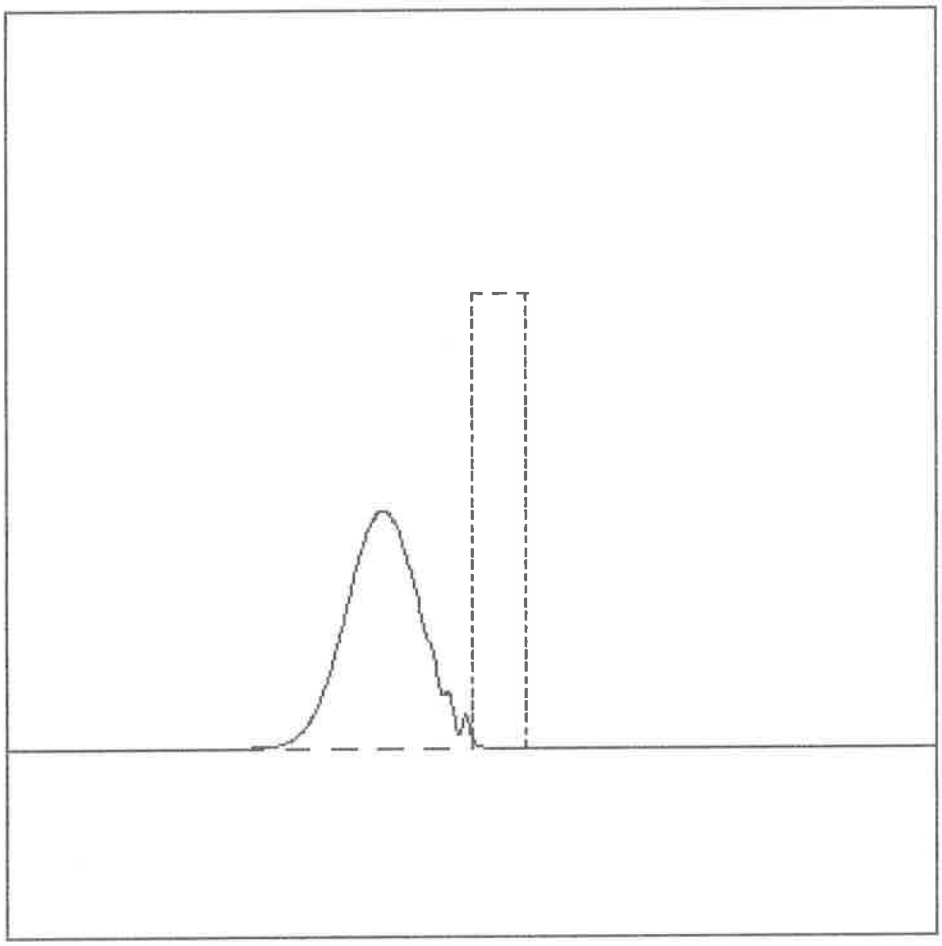
Initial position of C series and D series

