Quantum Scattering Problem on Computers — a term project for 22.113

Li Ju

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Contents

Chapter 1

Introduction

As a term project for MIT course 22.113 *Nuclear and Atomic Collision Phenomena*, I investigated the computational approaches to various kinds of quantum scattering problems. My motivation is first to understand the analytic formulations on which these computational methods are made possible, and then to implement them on the computer and get correct results. Two characteristic problems were chosen:

1) The quantum scattering problem for arbitary central pair potential.

2) Time-dependent 1D and 2D Schrodinger Equation.

These problems, in general, are not very complicated. But we can learn something from these nice "little" ones, and solve more complex problems in the future.

Reference Books:

1) *Computational Physics*
by Steven E.Koonin, 1986 Addison-Wesley.

2) *Computational Methods in Physics & Engineering*
by Samual S.M.Wong, 1992 Prentice-Hall.

3) *Numerical Recipes in C — The Arts of Scientific Computing.*
2nd Edition, 1992 Cambridge University Press.

Chapter 2

Central Pair Scattering

2.1 Theoretical Formulation

Denote the pairwise central potential as $V(r)$, the problem for two-body quantum scattering can be routinely transformed into the one body Schrodinger equation:

$$(\frac{-\hbar^2}{2\mu}\nabla^2 + V(r))\psi(\vec{r}) = E\psi(\vec{r})$$

where μ is the effective mass

$$\mu = \frac{mM}{m+M} \tag{2.1}$$

Let $k = \sqrt{2\mu E}/\hbar$. The asymptotic behaviour of the scattered plane wave is

$$\psi(\vec{r}) \longrightarrow e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \tag{2.2}$$

and the corresponding differential cross section is

$$\sigma(\theta) = \frac{dN/d\Omega}{J_{in}} = |f(\theta)|^2 \tag{2.3}$$

Because $V(r)$ is pairwise, $[\mathcal{H}, \mathcal{J}] = 0$. The angular momentum and the Hamiltonian can be diagonalized concurrently, so

$$\psi(r,\theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta) \tag{2.4}$$

with $u_l(r)$ satisfies

$$\frac{d^2u_l(r)}{dr^2} + [k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu V(r)}{\hbar^2}]u_l(r) = 0 \tag{2.5}$$

The general solution to this equation is of the form

$$u_l(r) = B_l r j_l(kr) + C_l r n_l(kr) \tag{2.6}$$

where $j_l(r)$ and $n_l(r)$ are the regular and irregular (Neumann function) spherical Bessel functions. The asymptotic behaviour of $u_l(r)$ at $kr \gg 1$ is

$$\begin{aligned} u_l(r) &\longrightarrow \frac{B_l}{k}\sin(kr - \frac{l\pi}{2}) - \frac{C_l}{k}\cos(kr - \frac{l\pi}{2}) \\ &= \frac{a_l}{k}\sin(kr - \frac{l\pi}{2} + \delta_l) \end{aligned} \tag{2.7}$$

so

$$\psi(r,\theta) \longrightarrow \sum_{l=0}^{\infty} i^l(2l+1)a_l P_l(\cos\theta)\frac{\sin(kr - l\pi/2 + \delta_l)}{kr} \tag{2.8}$$

There's also an frequently used expansion of plane wave into spherical harmonics:

$$\begin{aligned} \exp(ikr\cos\theta) &= \sum_{l=0}^{\infty} i^l(2l+1)j_l(kr)P_l(\cos\theta) \\ &\longrightarrow \sum_{l=0}^{\infty} i^l(2l+1)P_l(\cos\theta)\frac{\sin(kr - l\pi/2)}{kr} \end{aligned} \tag{2.9}$$

Compare with (2.2), we see that in order to achieve the predicted scattering behaviour, there should be

$$a_l\sin(kr - l\pi/2 + \delta_l) - \sin(kr - l\pi/2) = f_l e^{ikr} \tag{2.10}$$

and f_l should not be a function of r, so

$$a_l\frac{e^{ikr - il\pi/2 + i\delta_l} - e^{-ikr + il\pi/2 - i\delta_l}}{2i} - \frac{e^{ikr - il\pi/2} - e^{-ikr + il\pi/2}}{2i} = f_l e^{ikr}$$

The e^{-ikr} terms on the right hand side must vanish, so

$$a_l = e^{i\delta_l} \tag{2.11}$$

and we get

$$f_l = \exp(\frac{-il\pi}{2})\frac{e^{2i\delta_l} - 1}{2i} = (-i)^l e^{i\delta_l}\sin\delta_l \tag{2.12}$$

So the scattered wave is

$$f(\theta)\frac{e^{ikr}}{r} = \sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)\frac{\exp(ikr)}{kr} \tag{2.13}$$

and the differential cross section is just

$$\sigma(\theta) = \frac{1}{k^2}|\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)|^2 \tag{2.14}$$

and the total cross section is

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{2.15}$$

Although the sums above extends over all l, we can select a reasonable cutoff in the sense that when

$$\frac{l_{max}(l_{max}+1)\hbar^2}{2\mu r_{max}^2} \gg E$$

the l_{max} partial wave decrease so quickly even at the surface of the potential field that it became negligible, which leads to the approximation of

$$l_{max} \sim kr_{max} \tag{2.16}$$

This estimate is usually slightly low.

2.2 Computational Method

To find the phase shift for each partial wave, we solve the equation

$$\frac{d^2u_l(r)}{dr^2} + [k^2 - \frac{l(l+1)}{r^2} - \frac{2\mu V(r)}{\hbar^2}]u_l(r) = 0 \tag{2.17}$$

numerically using the **Numerov Method**, which is a particular simple and efficient method in intergrating 2nd-order differential equations.