$t = 200$



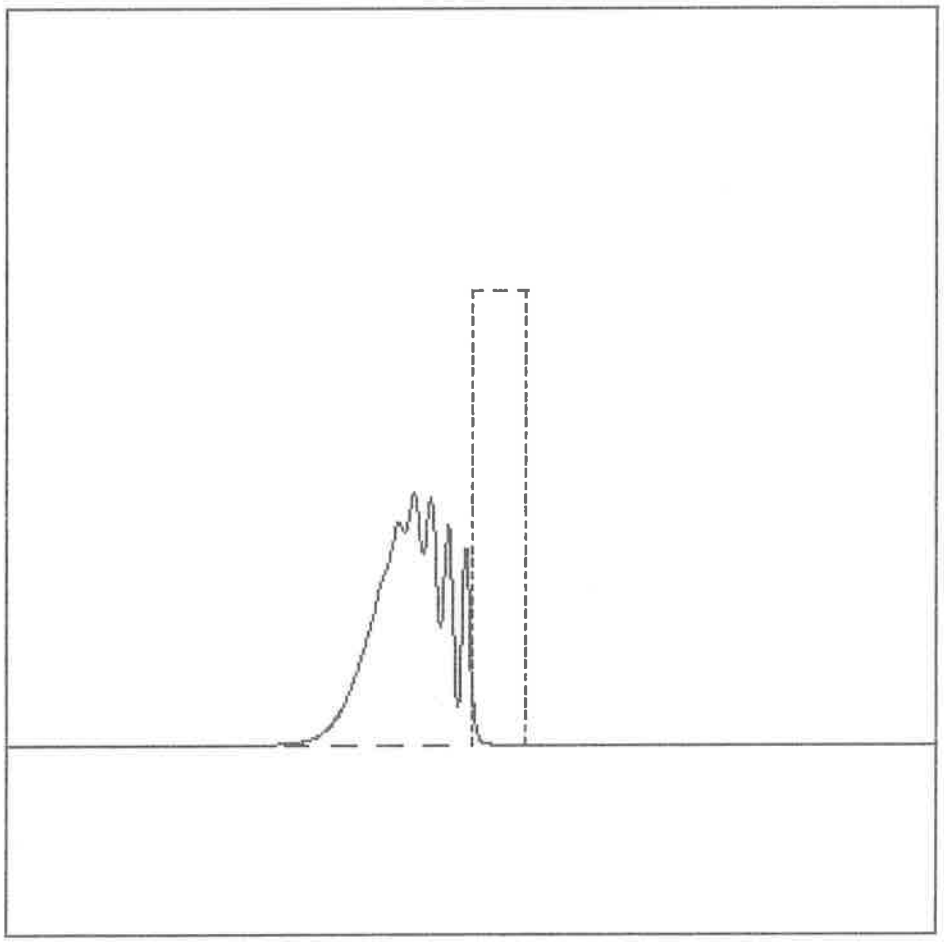
C

$t = 250$



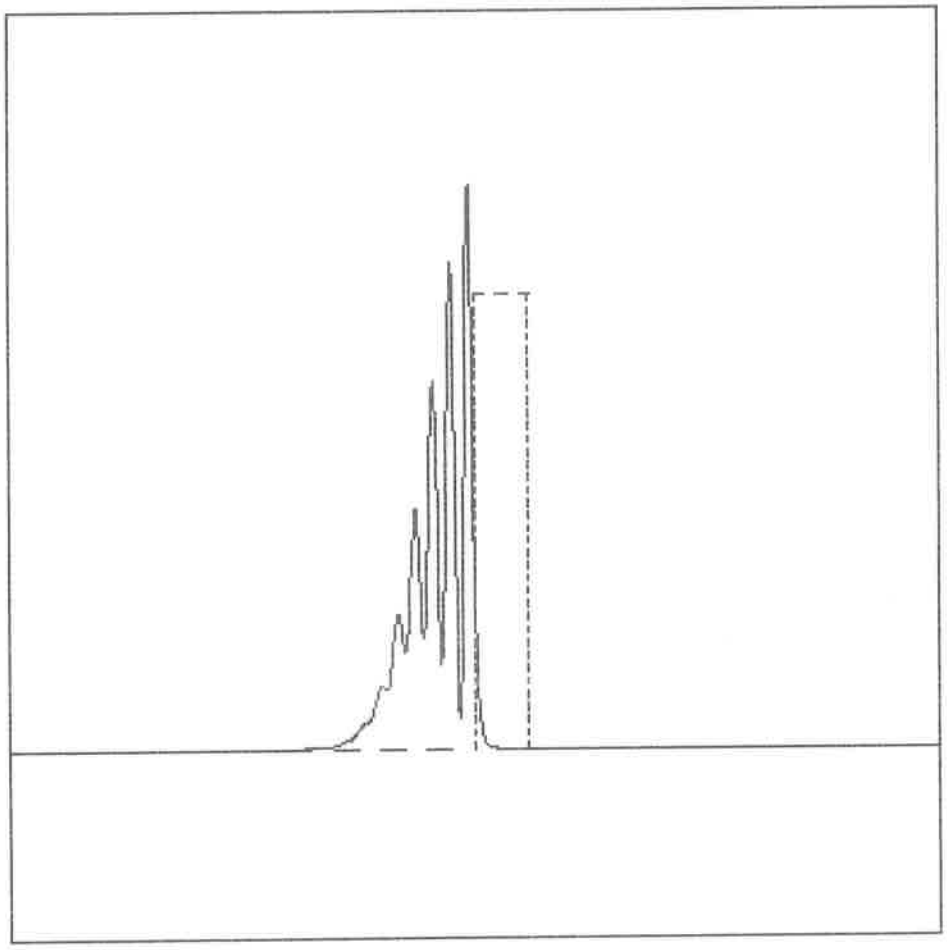
C

$t = 300$



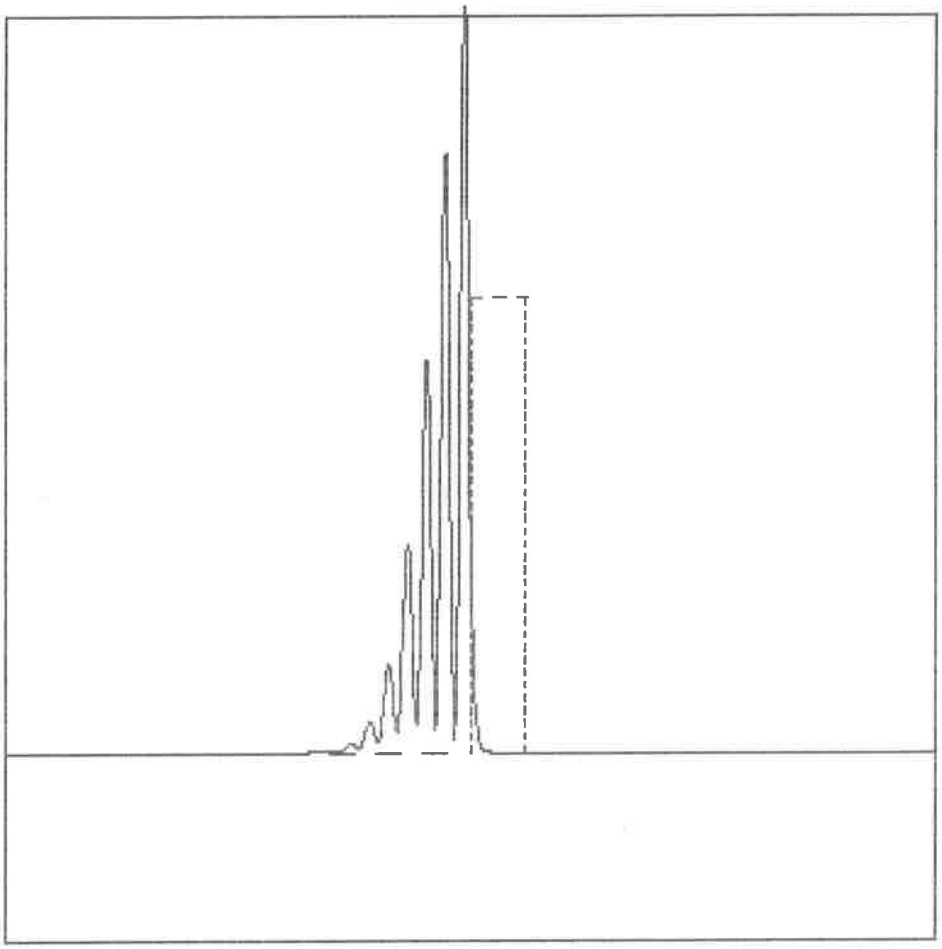
C

$t = 350$



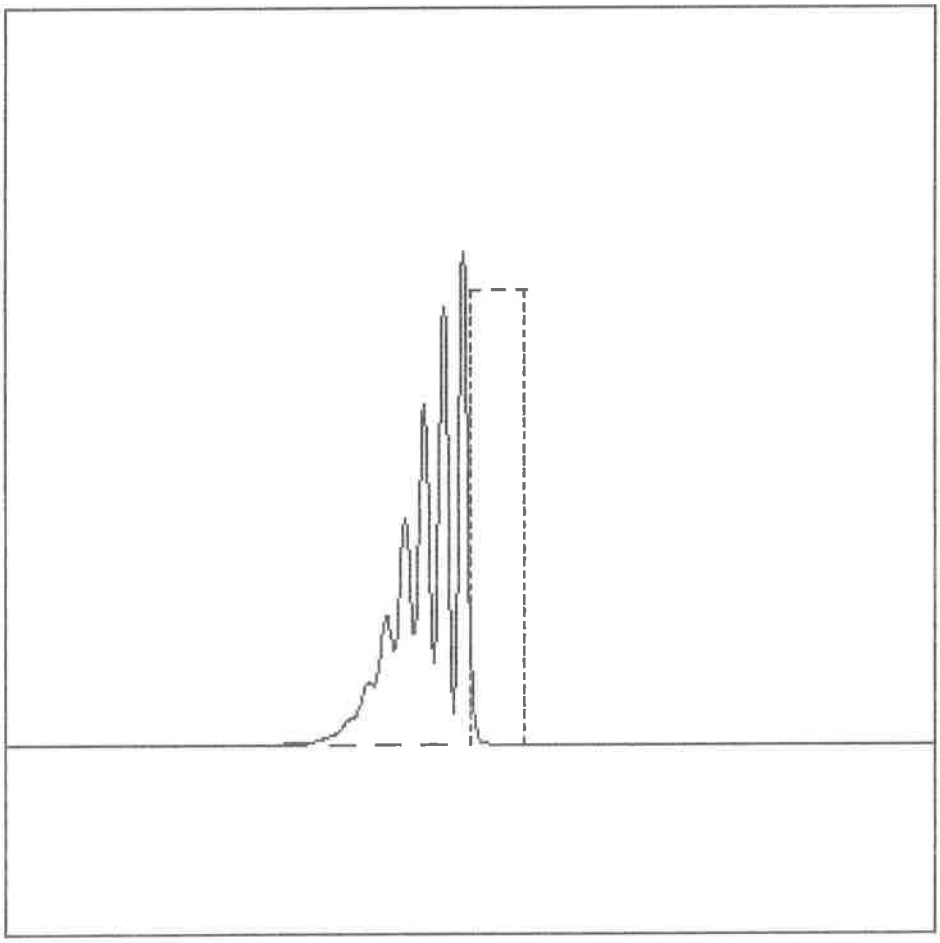
C

$t = 440$



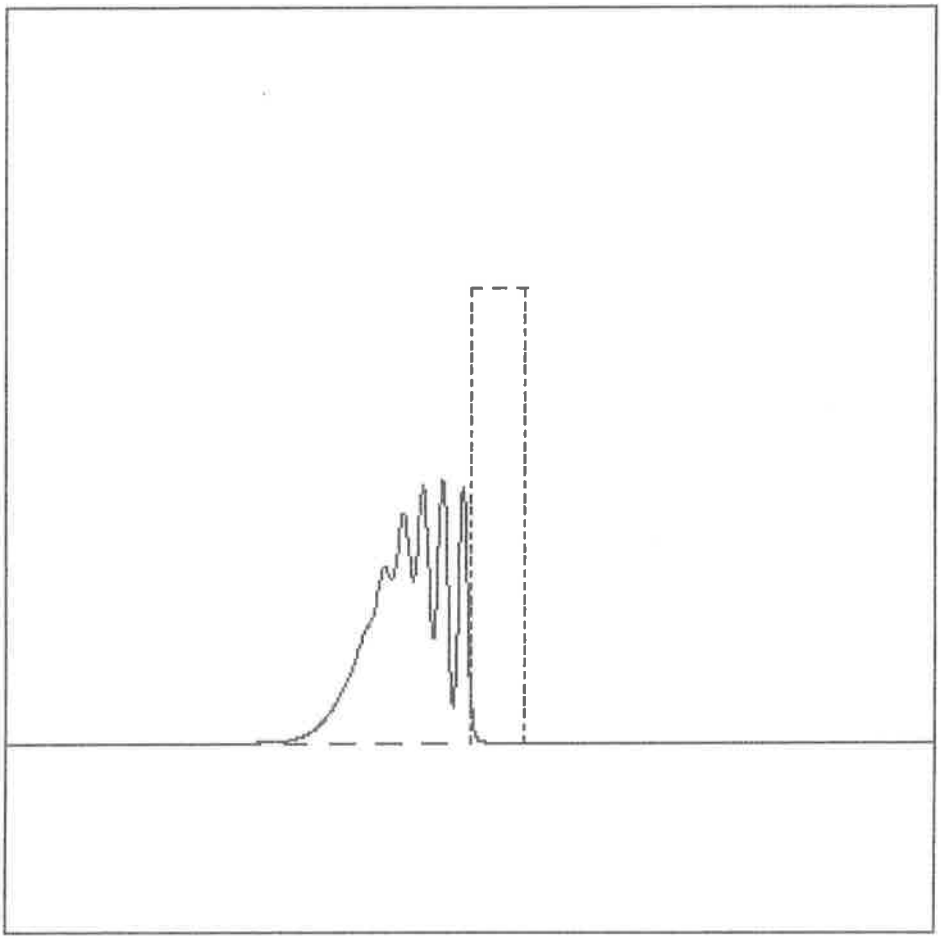
C

$t = 480$



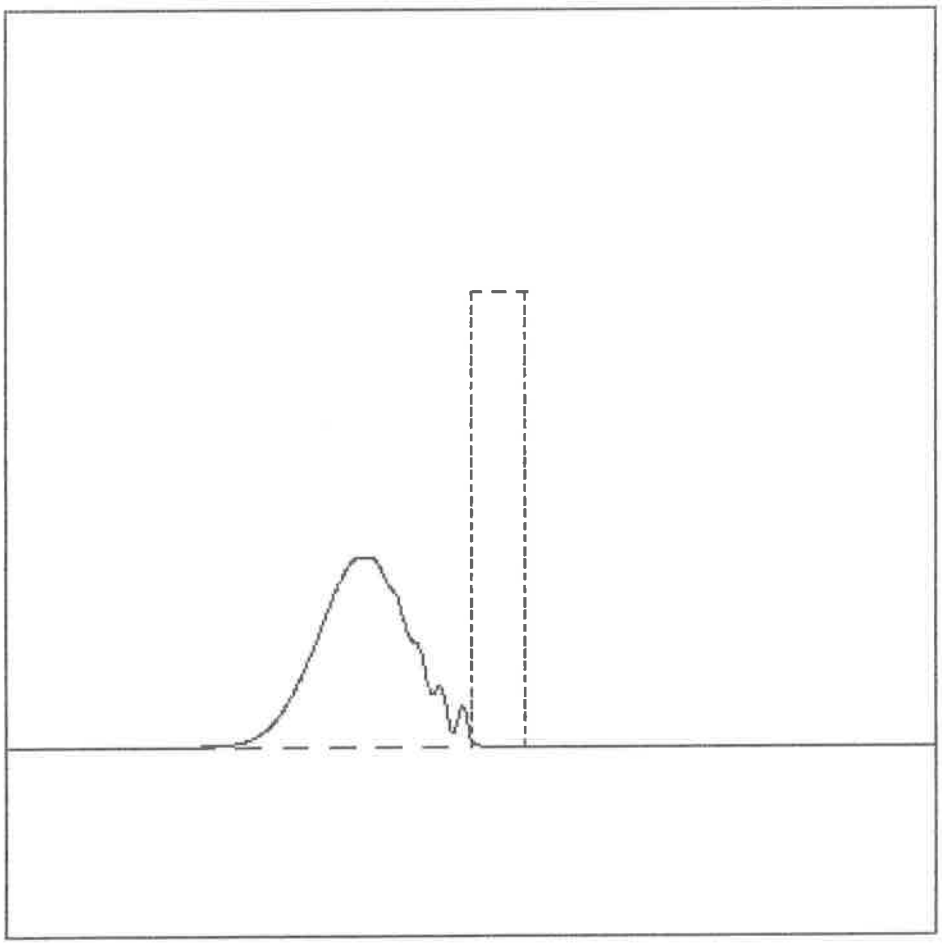
C

$t = 520$