Numerov Method: For equations with the general form

$$\frac{d^2y}{dx^2} + k(x)y = S(x) \tag{2.18}$$

the method gives

$$(1 + \frac{h^2}{12}k_{n+1})y_{n+1} - 2(1 - \frac{5h^2}{12}k_n)y_n + (1 + \frac{h^2}{12}k_{n-1})y_{n-1}$$

$$= \frac{h^2}{12}(S_{n+1} + 10S_n + S_{n-1}) + O(h^6) \tag{2.19}$$

Notice the local error of $O(h^6)$, which is one order more accurate than the fourth-order Runge-Kutta method.

Since for our particular problem, $S(x) = 0$, it's a linear differential equation. And we know that $u_l(r = 0) = 0$, so the choice of $u_l(r = h)$ became totally arbitary, because we can always normalize the entire partial wave later if neccesary. (However, $u_l(r = h)$ is often chosen to be a small number to avoid overflow at greater r).

We intergrate the equation to a certain point r_1 where $V(r_1)$ is small enough so that the wave function can be regarded as approaching asymptotic behaviour. So

$$u_l(r_1) \approx Akr_1[\cos(\delta_l)j_l(kr_1) - \sin(\delta_l)n_l(kr_1)] \tag{2.20}$$

We continue intergrating to a larger radius $r_2 > r_1$, it also has

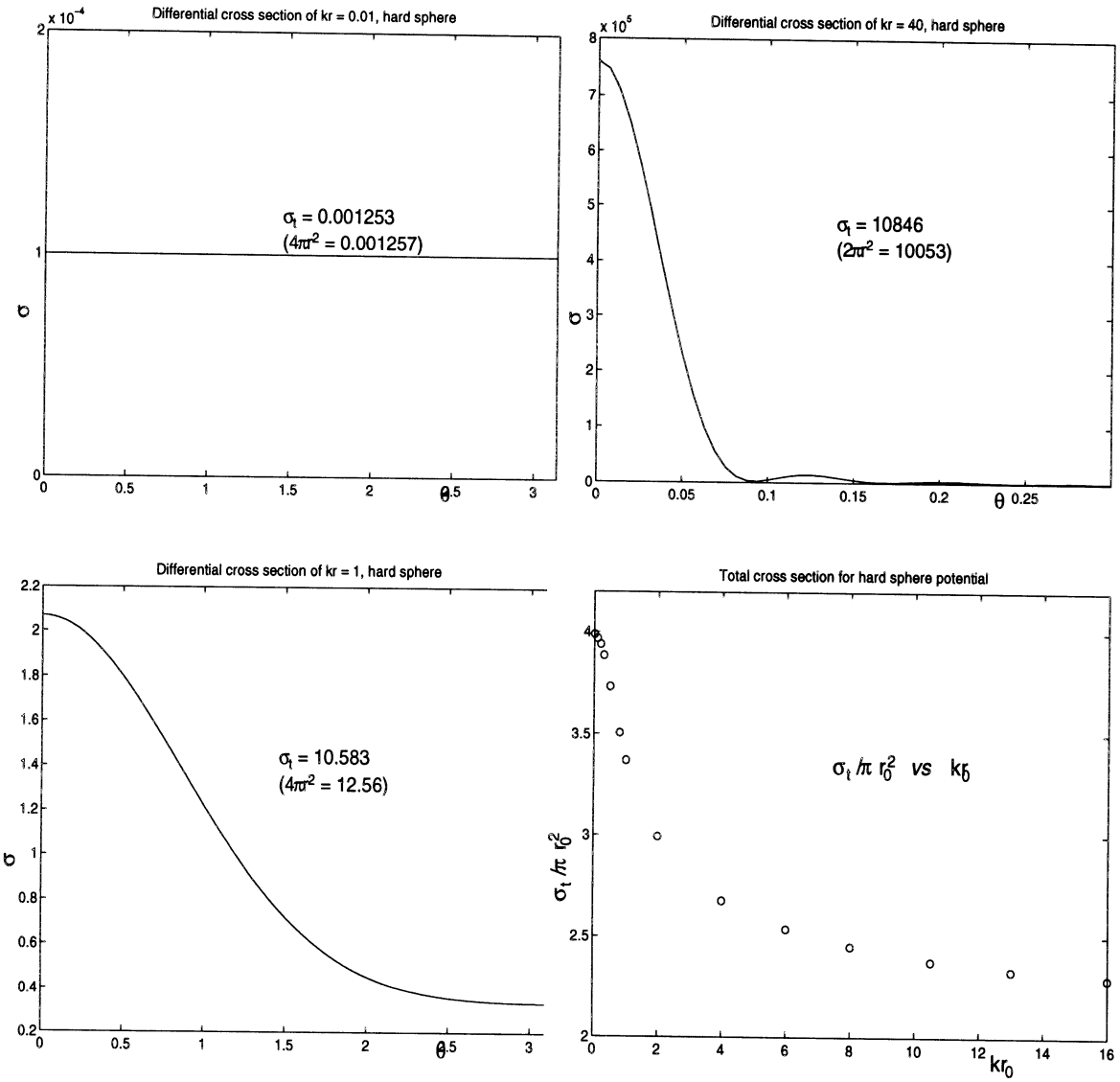
$$u_l(r_2) \approx Akr_2[\cos(\delta_l)j_l(kr_2) - \sin(\delta_l)n_l(kr_2)] \tag{2.21}$$

We can interpolate δ_l from these two points, after some manipulations we get

$$G = \frac{r_1u_l(r_2)}{r_2u_l(r_1)}$$

$$\delta_l = \tan^{-1}(\frac{Gj_l(r_1) - j_l(r_2)}{Gn_l(r_1) - n_l(r_2)})$$

2.3 Results



In this section we'll mainly show the computation results for hard sphere potential. (Although arbitary central potential is easily applicable, there don't exist much to compare with.) In classical mechanics we've shown that the total cross section for hard sphere collision is πr^2, with r as the radius of the sphere. In quantum mechanics, however, the result is quite different: For $kr \ll 1$, $\sigma_t \to 4\pi r^2$, and there will only be significant contribution from $l = 0$ so the scattering is isotropic, i,e, the differntial cross section is a constant. This is clearly shown in Fig.1.