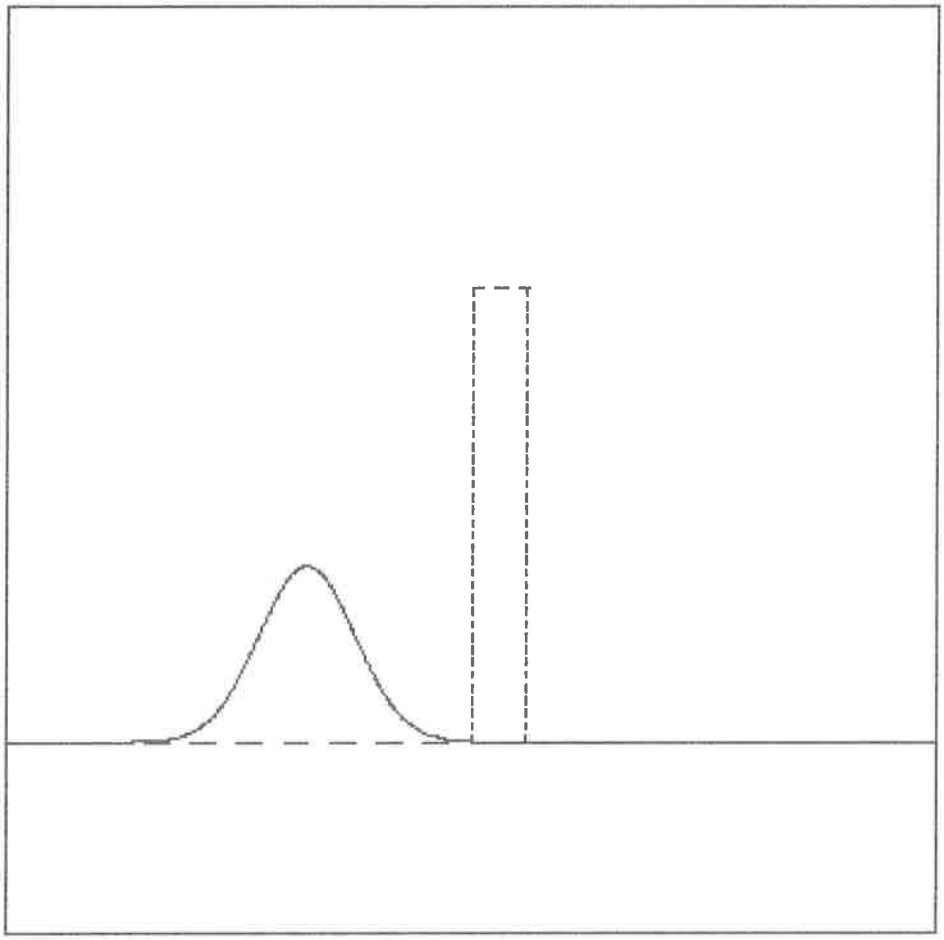
C

$t = 600$



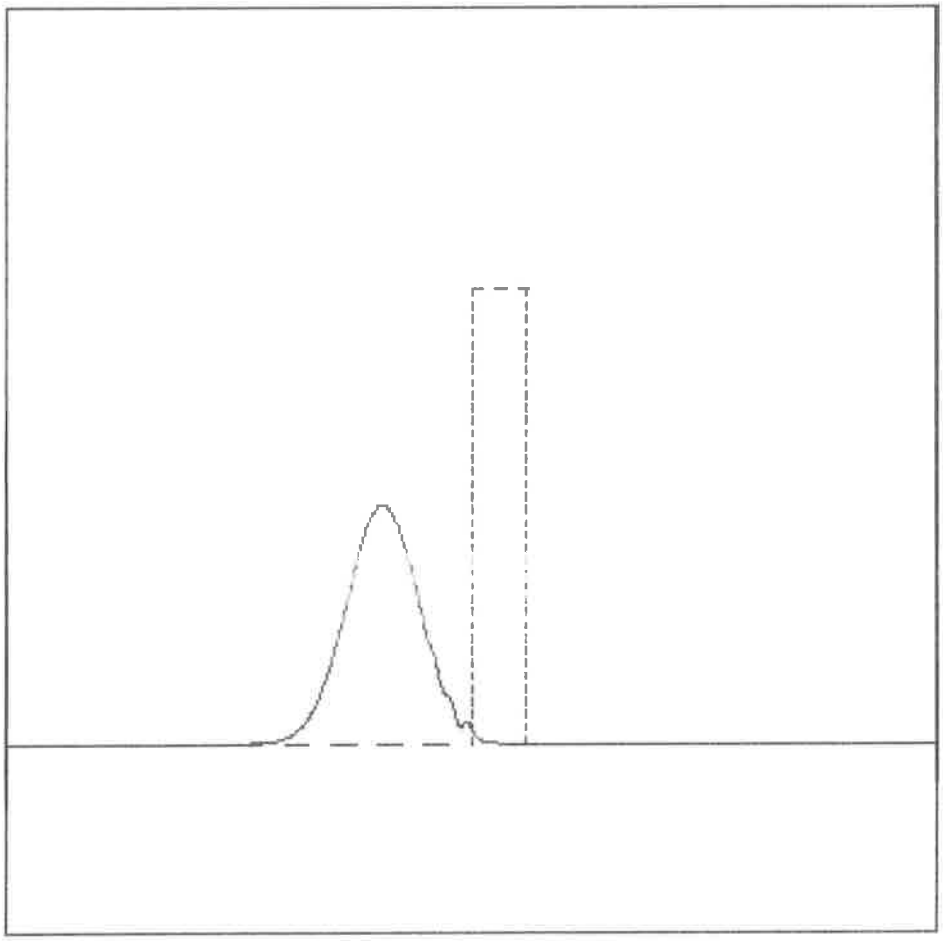
c

$t = 700$



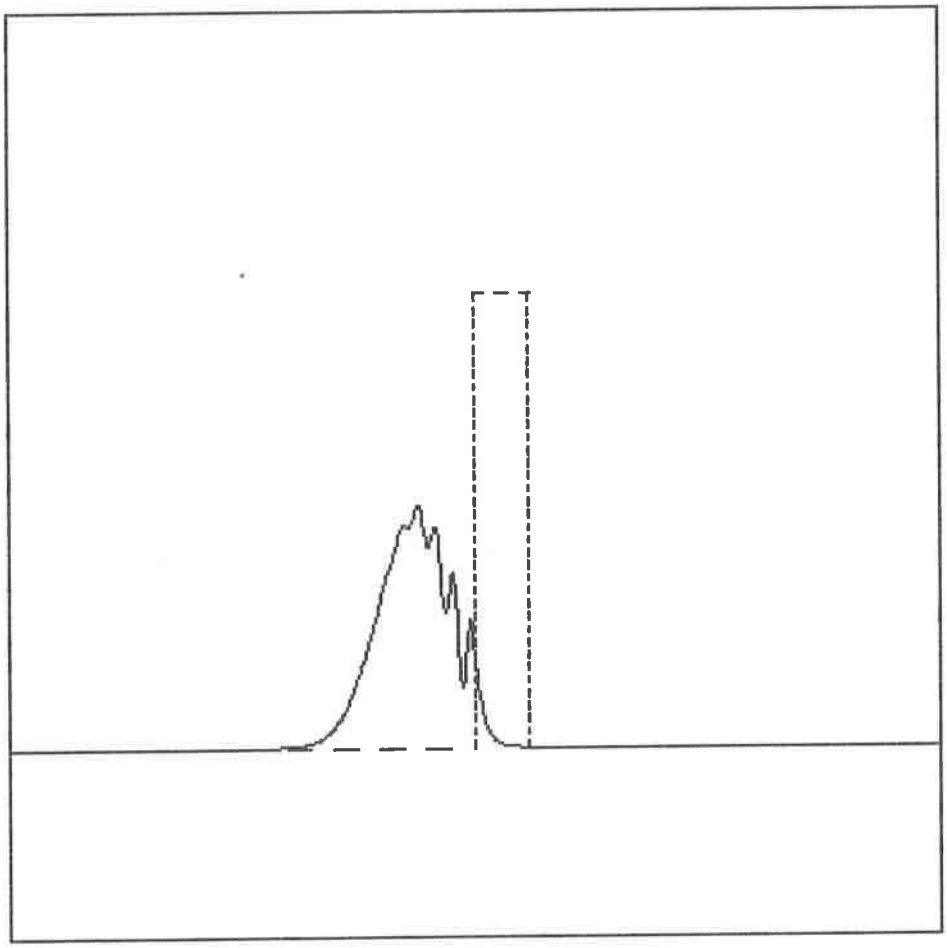
C

$t = 250$



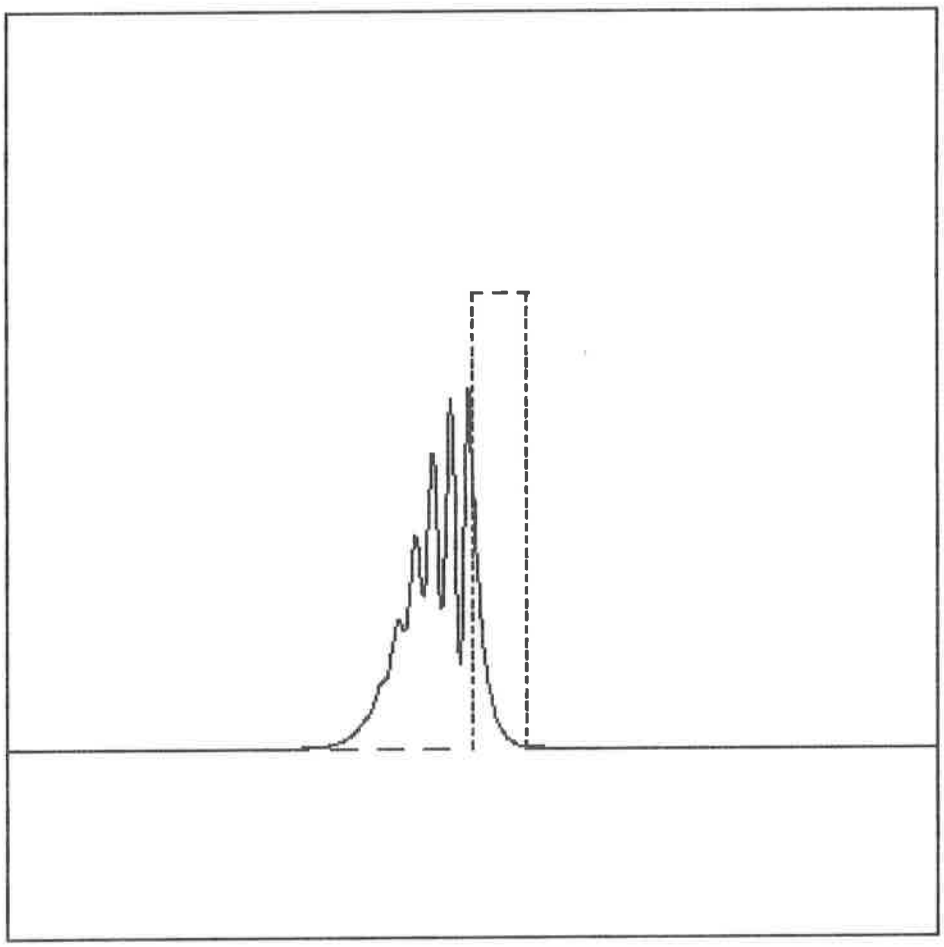
▷ Simulation results of a gaussian wave packet scattering from a square barrier. The average energy is equal to the barrier height.