When $kr \gg 1$, $\sigma_t \to 2\pi r^2$, and the differential cross section is highly condensed in the front. The computation result is shown in Fig.2.

The intermediate state of $kr = 1$ is shown in Fig.3.

Fig.4 is the $\sigma_t/\pi r^2$ versus kr curve, it start at $kr = 0$ with the value of 4, and then come down to 2 as $kr \to \infty$. This curve is not directly available from theory, but should be quite important. We can call it our first score.

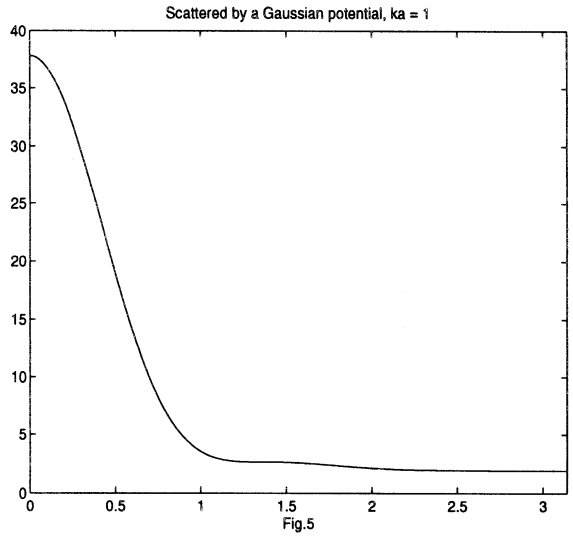


Fig.5

Fig.5 is the scattering by a Guassian potential:

$$V(r) = \exp(-(kr)^2/\alpha^2) \tag{2.22}$$

Here α is chosen to be 1, corresponding to situation of hard sphere collison with $kr = 1$. One should note the unusual tail inflextion at $\theta \simeq 1$.

Chapter 3

Time Dependent Schrodinger Equation

The Time Dependent Schrodinger Equation (TDSE) is

$$i\hbar\frac{\partial\psi}{\partial t} = \mathcal{H}\psi = (\frac{-\hbar^2}{2\mu}\nabla^2 + V(\vec{r}))\psi \tag{3.1}$$

Using reduced length and time unit we transform the equation into

$$i\frac{\partial\psi}{\partial t} = \mathcal{H}\psi = (-\nabla^2 + V(\vec{r}))\psi \tag{3.2}$$

Such partial differential equation with 1st-order time derivative is classified as *parabolic*, with respect to *elliptic* equations (0th order) and *hyperbolic* equations (2nd order). Another kind of parabolic differential equations is the diffusion equation.

Under discretization, the 2nd order derivative becomes

$$\frac{\partial^2\phi(x)}{\partial x^2} \longrightarrow \frac{1}{h^2}\{\phi(x+h) - 2\phi(x) + \phi(x-h)\} + \mathcal{O}(h^2) \tag{3.3}$$

and the general solution for (3.2) can be written as

$$\psi(x,t) = \exp(-it\mathcal{H})\psi(x,0) \tag{3.4}$$

The propagation operator can be approximated in the small time limit as

$$\exp(-i\tau\mathcal{H})\psi(x,0) = (1 - i\tau\mathcal{H})\psi(x,0) + \mathcal{O}(\tau^2) \tag{3.5}$$

The right hand side of the equation can be directly evaluated using (3.3). It is called the *explicit* scheme for the solution of parabolic equations. However, this scheme has severe limitations, that is, when the time constant τ get large, the scheme become unstable. This

can be easily understood if we consider the eigenfunctions of $\mathcal{H}$ under current boundary conditions:

$$\mathcal{H}\psi_n = \epsilon_n \psi_n \tag{3.6}$$

Since $\mathcal{H}$ is discretized, the number of eigenmodes for (3.6) isn't infinity as in continuum space, but equals to the N, the degree of discretization in space domain. Let's consider the highest eigenvalue (energy level), under rough approximation

$$\epsilon_N \approx (\frac{\pi}{h})^2 \tag{3.7}$$

because π/h is the edge of the first Brillouin zone, and we treat it as a free particle. We can see that when $\tau\epsilon_N$ is in the order of unity, the expansion (3.5) become invalid and those high eigenvalued modes (actually noise) would be endlessly amplified until the system breaks down. So the criterea of stabilty for the explicit scheme is

$$\tau(\frac{\pi}{h})^2 \ll 1 \tag{3.8}$$

Since h is usually chosen to be small in order to minimize the error in (3.3), we had to pick very small τ to stablize the scheme, thus making the observation of a time evolution process very difficult.

There is a much better scheme called the **Crank-Nicholson method**: we can approximate the propagation operator of (3.4) in the **Cayley form** as

$$\exp(-i\tau\mathcal{H}) = \frac{1 - \frac{1}{2}i\tau\mathcal{H}}{1 + \frac{1}{2}i\tau\mathcal{H}} + \mathcal{O}(\tau^3) \tag{3.9}$$

We observe that this form is one order more accurate than the explicit scheme. What's more, it's an unitary operator and therefor the amplitude of each eigenvalue component will always remain the same as the initial amplitude, because

$$\left|\frac{1 - \frac{1}{2}i\tau\epsilon_n}{1 + \frac{1}{2}i\tau\epsilon_n}\right| = 1 \tag{3.10}$$

This property is called *norm conserving* and it is the fundamental attribute of the Schrodinger wave equation. One direct conclusion is that the scheme is always **stable**, even when $\tau\epsilon_N \sim 1$, provided that the initial amplitude of the high k components are small, they will still cause little error later. What count are those components in the low k regime with large amplitudes, where $\tau\epsilon$ is small and the expansion is valid.