$t = 300$



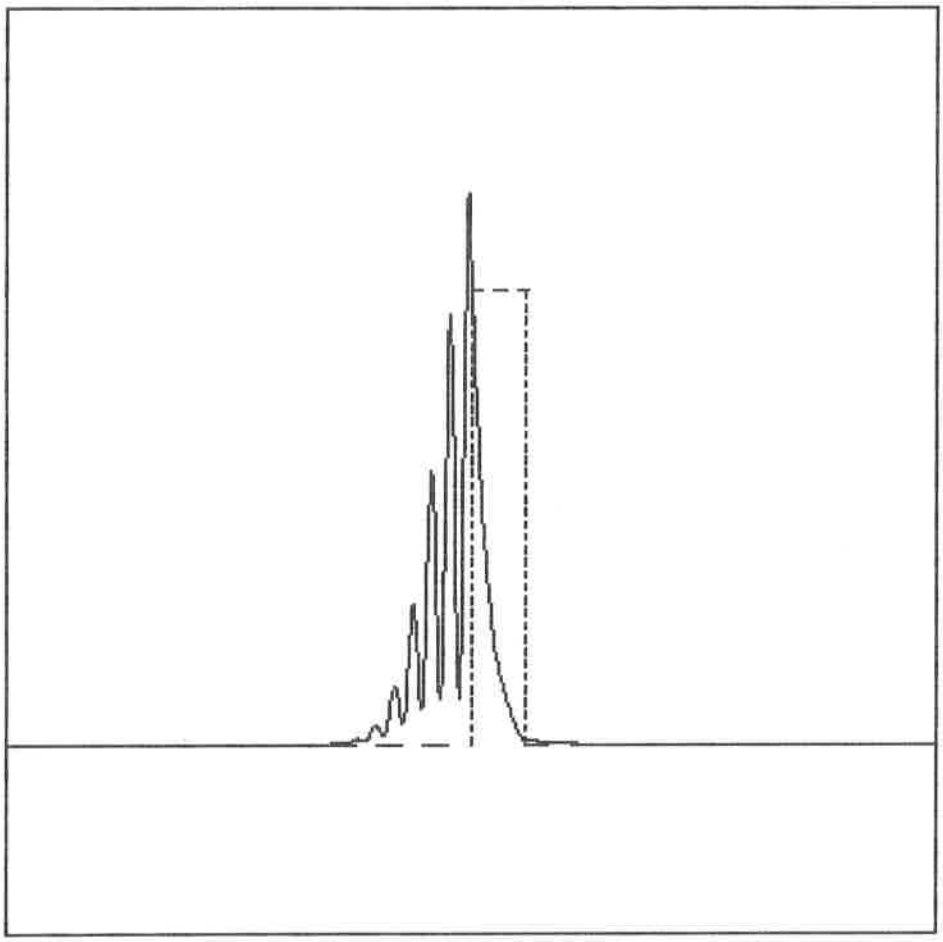
D

$t = 350$



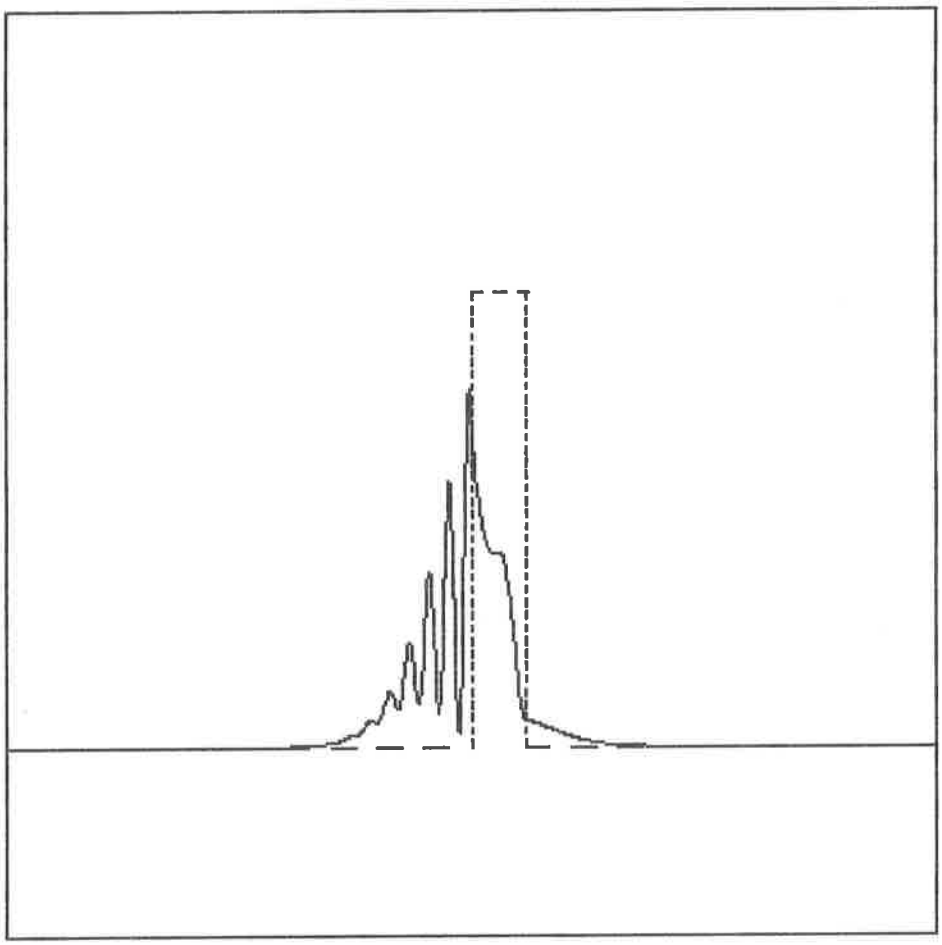
D

$t = 400$



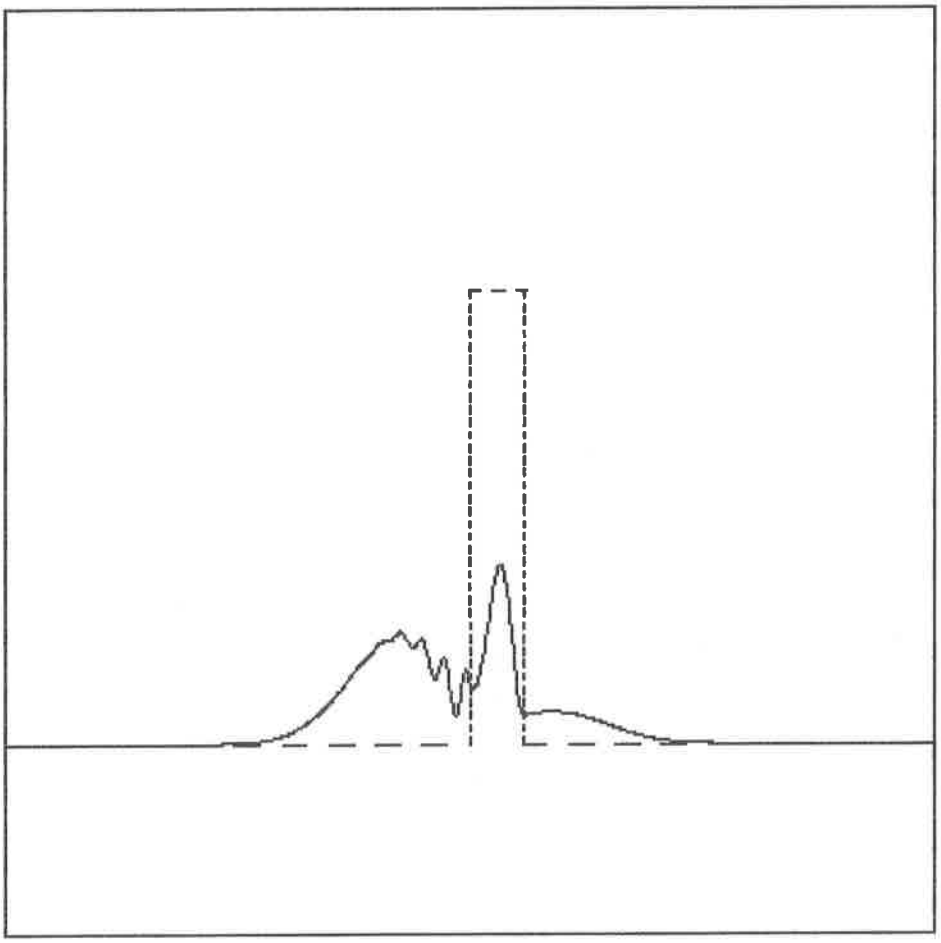
D

$t = 500$



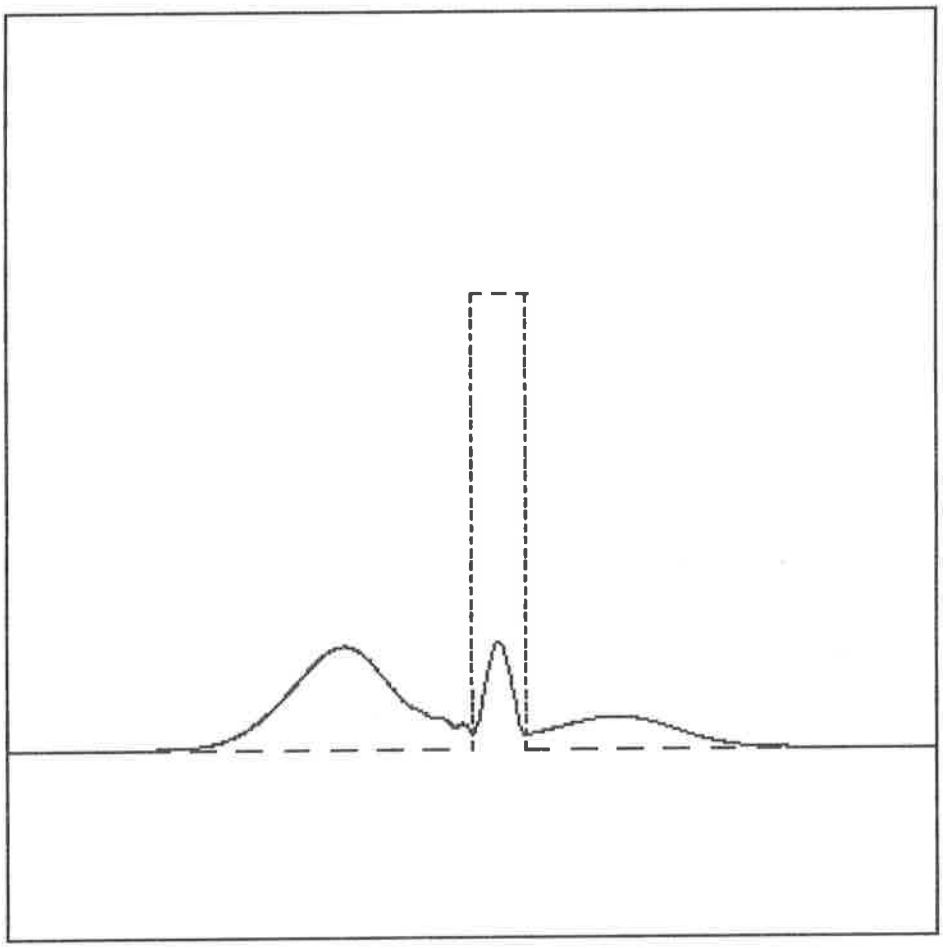
D

$t = 600$



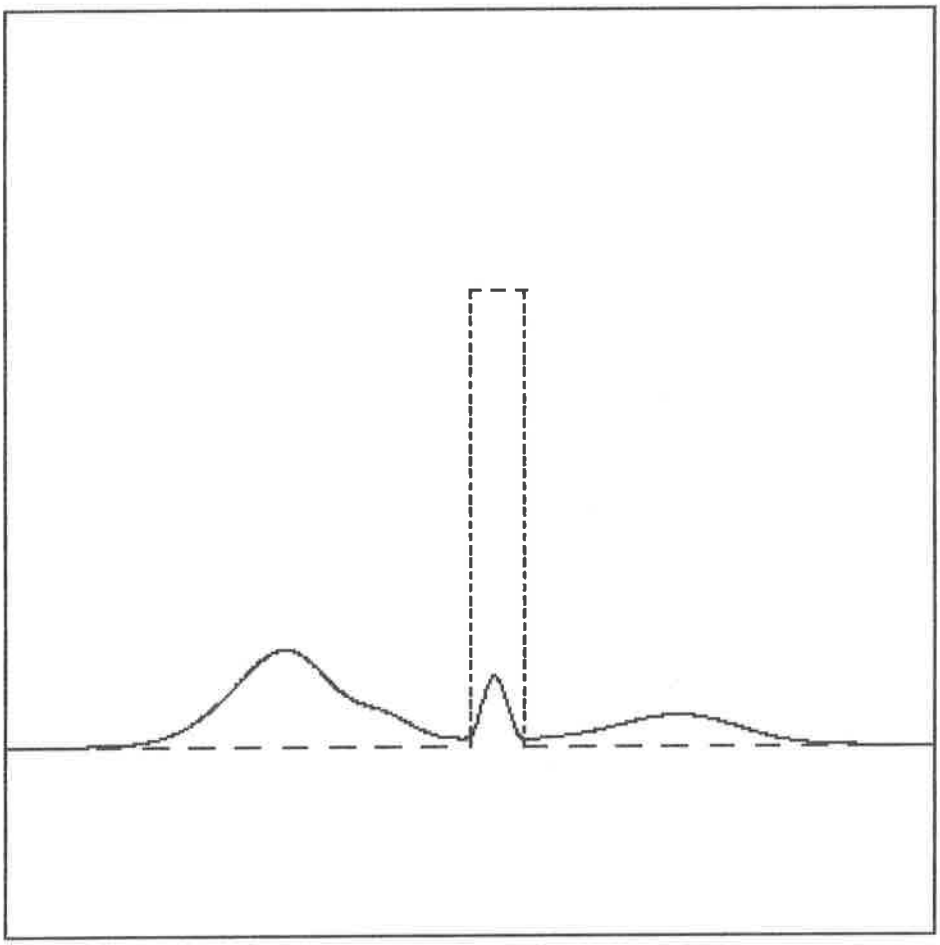
D

$t = 700$



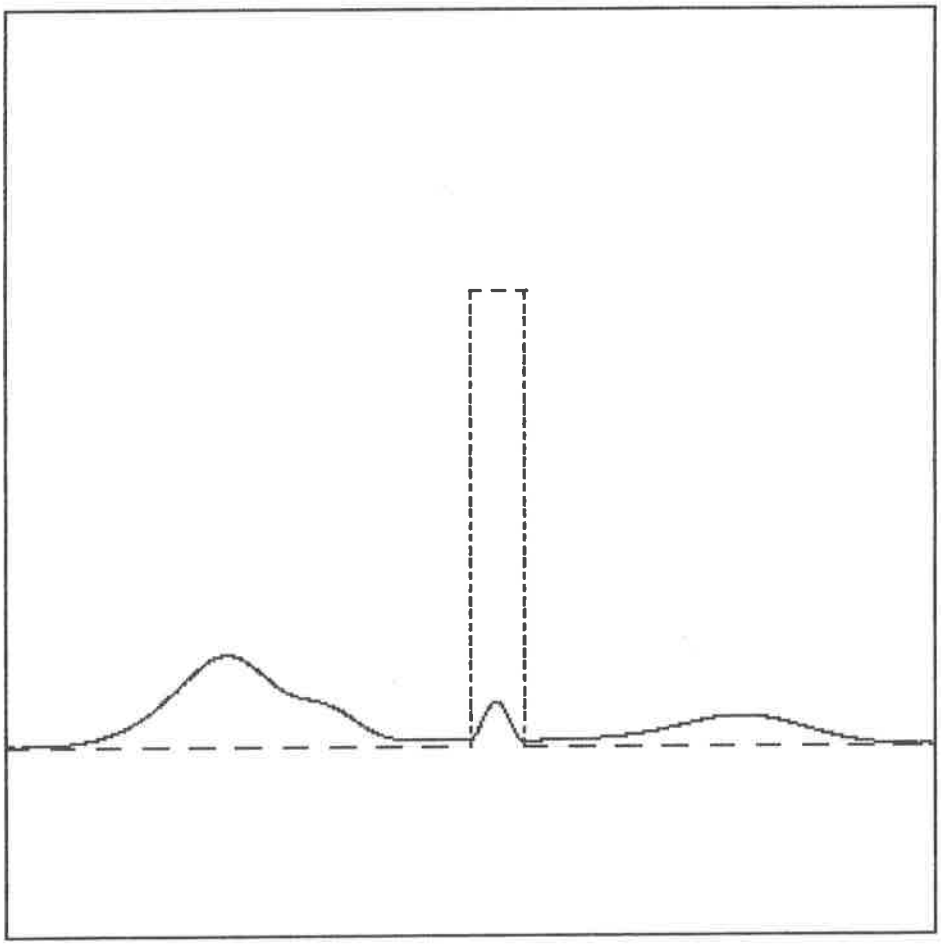
D

$t = 800$



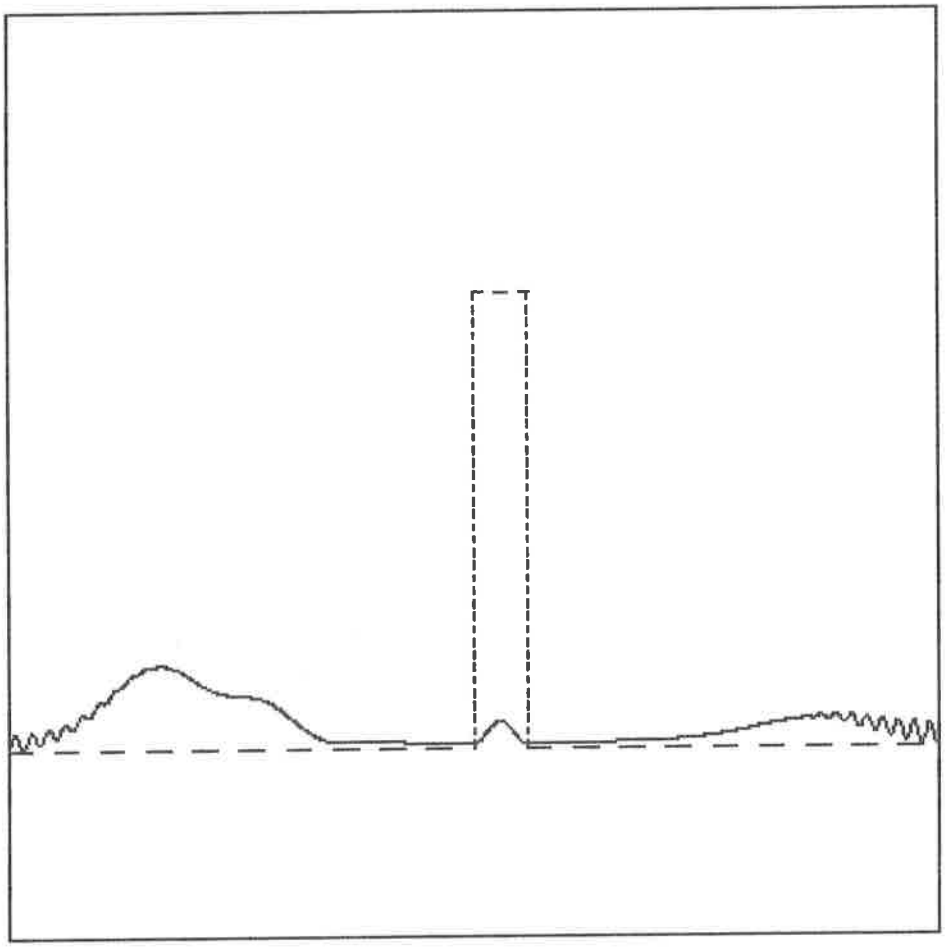
D

$t = 900$



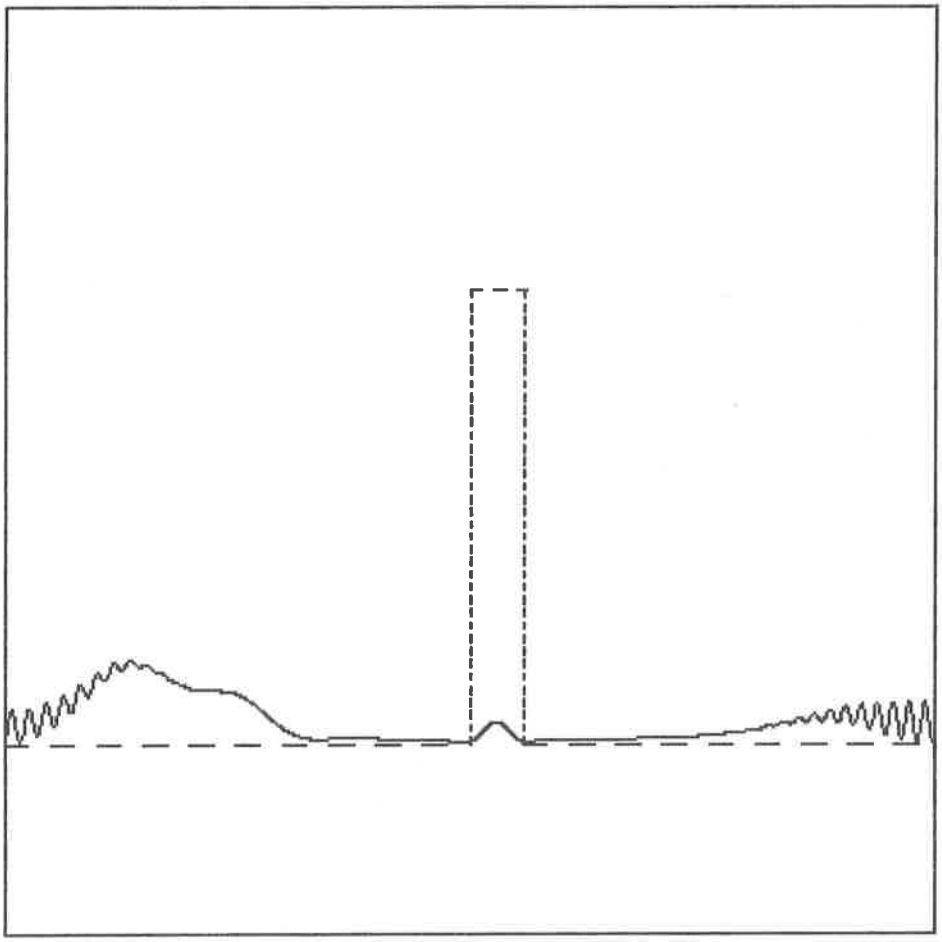
D

$t = 1020$



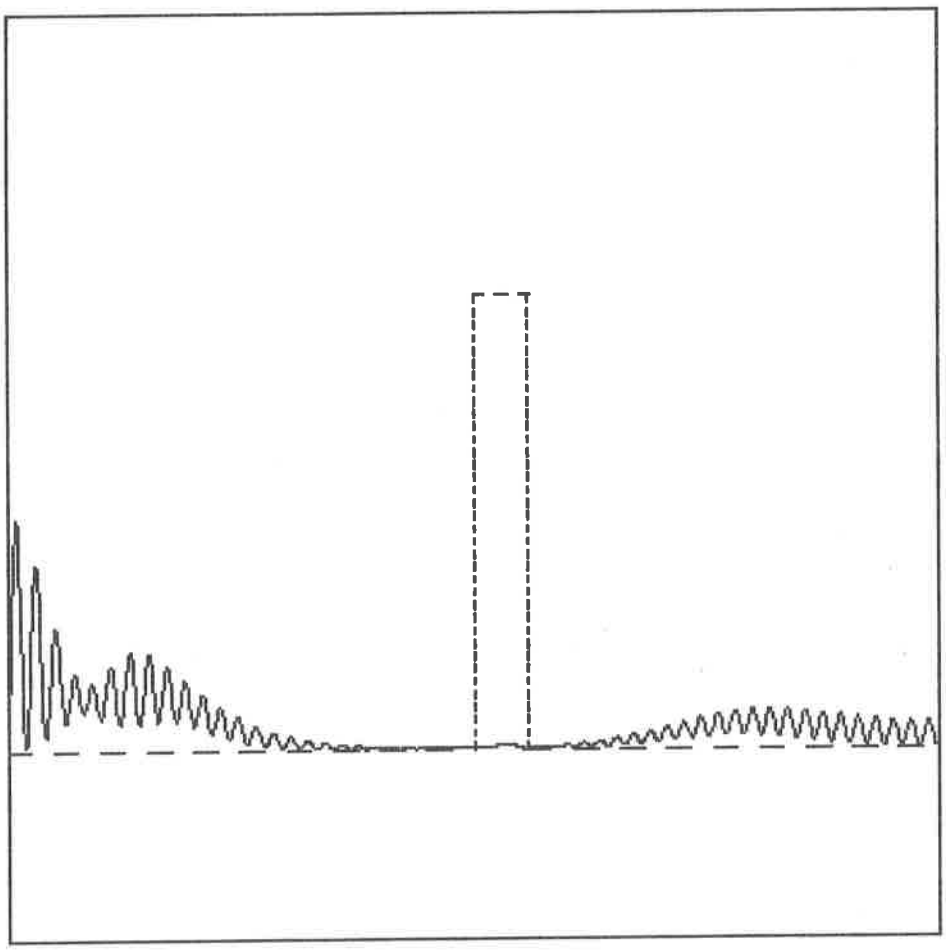
D

$t = 1050$



D

$t = 1500$



D

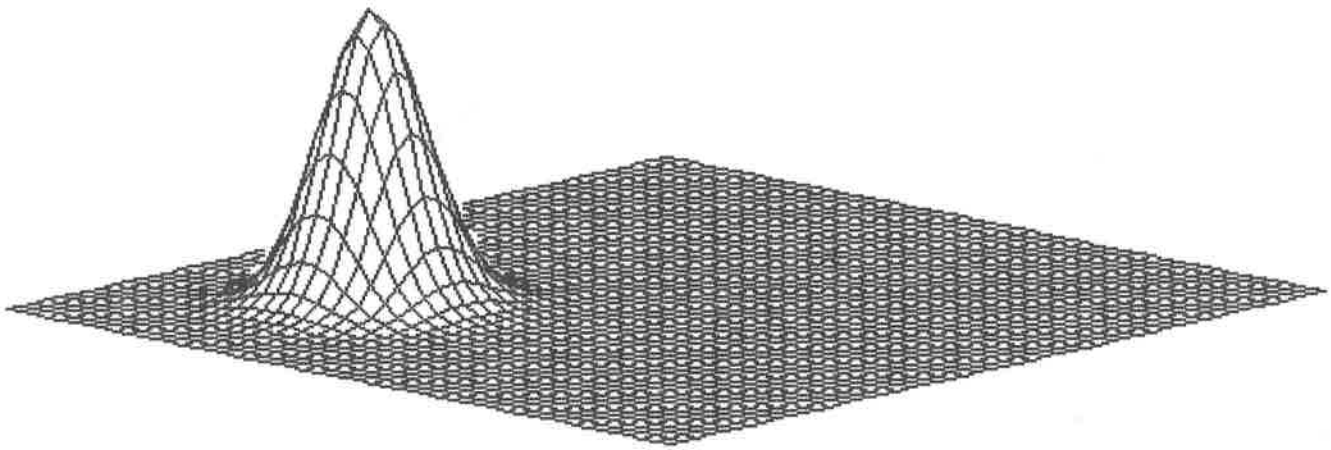
§ 6.4 Two-dimensional Simulation Pictures

Below is a tabulation of relevant parameters of two-dimensional simulation pictures

	σ_0	k_0	a	V
E Series	0.08	90.0	0.08	$-2k_0^2$
F series	0.08	90.0	0.08	$-k_0^2$
G series	0.08	90.0	0.08	$2k_0^2$

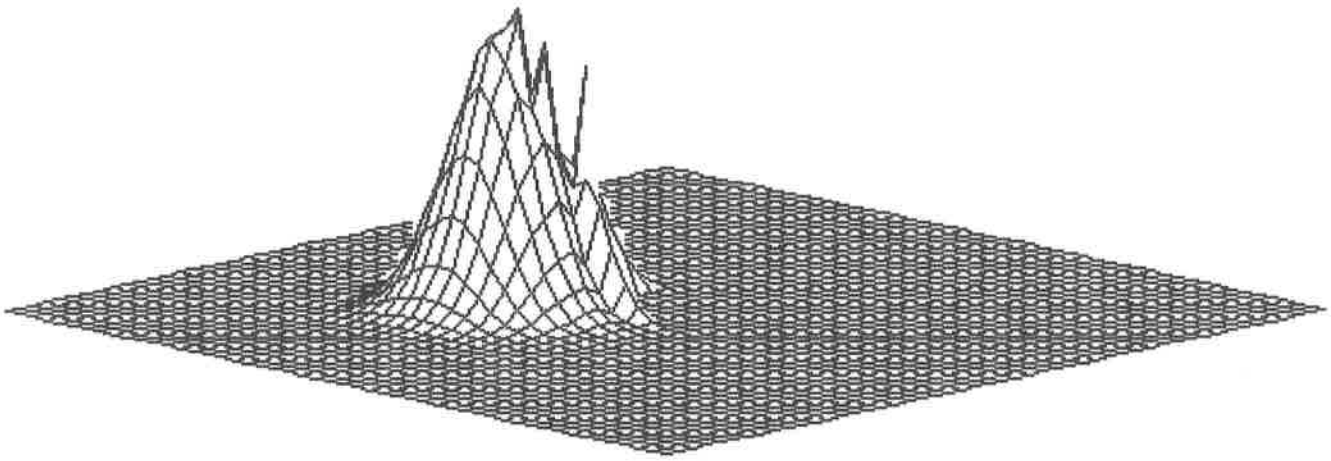
where σ_0 is the wave packet initial width, k_0, the average momentum, a, the radius and V the maximum of potential. The potential is cylinderically shaped

The transimission, reflection aspects in these cases have new degrees of freedom. Wave packets are scattered more in some directions are less others. The cross section, introduced in § 4.5, is a physical quantity that accounts for these degrees of freedom.