However, this is an *implicit* scheme because the Cayley operator can't be directly evaluated. We can rewrite (3.9) as

$$\{1 + \frac{1}{2}i\tau\mathcal{H}\}\psi(x_j, t+\tau) = \{1 - \frac{1}{2}i\tau\mathcal{H}\}\psi(x_j, t) \tag{3.11}$$

For one dimensional case

$$\mathcal{H} = -\frac{d^2}{dx^2} + V(x) \tag{3.12}$$

so

$$\{1+\frac{i\tau}{2}V(x_j)-\frac{i\tau}{2}\frac{d^2}{dx^2}\}\psi(x_j,t+\tau)=\{1-\frac{i\tau}{2}V(x_j)+\frac{i\tau}{2}\frac{d^2}{dx^2}\}\psi(x_j,t) \tag{3.13}$$

After some rearrangements we get the following equation

$$A_i^-\psi'_{i-1}+A_i^0\psi'_i+A_i^+\psi'_{i+1}=b_i \tag{3.14}$$

with

$$A_i^-=A_i^+=\frac{-i\tau}{2h^2} \tag{3.15}$$

$$A_i^0=1+\frac{i\tau}{2}V_i+\frac{i\tau}{h^2} \tag{3.16}$$

$$b_i=(2-A_i^0)\psi_i-A_i^+\psi_{i+1}-A_i^-\psi_{i-1} \tag{3.17}$$

This forms a set of $N\times N$ linear equations, which usually requires N^2 operations even in applying the inversion matrix each time. Fortunately, the following algorithm (Gaussian elimination and back-substitution) provides a very efficient solution (of the order N operations) for the tri-diagonal system as (3.14).

Using **C** language convention, let's represent the space in an $N+1$ matrix: the Dirichlet boundary condition is imposed on ψ'_0 and ψ'_N, which might be time dependent. We assume that solution of (3.14) satisfies relations of the form

$$\psi'_{i+1}=\alpha_i\psi'_i+\beta_i \tag{3.18}$$

and substitute it into (3.14)

$$A_i^-\psi'_{i-1}+A_i^0\psi'_i+A_i^+(\alpha_i\psi'_i+\beta_i)=b_i \tag{3.19}$$

This is of the same form as (3.18) except one regresion of index, so comparing with the assumed relation for ψ'_{i-1}, we identify the backward recursion relationship for α_{i-1} and β_{i-1} to be

$$\begin{aligned}\gamma_i &= -1/(A_i^0+A_i^+\alpha_i)\\ \alpha_{i-1} &= \gamma_i A_i^-\\ \beta_{i-1} &= \gamma_i(A_i^+\beta_i-b_i)\end{aligned} \tag{3.20}$$

In order to satisfy the boundary condition at ψ'_N, we let

$$\alpha_{N-1}=0 \quad \beta_{N-1}=\psi'_N \tag{3.21}$$

and make a backsweep from here to get $\alpha_i,\beta_i(i=N-2,0)$. After that we do a forward sweep from $i=0$ to $N-1$ to get the new wave function.

3.1 One Dimensional Scattering of a Wave Packet

There are several possibilities in selecting the initial form of the wave function. The recommendation of Goldberg, Schey, and Schwartz is to use a Guassian wave packet:

$$\Psi(x, t = 0) = \exp(ik_0 x - (x - x_c)^2/2\sigma_0^2) \tag{3.22}$$

The wave packet has a group velocity of k_0, but it will also spread out by itself(dispersion) as time evolves. We let it collide with an square barrier potential to see what happens.

The total length of the scenario was chosen to be 1, and was divided into 1000 equal parts, so $h = 0.001.\sigma_0 = 40$ and k_0 was chosen to be 50π, and τ was chosen to be 2×10^{-6}, so the expansion parameter in the spectrum center is about $k_0^2\tau \sim 0.05$, which is marginally satisfactory since the Cayley form perserves 2nd order accuracy. The height of the potential barrier was in the order 10^4 to match the kinetic energy, and the width to be of 0.05, thus about 50 mesh sites.

Shown in Fig.1 is the case of $V = 50000$, which is about twice the energy of the incoming wave — so it's mostly bounced back when hitting the barrier.

Fig.2 is the case where the kinetic energy is one time higher than the potential barrier, so it passed through quite easily.

In Fig.3 $V = 50000$, which is the same as the first case. But instead of Gaussian form, the initial wave pack is a square. Since there are usually more high-frequency components contained in a discontinous function, there are more wave components passing through than the first case.

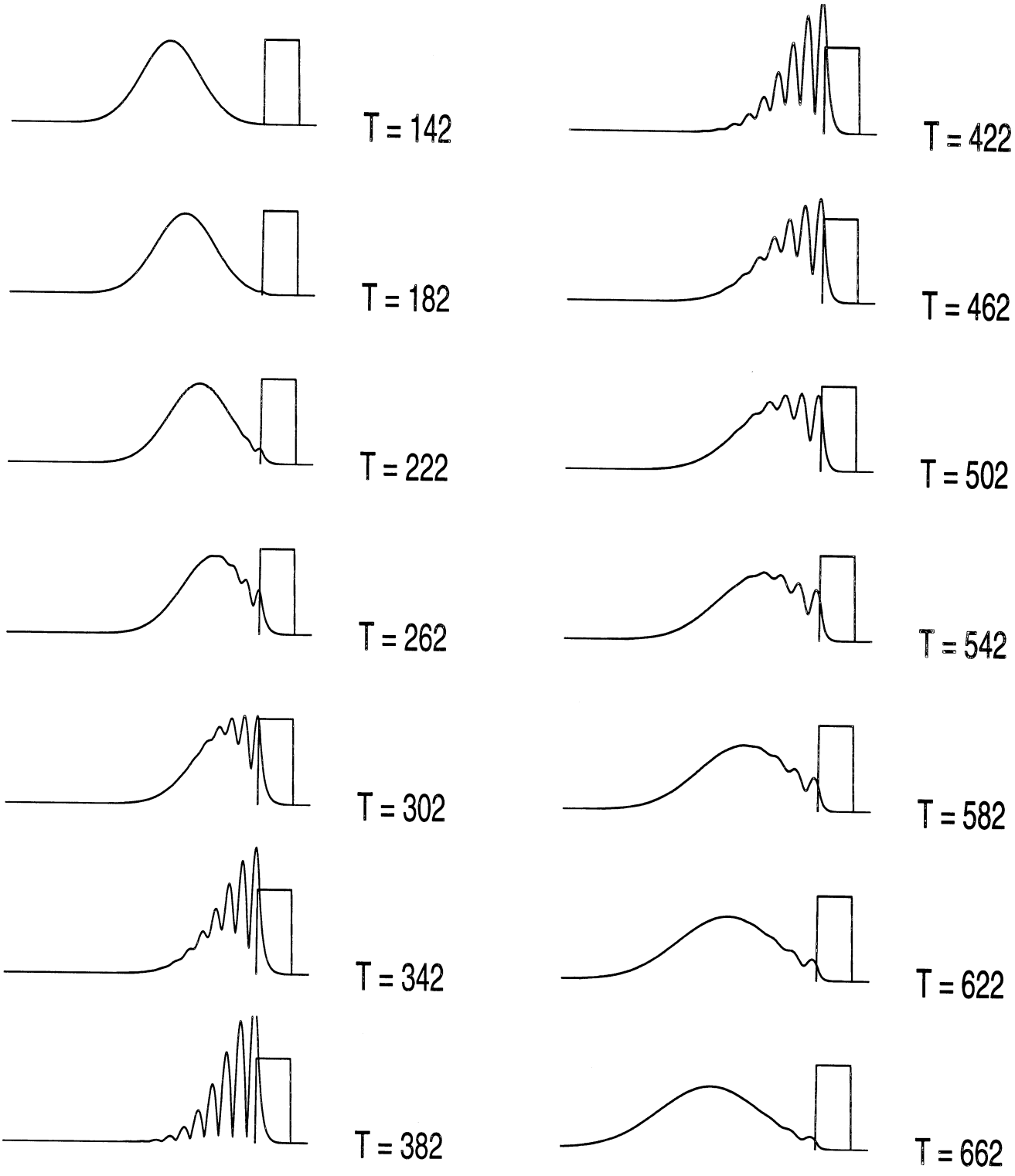


Fig.1 k = 150, V = 50000

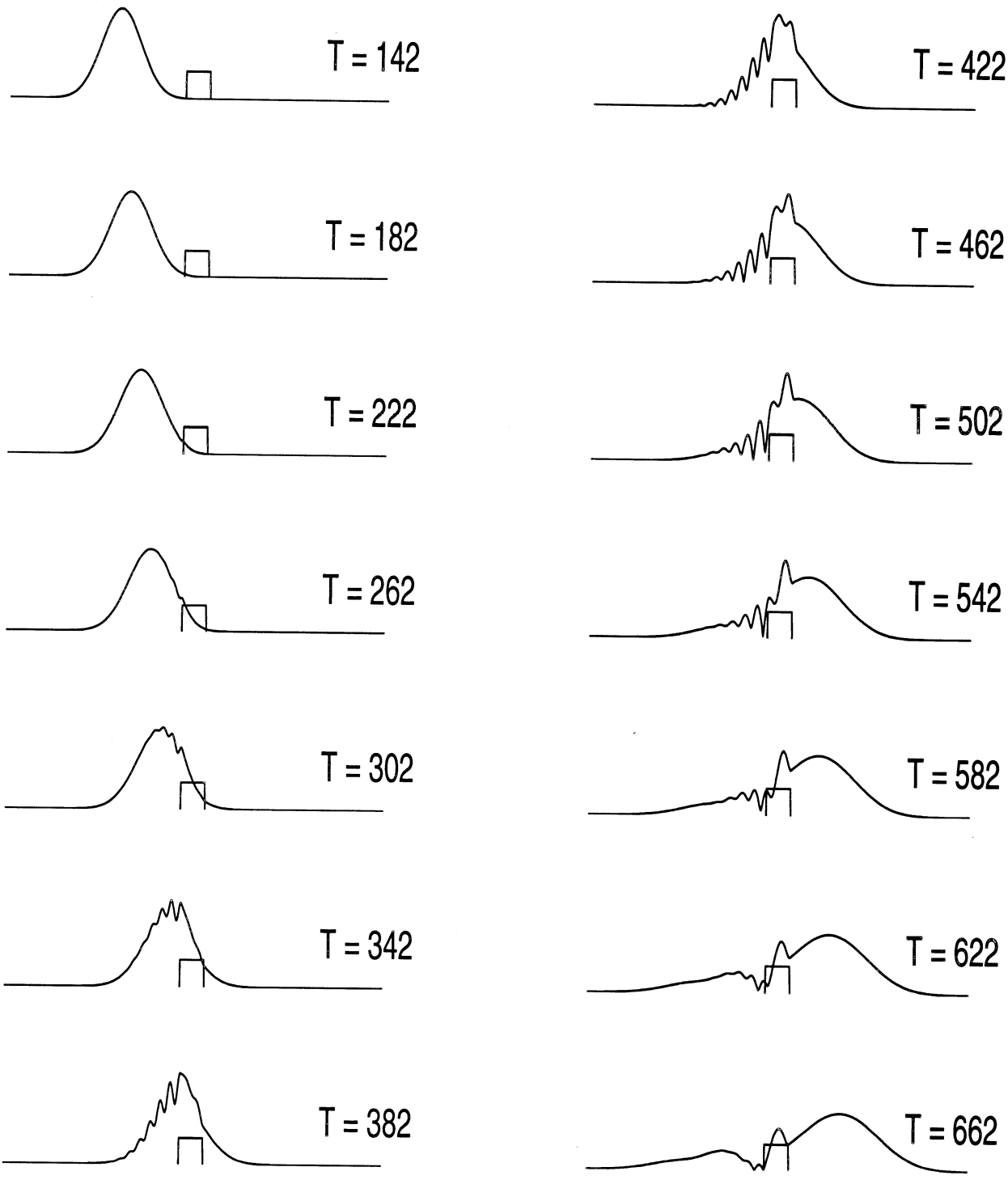


Fig.2 k = 150, V = 12000

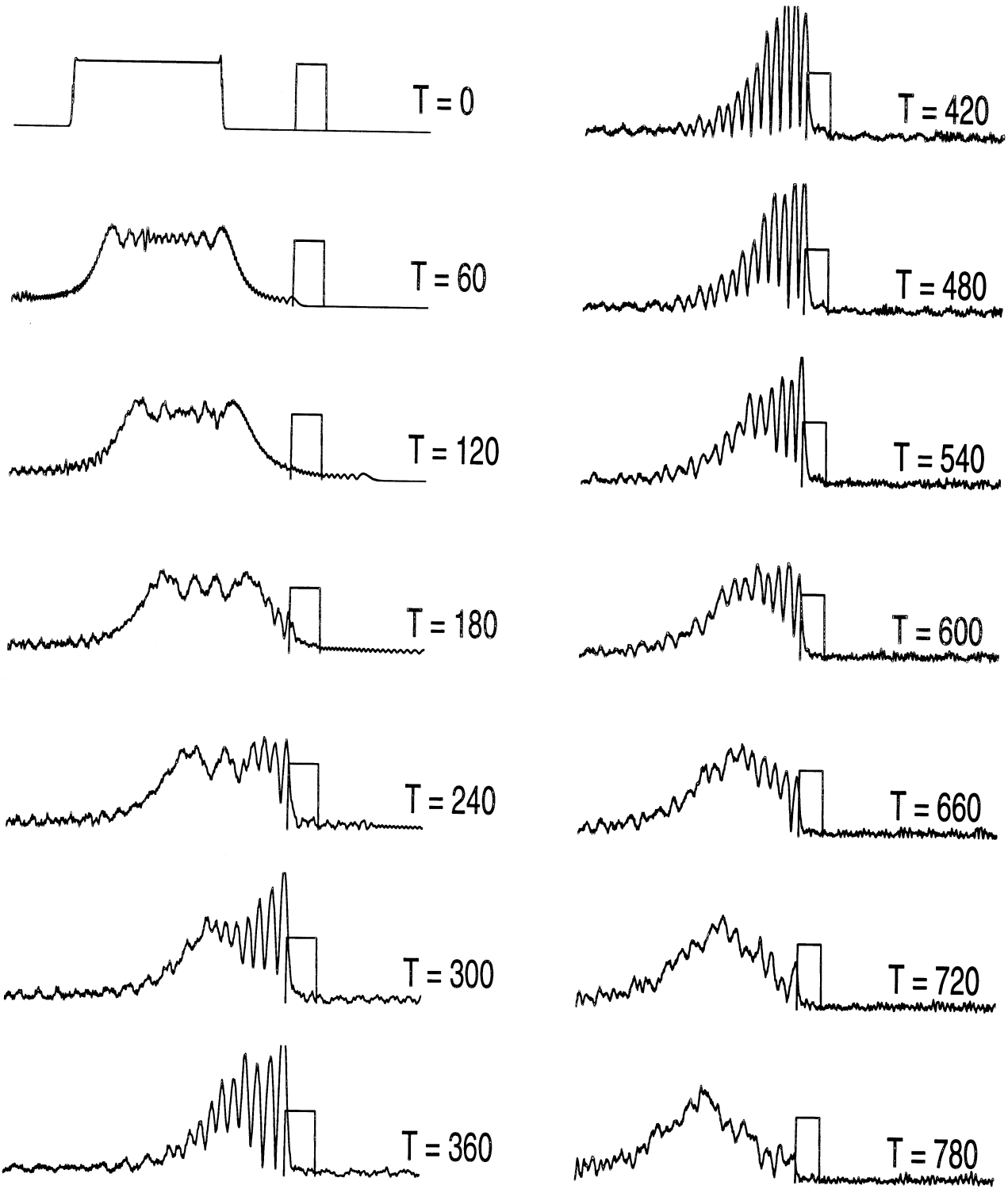


Fig.3 k = 150, V = 50000 (Plane Wave)

3.2 Two dimensional TDSE

There are complications in the two dimensional TDSE: we can no longer solve the implicit equations using the efficient back-substitution method for tri-diagonal systems as in the one dimensional case, because the discretization

$$\nabla^2\psi_{i,j} = \frac{1}{h^2}(\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1} - 4\psi_{i,j}) + \mathcal{O}(h^2) \tag{3.23}$$

involves more than 3 variables. However, we can always seperate $\mathcal{H}$ into $\mathcal{H}_x + \mathcal{H}_y$, and apply each Cayley operator onto the system seperately. We'll analyze the accuracy of such factorization down below:

Since

$$\mathcal{H} = -\frac{d^2}{dx^2} - \frac{d^2}{dy^2} + V(x,y) \tag{3.24}$$

Let's define

$$\begin{aligned} \mathcal{H}_x &= -\frac{d^2}{dx^2} + V_1(x,y) \\ \mathcal{H}_y &= -\frac{d^2}{dy^2} + V_2(x,y) \\ V(x,y) &= V_1(x,y) + V_2(x,y) \end{aligned} \tag{3.25}$$

so

$$\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y \tag{3.26}$$

and

$$\begin{aligned} \exp(-i\tau\mathcal{H}) &= \exp(-i\tau\mathcal{H}_x - i\tau\mathcal{H}_y) \\ &= 1 - i\tau\mathcal{H}_x - i\tau\mathcal{H}_y + \frac{1}{2}(i\tau\mathcal{H}_x + i\tau\mathcal{H}_y)^2 + \mathcal{O}(\tau^3) \end{aligned} \tag{3.27}$$