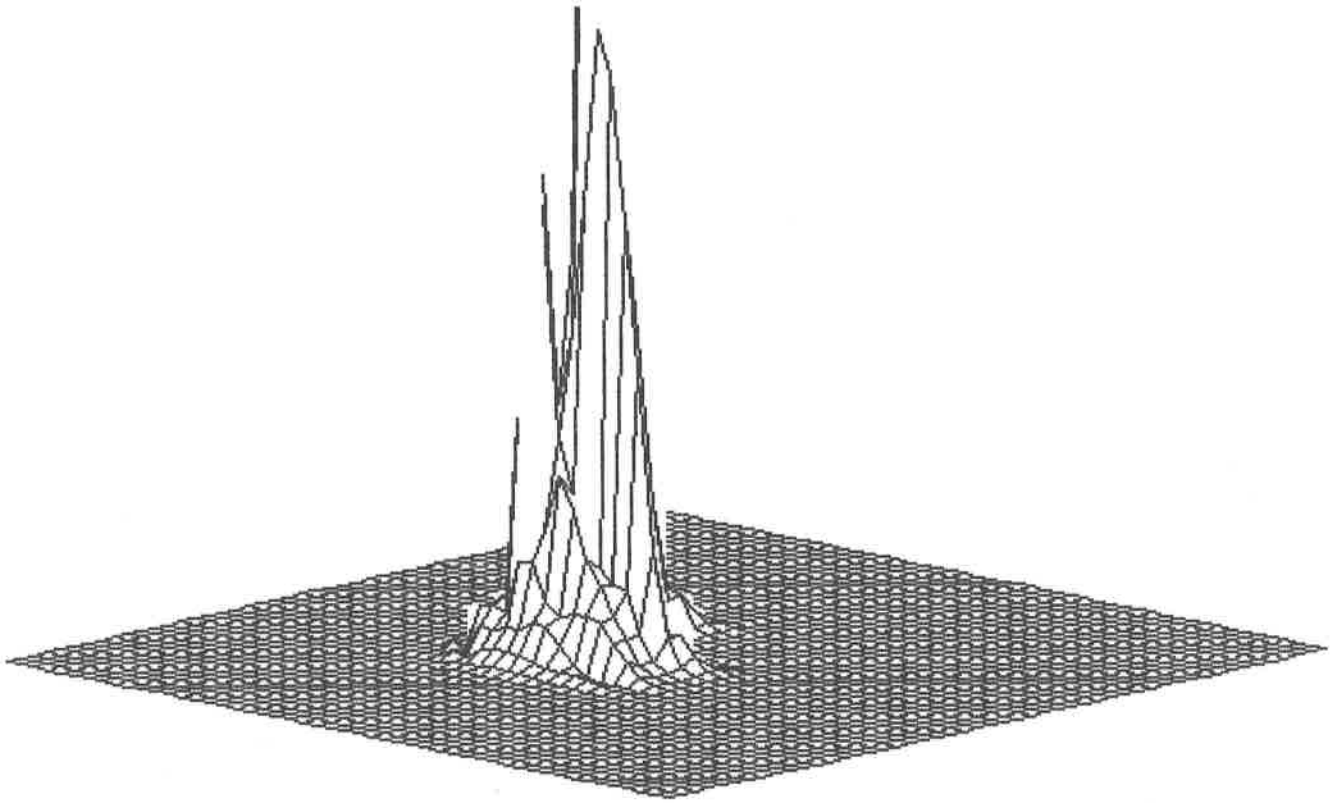
Initial Position

$t = 8$



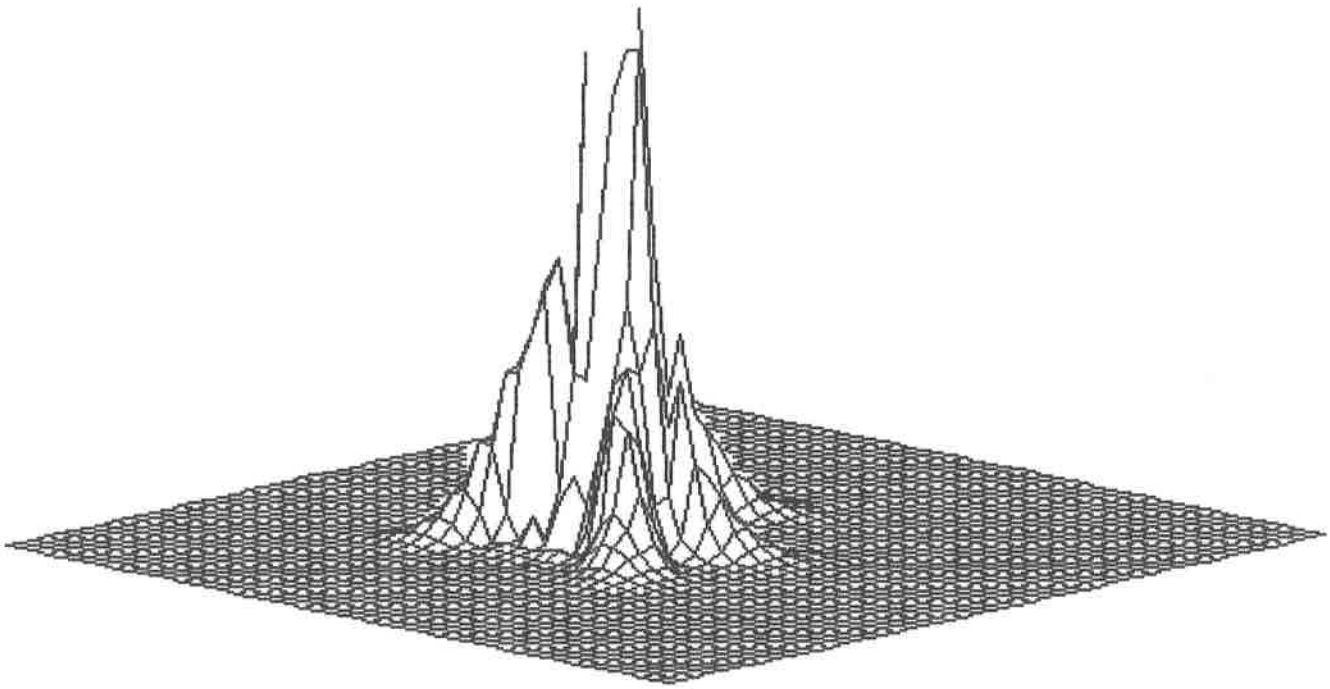
E

$t = 12$



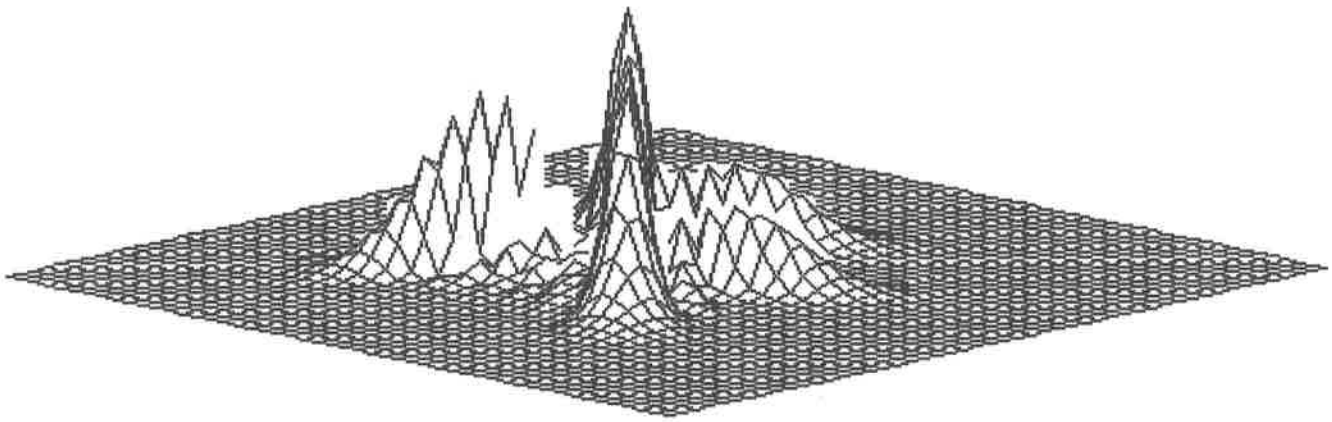
E

$t = 16$



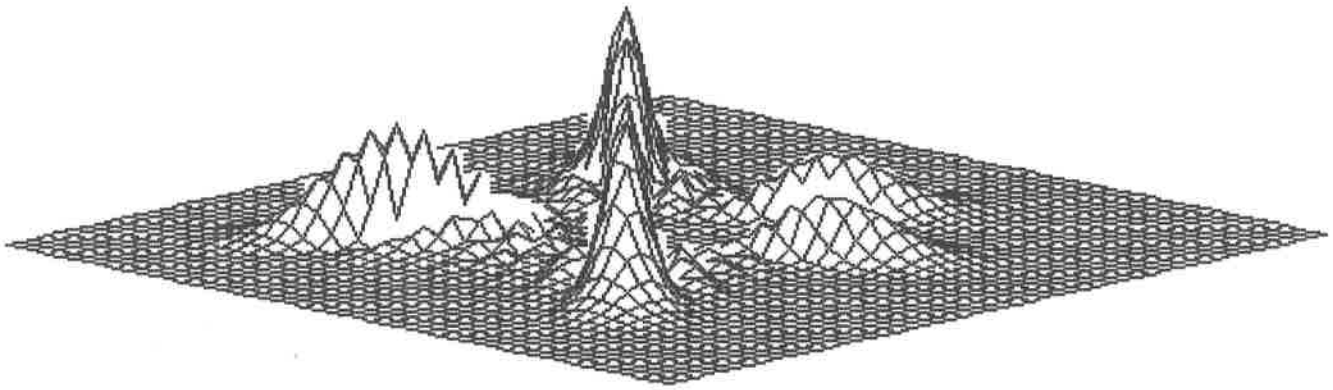
E

$t = 20$



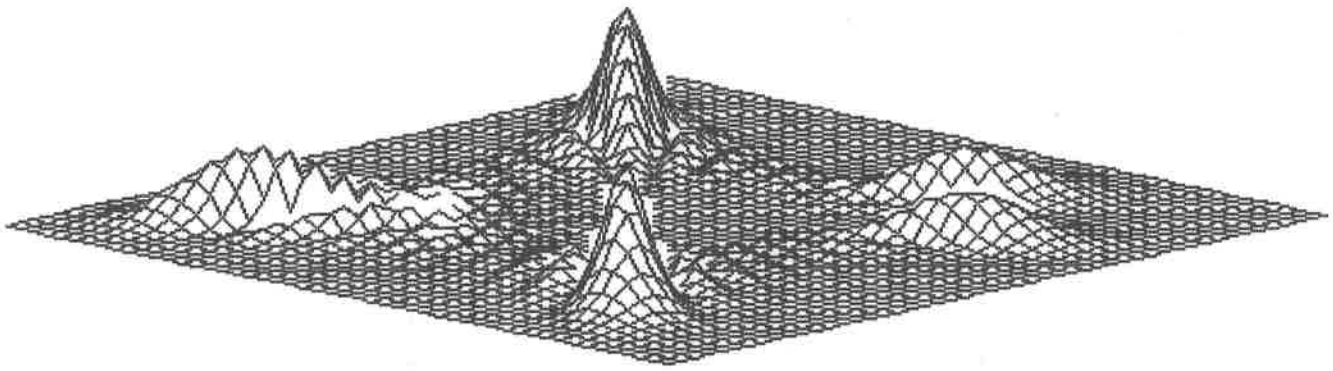
三

$t = 24$



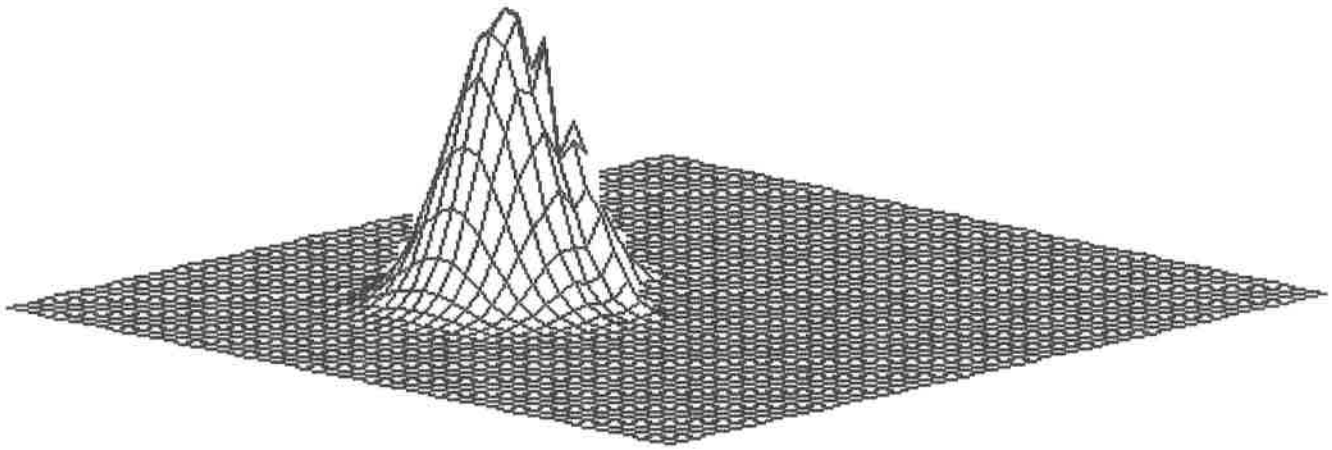
E

$t = 30$



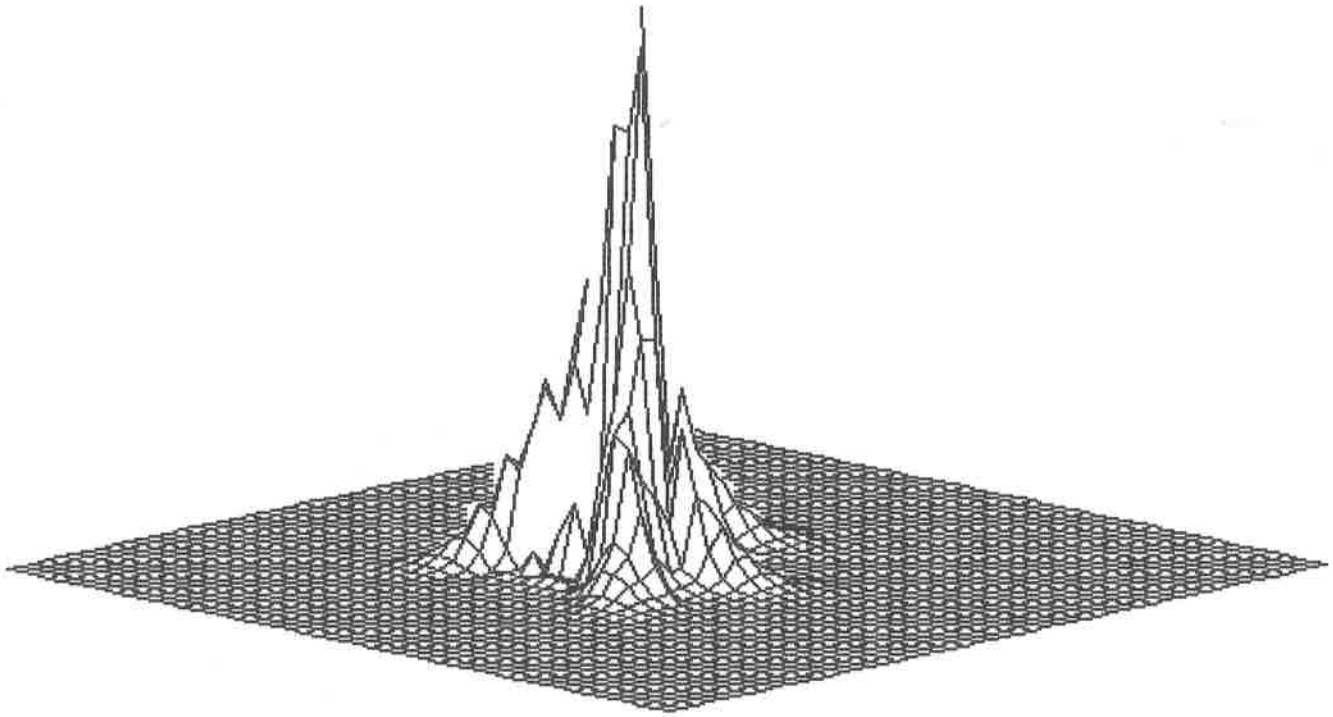
E

$t = 8$



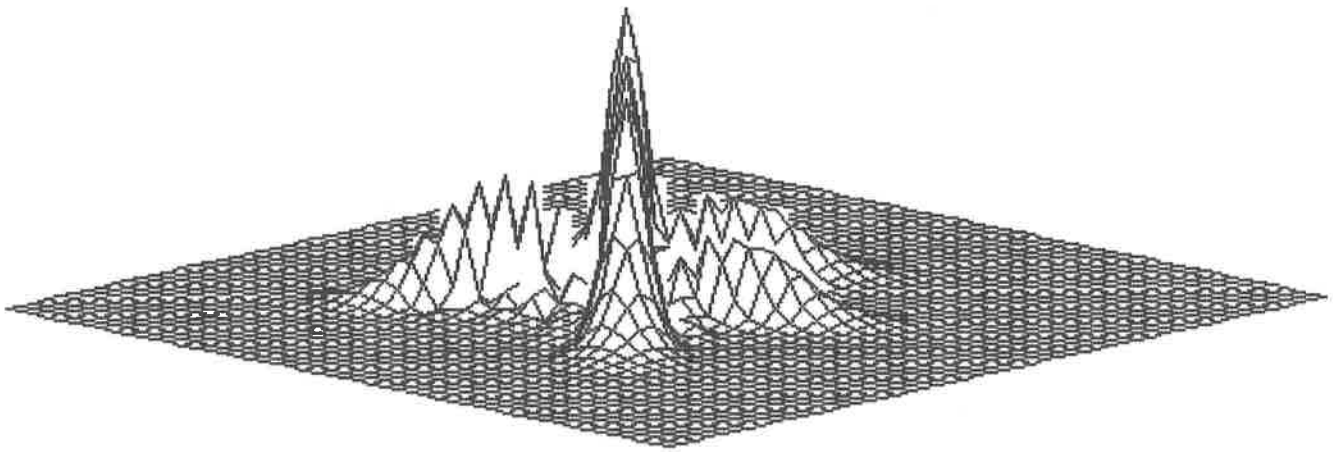
F

$t = 12$



F

$t = 16$

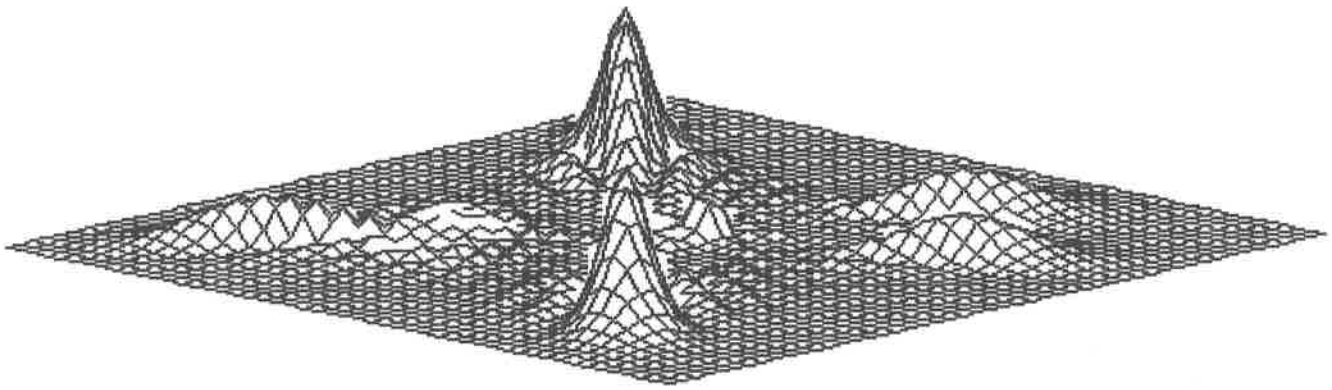


F

$t = 20$

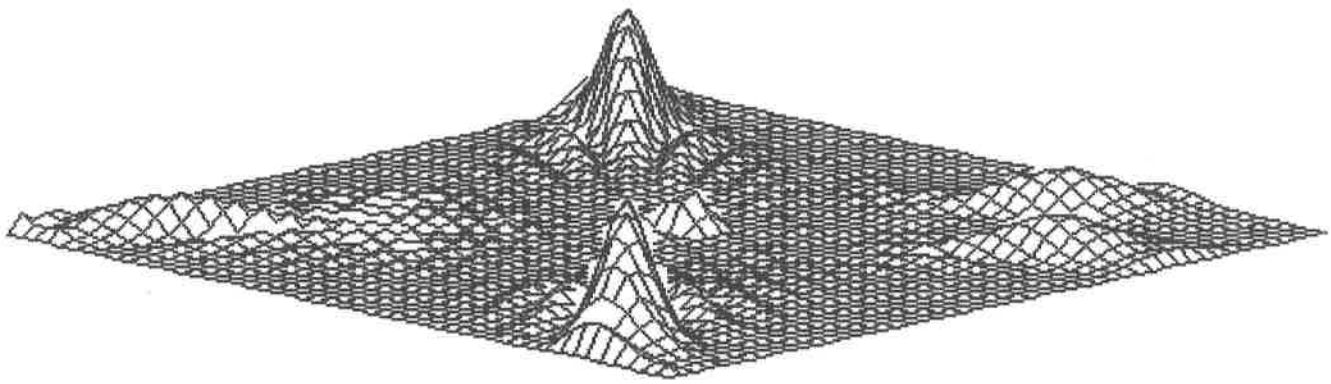
F

$t = 24$



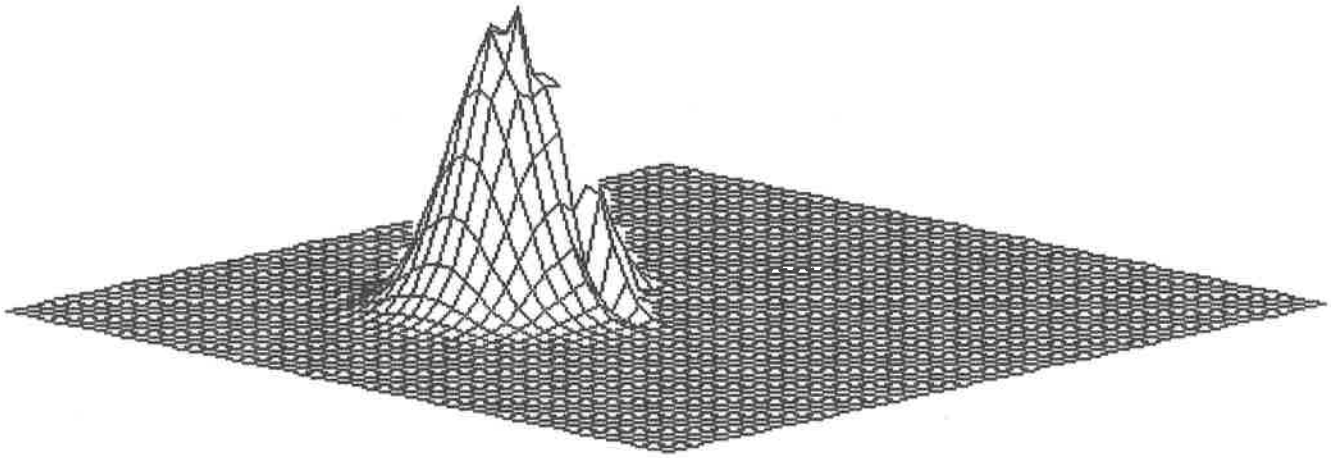
F

$t = 30$



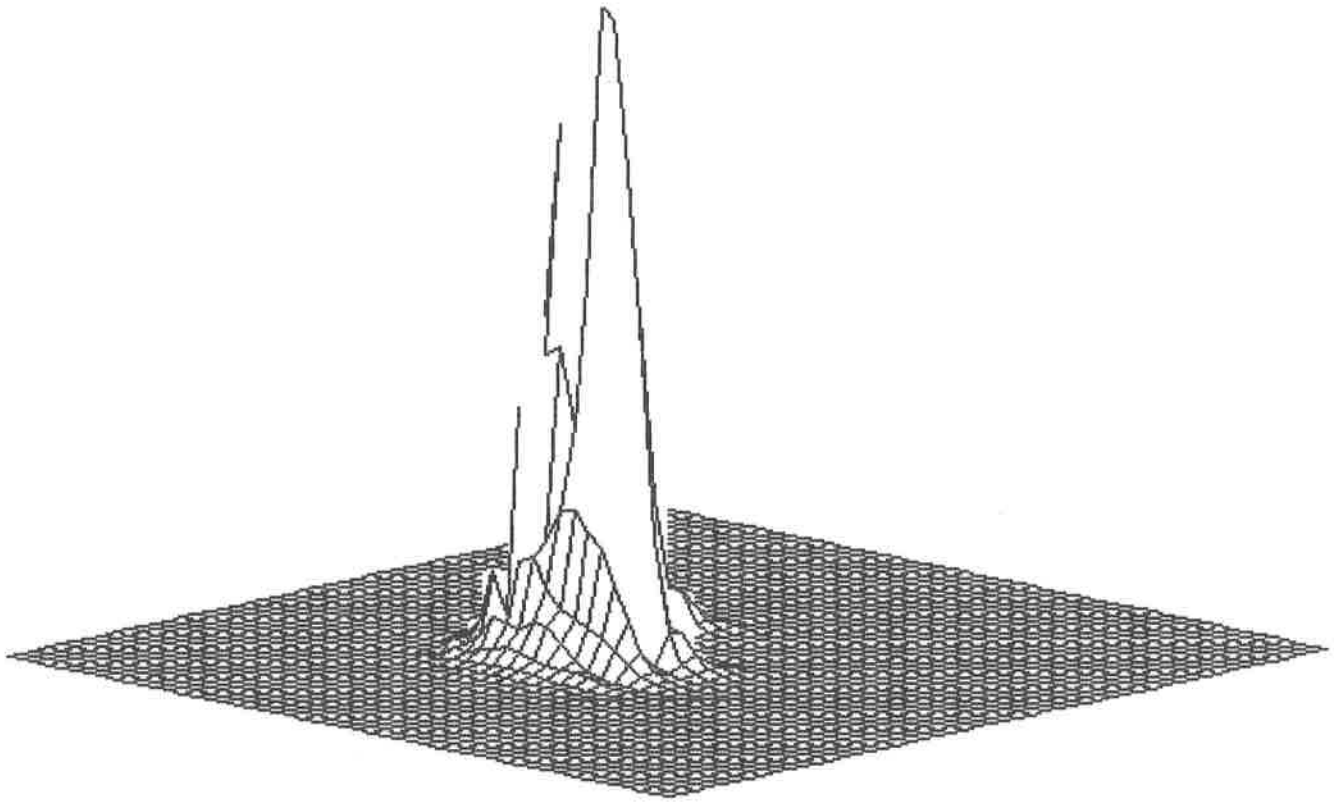
F

$t = 8$



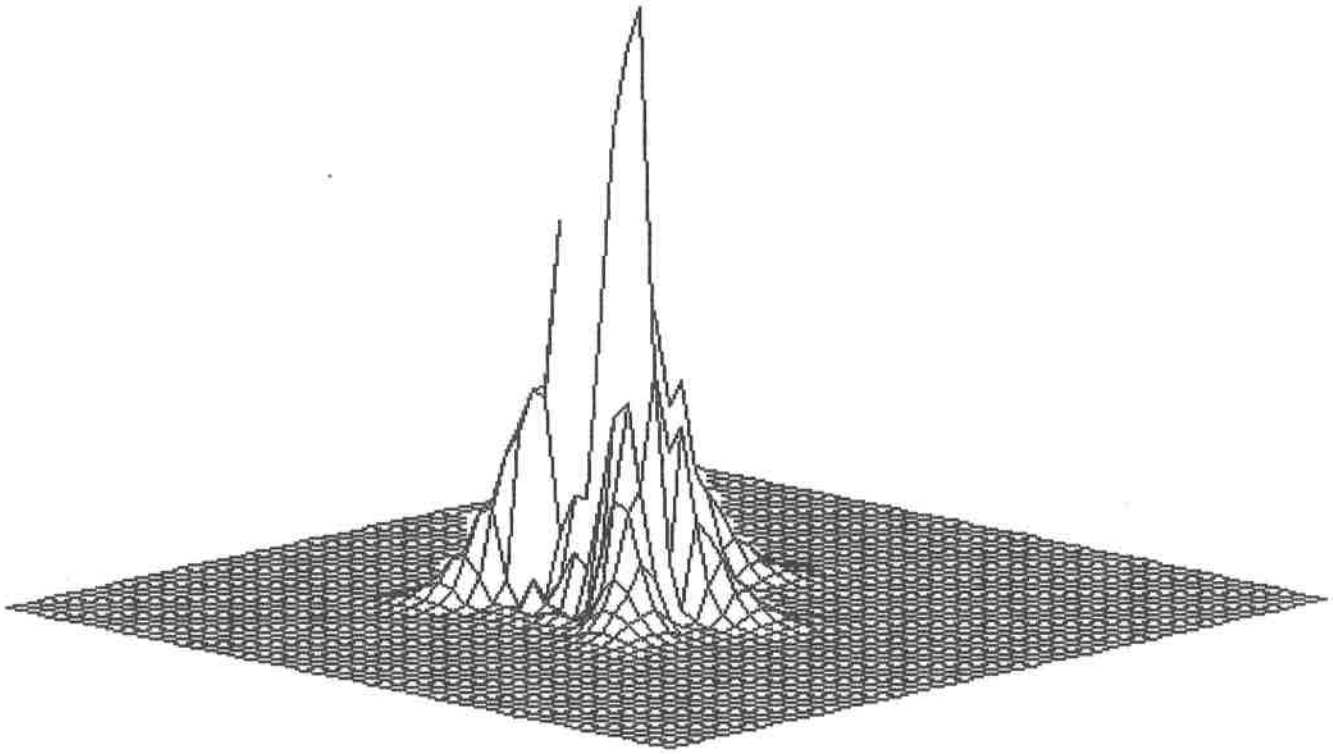
G_T

$t = 12$



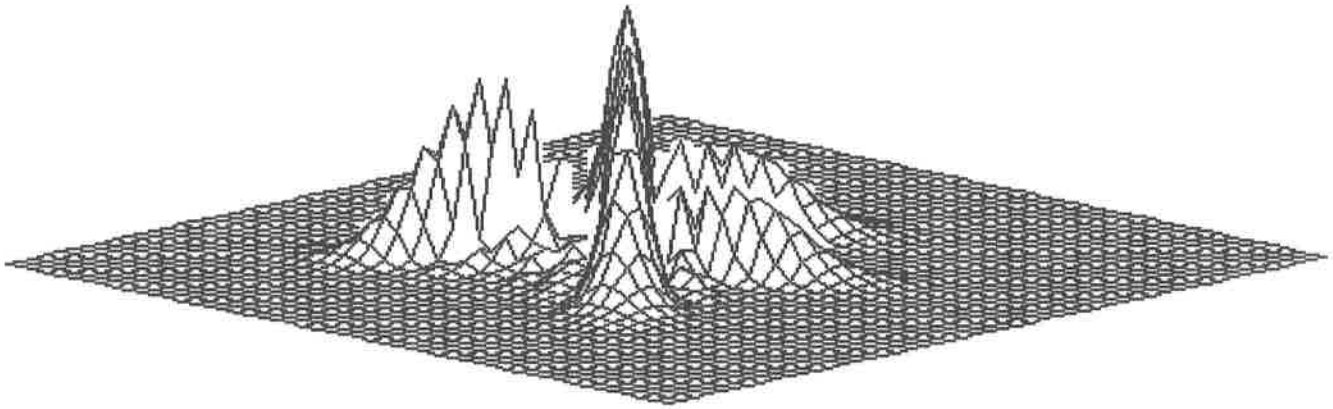
G

$t = 16$



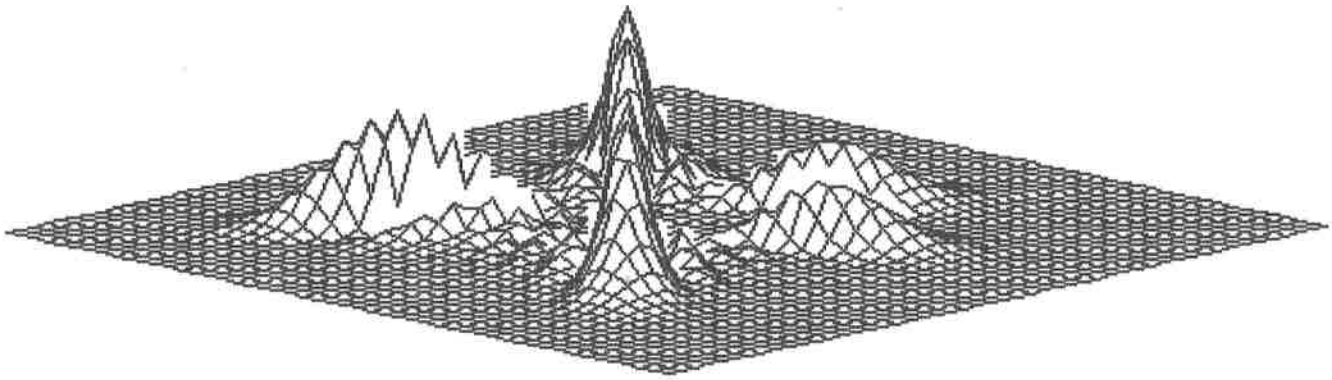
G_T

$t = 20$



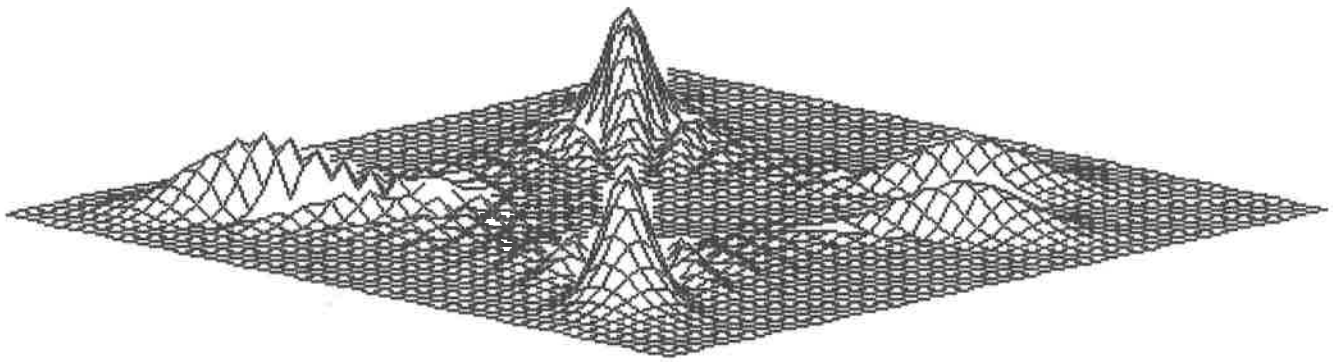
G_T

$t = 24$



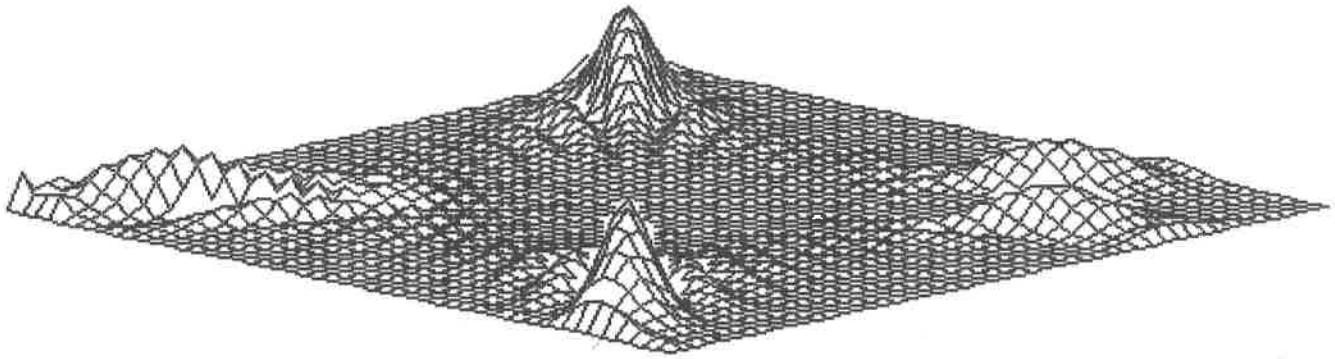
G

$t = 30$



G

$t = 34$



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Chapter 7 Concluding Remarks

§ 7.1 Klein – Gordan Equation

§ 7.2 Miscellaneous

§ 7.3 Conclusions

§7.1 Klein Gordan Equation

Another equation which may be treated with the same methodology is Klein - Gordan equation (See [Da 76] for details) It describes a spin zero particle.