Because

$$\begin{aligned} \frac{1 - \frac{1}{2}i\tau\mathcal{H}_x}{1 + \frac{1}{2}i\tau\mathcal{H}_x} &= (1 - \frac{1}{2}i\tau\mathcal{H}_x)[1 - \frac{1}{2}i\tau\mathcal{H}_x + (\frac{1}{2}i\tau\mathcal{H}_x)^2] + \mathcal{O}(\tau^3) \\ &= 1 - i\tau\mathcal{H}_x + \frac{1}{2}(i\tau\mathcal{H}_x)^2 + \mathcal{O}(\tau^3) \end{aligned} \tag{3.28}$$

so

$$\begin{aligned} (\frac{1 - \frac{1}{2}i\tau\mathcal{H}_x}{1 + \frac{1}{2}i\tau\mathcal{H}_x})(\frac{1 - \frac{1}{2}i\tau\mathcal{H}_y}{1 + \frac{1}{2}i\tau\mathcal{H}_y}) &= [1 - i\tau\mathcal{H}_x + \frac{1}{2}(i\tau\mathcal{H}_x)^2][1 - i\tau\mathcal{H}_y + \frac{1}{2}(i\tau\mathcal{H}_y)^2] + \mathcal{O}(\tau^3) \\ &= 1 - i\tau\mathcal{H}_x - i\tau\mathcal{H}_y + \frac{1}{2}(i\tau\mathcal{H}_x)^2 + \frac{1}{2}(i\tau\mathcal{H}_y)^2 - \tau^2\mathcal{H}_x\mathcal{H}_y + \mathcal{O}(\tau^3) \end{aligned} \tag{3.29}$$

Comparing with (3.27)

$$\exp(-i\tau\mathcal{H}) = (\frac{1-\frac{1}{2}i\tau\mathcal{H}_x}{1+\frac{1}{2}i\tau\mathcal{H}_x})(\frac{1-\frac{1}{2}i\tau\mathcal{H}_y}{1+\frac{1}{2}i\tau\mathcal{H}_y}) + \frac{\tau^2}{2}[\mathcal{H}_x, \mathcal{H}_y] + \mathcal{O}(\tau^3) \tag{3.30}$$

We can see that the error caused by this two-step process is in the order of τ^2, thus destroying one order of accuracy. Nevertheless, we'll adopt this method because otherwise the cost would become unbearable.

One may intuitively suggest picking $V_1(x,y)$ and $V_2(x,y)$ such that $[\mathcal{H}_x, \mathcal{H}_y] = 0$. Indeed, that's the purpose of the author at the first time to split $V(x,y)$ into two parts. However, after some manipulations it's found to be generally impossible, because the commutation of d^2/dx^2 with a scaler function would generate free d/dx operators, which can't be offset by simple manipulations. Another idea is to symmetrize the right hand side of (3.30) and use the fact that

$$\exp(-i\tau\mathcal{H}) = (\frac{1-\frac{1}{2}i\tau\mathcal{H}_x}{1+\frac{1}{2}i\tau\mathcal{H}_x})(\frac{1-\frac{1}{2}i\tau\mathcal{H}_y}{1+\frac{1}{2}i\tau\mathcal{H}_y}) + (\frac{1-\frac{1}{2}i\tau\mathcal{H}_y}{1+\frac{1}{2}i\tau\mathcal{H}_y})(\frac{1-\frac{1}{2}i\tau\mathcal{H}_x}{1+\frac{1}{2}i\tau\mathcal{H}_x}) + \mathcal{O}(\tau^3) \tag{3.31}$$

However, that destroy the *norm conserving* property of the simple scheme (3.30), because the sum of two unitary operators isn't necessarily an unitary operator.

Next we'll analyze the influence of finite discretization in both space and time to our computation. One may immediately remember the dispersion relation derived by Huang in our first solid state physics course, and how the finite discretization of space (lattice sites) influence the behaviour of a should-be-continous wave. In general, suppose a wave component

$$\psi = \exp(ikx - i\omega t) \tag{3.32}$$

in free propagation (without potential). Under finite discretization of space:

$$\begin{aligned}
\mathcal{H}\psi &= \frac{-1}{h^2}[\exp(ik(x+h) - i\omega t) + \exp(ik(x-h) - i\omega t) - 2\exp(ikx - i\omega t)] \\
&= \frac{-1}{h^2}(\exp(ikh) + \exp(-ikh) - 2)\psi \\
&= \frac{2 - 2\cos(kh)}{h^2}\psi \\
&= \epsilon\psi
\end{aligned} \tag{3.33}$$

and under further discretization of time by putting it into the Cayley form (recursion relation), we get the following dispersion relation:

$$\exp(-i\omega\tau) = \frac{1-\frac{1}{2}i\tau\epsilon}{1+\frac{1}{2}i\tau\epsilon} \tag{3.34}$$

or

$$\begin{aligned}\omega(k) &= \frac{2}{\tau}\tan^{-1}\left(\frac{\tau - \tau\cos(kh)}{h^2}\right) \\ &= k^2 - \frac{1}{12}h^2k^4 + \left(\frac{1}{360}h^4 - \frac{1}{12}\tau^2\right)k^6 + \mathcal{O}(k^8)\end{aligned} \tag{3.35}$$