$$\frac{\hbar^2}{c^2}\frac{\partial^2\Psi}{\partial t^2} - \hbar^2\nabla^2\Psi = m^2c^2\Psi \qquad (1)$$

Since it is a hyperbolic differential equation, it has an extra degree of freedom. We may write

$$\Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$$

Then

$$\begin{cases} i\hbar\frac{\partial\varphi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2(\varphi+\chi) + mc^2\varphi & (2a) \\ i\hbar\frac{\partial\chi}{\partial t} = \frac{\hbar^2}{2m}\nabla^2(\varphi+\chi) - mc^2\varphi & (2b) \end{cases}$$

Introduce

$$\hat{\tau}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \hat{\tau}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \hat{\tau}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

We can rewrite the coupled equations (2a) and (2b) as

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_{KG}\Psi \qquad (3)$$

with

$$\hat{H}_{KG} = (\hat{\tau}_3 + i\hat{\tau}_2)\left(\frac{-\hbar^2}{2m}\nabla^2\right) + mc^2\hat{\tau}_3$$

We shall work in a unit such that

$$\hbar = 1 \qquad c = 1 \qquad m = \tfrac{1}{2} \tag{4}$$

Solving (3) formally, we obtain the evolution operator

$$\Psi(\mathbf{x},t) = \exp(-it\hat{H}_{KG})\,\Psi(\mathbf{x},0) \tag{5}$$

The method mentioned in § 6.1 may be used again to solve (5) numerically, ensuring that unitary of the difference equation is preserved.

Another way is to start with

$$\left.\begin{aligned} \varphi &= a + ib \\ \chi &= c + id \end{aligned}\right\} \tag{6}$$

Substitute (4) and (6) into (2a) and (2b), we get

$$\left\{\begin{aligned} -\frac{\partial b}{\partial t} &= -\nabla^2(a+c) + \tfrac{1}{2}a && \text{(i)} \\ \frac{\partial a}{\partial t} &= -\nabla^2(b+d) + \tfrac{1}{2}b && \text{(ii)} \\ -\frac{\partial d}{\partial t} &= \nabla^2(a+c) - \tfrac{1}{2}c && \text{(iii)} \\ \frac{\partial c}{\partial t} &= \nabla^2(b+d) - \tfrac{1}{2}d && \text{(iv)} \end{aligned}\right.$$

Define

$$\alpha_+ = a + c$$
$$\alpha_- = a - c$$
$$\beta_+ = b + d$$
$$\beta_- = b - d$$

(iii) − (i) :

$$\frac{\partial (b-d)}{\partial t} = 2\nabla^2 (a+c) - \frac{1}{2}(a+c)$$

(ii) + (iv) :

$$\frac{\partial (a+c)}{\partial t} = \frac{1}{2}(b-d)$$

$$\therefore \quad \frac{\partial (b-d)}{\partial t} = 2\frac{\partial^2}{\partial t^2}(a+c)$$

Hence $$\frac{\partial^2}{\partial t^2}\alpha_+ = \nabla^2 \alpha_+ - \frac{1}{4}\alpha_+$$

(ii) − (iv) :

$$\frac{\partial (a-c)}{\partial t} = -\nabla^2 (b+d) + \frac{1}{2}(b+d) \qquad (*)$$

(i) + (iii)

$$\frac{\partial (b+d)}{\partial t} = -\frac{1}{2}(a-c) \qquad (**)$$

We partial differentiate (*) with respective to t.

$$\frac{\partial^2}{\partial t^2}(a-c) = -\nabla^2 \frac{\partial}{\partial t}(b+d) + \frac{1}{2}\frac{\partial}{\partial t}(b+d)$$

Substitute (**) into the above expression,

$$\frac{\partial^2}{\partial t^2}\alpha_- = \nabla^2 \alpha_- - \frac{1}{4}\alpha_-$$

Similarly we can derive an expression for β_+ and

β- as well. It is interesting to note that they obey the same differential equation.

$$\left(\frac{\partial^2}{\partial t^2} - \nabla^2 \right) \psi(x,t) = -\frac{1}{4} \psi(x,t) \qquad (7)$$

I had tried solving equations (3) and (7) numerically. But I did not have time to ponder over the numerical results and present them. My aim was to produce pictures of the dynamical process of particle-antiparticle annihilation

§7.2 Miscellaneous.

Other than Klein-Gordon equation, Dirac equation (See [Da76]) may be solved numerically. These fundamental equations of motion which describe spin zero and spin $\frac{1}{2}$ particles relativistically are more difficult to deal with, because a gaussian wave packet may alter its wave form drastically.

Another area of interest is a direct application of Schrödinger equation to a quantum mechanical system composed of many sub-systems. For example, Hartree-Fock equation (See [BKN76]) is a good approximation of wide variety of nuclear dynamical phenomena. If one really is serious about the behaviour of elementary particles, one has to go beyond quantum mechanics. Quantum field theory is the best means of studying these particles at this moment. Computer simulations in quantum field theory are not done extensively, because the mathematical models are too complex and the number of degrees of freedom is formidable.

It must be realised that a computer is more than a calculating machine. We can teach computer how to deduce. And we can let computer perform numerous deductions of the possible conformal structures of protein molecules from their constituent amino acids. This category of research is still at the rudimentary stage, despite the great significance of determing three-dimensional bio-molecules.

As has been mentioned, computer is only a tool.

The application aspects of it must not supersede the essence and foundation of scientific inquiries.

§ 7.3 Conclusion

In this paper, I had managed to present a short, elementary but self-contained discussion on the basics of quantum mechanics. Simulation pictures were produced to make understanding quantum mechanics simple and intuitive for beginners. Difficult mathematics was avoided as far as possible so that physical insights of quantum mechanics are easy to grasp.

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Appendix A Fourier Series and Fourier Transform

Let $f(x)$ be a periodic function with a fundamental period of L. ie

$$f(x+L) = f(x)$$

If $f(x)$ is a piecewise smooth function, it may be expanded as follows

$$f(x) = \sum_{-\infty}^{+\infty} c_n e^{ik_n x}$$

with $k_n = n\frac{2\pi}{L}$

$$c_n = \frac{1}{L}\int_{x_0}^{x_0+L} f(x)\, e^{-ik_n x}\, dx$$

x_0 being an arbitrary real number

We want to check if the expansion converges towards $f(x)$.
Let's consider a finite sum $\sum_{n=-N}^{N} c_n e^{ik_n x}$ and calculate

$$J = \frac{1}{L}\int_{x_0}^{x_0+L} \left| f(x) - \sum_{n=-N}^{N} c_n e^{ik_n x} \right|^2 dx$$

$$= \frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2 dx - 2\sum_{-N}^{N} c_n c_n^* + \sum_{-N}^{N} c_n c_n^*$$

$$= \frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2 dx - \sum_{-N}^{N} |c_n|^2$$

Since $J \geq 0$, we have Bessel's inequality

$$\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2 dx \geq \sum_{-N}^{N} |c_n|^2$$

When $N \to \infty$, because $\{e^{ik_n x}\}$ is complete orthonormal, we have the well-known Parseval relation

$$\frac{1}{L}\int_{x_0}^{x_0+L} |f(x)|^2 = \sum_{n=-\infty}^{\infty} |c_n|^2$$

Consider a function $f(x)$ which is periodic within the interval $-L/2 \leq x \leq \frac{L}{2}$. We denote $f(x)$ in this interval as $f_L(x)$, which we expand into Fourier series

$$f_L(x) = \sum_{n=-\infty}^{+\infty} c_n e^{ik_n x}$$

with $$k_n = \frac{2n\pi}{L}$$

and $$c_n = \frac{1}{L}\int_{x_0}^{x_0+L} e^{-ik_n x} f_L(x)\, dx$$

$$= \frac{1}{L}\int_{-\frac{L}{2}}^{\frac{L}{2}} e^{-ik_n x} f(x)\, dx$$

When $L \to \infty$, $f_L(x) \longrightarrow f(x)$. Therefore we shall consider this limit. Now,

$$k_{n+1} - k_n = \frac{2\pi}{L}$$

$$\therefore \quad L = \frac{k_{n+1} - k_n}{2\pi}$$

$$\therefore \quad f_L(x) = \sum_{n=-\infty}^{+\infty} \frac{k_{n+1} - k_n}{2\pi} e^{ik_n x} \int_{-L/2}^{+\frac{L}{2}} e^{-ik_n \xi} f(\xi)\, d\xi$$

As $L \to \infty$, $k_{n+1} - k_n \to dk$, and k_n becomes a continuous variable k. We may write

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-ikx} f(x) \qquad \text{so that}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ikx} \tilde{f}(k)\, dk$$

Hence, we obtained the Fourier Transform pair.

Appendix B Sturm - Liouville Eigenvalue Problem

For $x \in [a,b]$,

$$(p(x)y')' - q(x)y + \lambda w(x)y = (L + \lambda\omega)y = 0 \qquad (1)$$

Here, a dash denotes differentiation with respect to x. $p(x)$, $q(x)$, $w(x)$ are real continuous function on $[a,b]$. λ is a constant. If there exist $y(x)$ which is not identical to 0, then λ is called eigenvalue and $y(x)$ eigenfunction. To make the discussion simple, we shall consider the case $p(x) > 0$ and $q(x) > 0$.

Let say $\lambda_1 \neq \lambda_2$ are two eigenvalues of $y_1(x)$ and $y_2(x)$ respectively.

$$(py_1')' - qy_1 + \lambda_1 w y_1 = 0 \qquad (2)$$

$$(py_2')' - qy_2 + \lambda_2 w y_2 = 0 \qquad (3)$$

Multiply (2) by $y_2(x)$ and (3) by $y_1(x)$. Subtract after multiplication and rearrange,

$$\{p(y_2y_1' - y_1y_2')\}' + (\lambda_1 - \lambda_2) w y_1 y_2 = 0$$

Integrate,

$$(\lambda_1 - \lambda_2)\int_a^b w y_1 y_2 \, dx = \int_a^b \{p(y_1y_2' - y_2y_1')\}' \, dx$$

$$= [p(y_1 y_2' - y_2 y_1')]_a^b = 0$$

since y_1 and y_2 satisfy the same boundary conditions.
Now $\lambda_1 - \lambda_2 \neq 0$, we deduce that

$$\int_a^b w y_1 y_2 \, dx = 0$$

Hence, we have proven that for all eigenfunctions,

$$\int_a^b y_m(x) y_n(x) w(x) \, dx = \text{constant } \delta_{mn} \qquad (4)$$

Let's proceed to prove that all eigenvalues are real
We shall show that

$$\lambda = \mu + i\nu \qquad (\nu \neq 0)$$

whose eigenfunction $y = u + iv$ will lead to contradiction In elementary linear algebra, we learn that if λ is an eigenvalue, then its complex conjugate is also an eigenvalue. The corresponding eigenfunctions are y and y^* Since $\lambda \neq \lambda^*$, we use (4)

$$0 = \int_a^b y y^* w \, dx = \int_a^b (u^2 + v^2) w \, dx$$

But u, v, w are real functions and $w \neq 0$ Therefore

$$u = v = 0$$

ie $y = 0$ This is a contradiction

We may redefine $y_n(x)$ such that the constant is equal to one Thus an orthonormal eigenfunction

system with real eigenvalues is obtained.
How do we know that the eigenvalues are discrete?
We shall go over to polar form. Let us define $\rho(x)$, and $\theta(x)$ such that:

$$\rho(x) = \left(y^2 + p^2 y'^2 \right)^{\frac{1}{2}}$$

$$y = \rho \sin\theta$$

$$py' = \rho \cos\theta$$

Thus we can express (1) as

$$\rho' = \rho \{ p^{-1} + q - \lambda w \} \sin\theta \cos\theta \qquad (5)$$

$$\theta' = p^{-1} \cos^2\theta + (\lambda w - q) \sin^2\theta \qquad (6)$$

Since (6) is only a differential equation of $\theta(x)$, we may solve it with an initial condition $\theta(a) = \mu$.
The most general boundary condition of (1) is

$$\alpha_1 y(a) + \beta_1 y'(a) = 0 \qquad (7)$$

$$\alpha_2 y(b) + \beta_2 y'(b) = 0 \qquad (8)$$

where $\alpha_1, \alpha_2, \beta_1$ and β_2 are arbitrary constants.
We choose μ and ν such that

$$\beta_1/\alpha_1 = -p(a) \tan\mu$$

$$\beta_2/\alpha_2 = -p(a) \tan\nu$$

then (7) and (8) becomes

$$p(a)\,y'(a)\sin\mu - y(a)\cos\mu = 0 \qquad (9)$$

$$p(b)\,y'(b)\sin\nu - y(b)\sin\nu = 0 \qquad (10)$$

Since $y = \rho\sin\theta$

$$\therefore \quad y(a) = \rho(a)\sin\theta(a) = \rho(a)\sin\mu$$

and $\quad py' = \rho\cos\theta$

$$\therefore \quad p(a)\,y'(a) = \rho(a)\cos\theta(a) = \rho(a)\cos\mu$$

Therefore (9) is satisfied by $\theta(a)$

On the other hand, we have

$$y(b) = \rho(b)\sin\theta(b)$$

$$p(b)\,y'(b) = \rho(b)\cos\theta(b)$$

If we set $\theta(b) = \nu + n\pi$, then boundary condition (10) is satisfied.

Therefore we see that $\theta(b)$ takes on discrete values. From (6) it is easy to see that $\theta(x)$ is dependent on λ. We write $\theta(x)$ as $\theta(x,\lambda)$ to show this fact.

Suppose that $\lambda_2 > \lambda_1$, then from (6)

$$\theta'(x,\lambda_2) - \theta'(x,\lambda_1) = (\lambda_2-\lambda_1) w \sin^2\theta > 0$$

$$\theta'(x,\lambda_2) = \theta'(x,\lambda_1) + c \qquad (11)$$

$$c = (\lambda_2-\lambda_1) w \sin^2\theta > 0$$

Since the initial condition of $\theta(x)$ is $\theta(a) = \mu$, We see that for $x > \mu$, by the continuity of $\theta(x)$ and (11) $\theta'(x,\lambda_2) > \theta'(x,\lambda_1)$. therefore we conclude that

$$\theta(x,\lambda_2) > \theta(x,\lambda_1)$$

Now making use of the monotonous property of $\theta(x)$, Suppose that we vary λ monotonously from $-\infty$, then $\theta(b,\lambda)$ is also monotonously increasing. At, say, $\lambda = \lambda_0$, boundary condition

$$\theta(b,\lambda_0) = \nu$$

is satisfied. Then λ_0 becomes our smallest eigenvalues. We can find other eigenvalues by

$$\theta(b,\lambda_n) = \nu + n\pi$$

Therefore we see that the eigenvalue takes on discrete values which are countably infinite in number