Obviously in the long wave length limit we have our

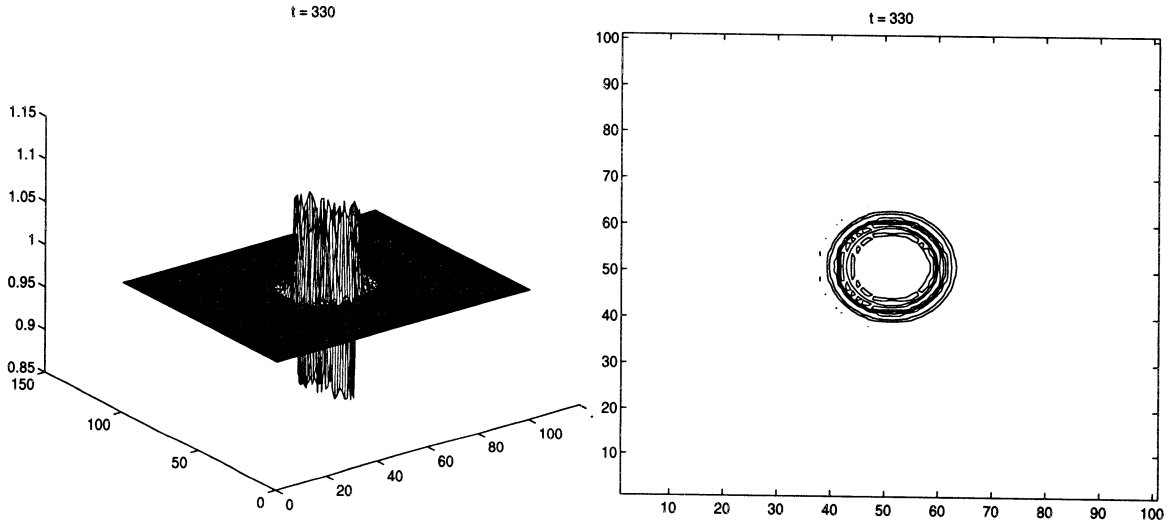
$$w(k) \simeq k^2 \tag{3.36}$$

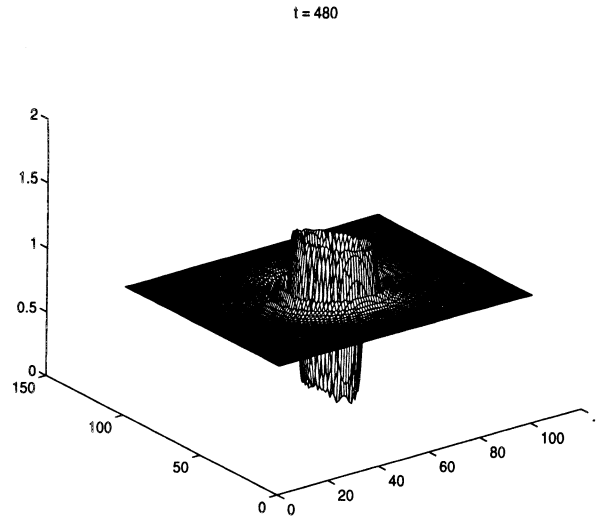
behaviour back. The question is how long is long, and that is answered by the other terms in (3.34).

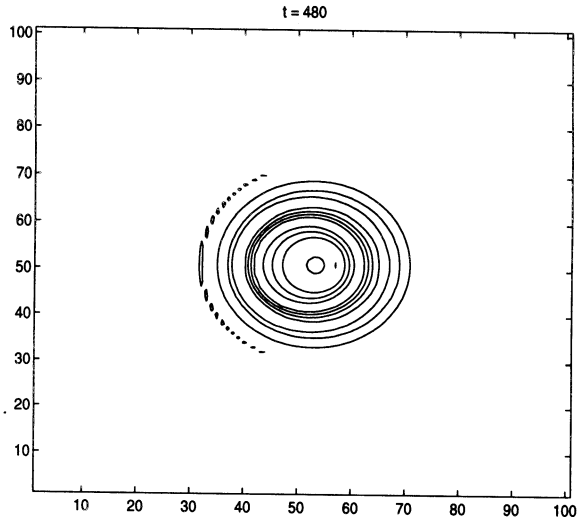
As an example of 2D TDSE implementation, the following scenario was devised: A 1.0×1.0 square was devided into a 500×500 mesh array. At $t = 0$ the initial condition was a steady plane wave flow in the X direction

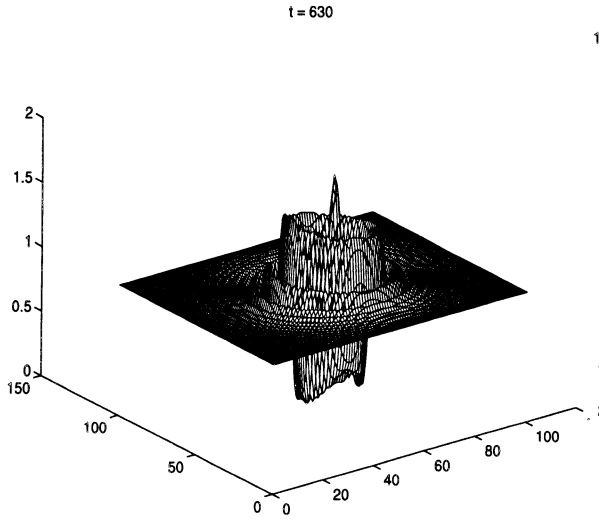
$$\psi(x, y) = \exp(ikx - i\omega t) \tag{3.37}$$

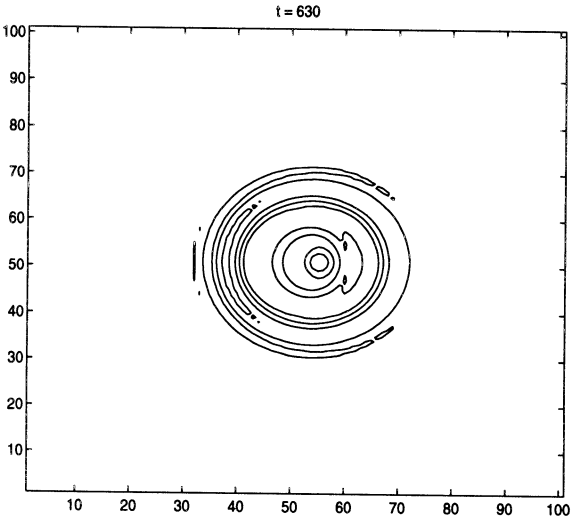
$k = 10\pi$ so the wavelength $\lambda = 1/5 = 100$ mesh points, which was considered to be enough for a sinusoidal function. τ was chosen to be 2×10^{-6} and ω can be calculated using dispersion relation (3.34). The boundary condition of (3.36) was imposed on 4 sides of the square, to simulate the enviroment of an infinite "river" of steady flow. (However, this would cause the biggest trouble later on.) Such situation would continue for 300τ to test the code, if it's working, then the plane wave would continue to be a plane wave and $|\psi(x, y, t < 300\tau)| = 1$. At $t = 300\tau$ something happens: a cylinder barrier of radius = 50 mesh points, height = 300000 suddenly jump out of nothing in the center, and stirs the flow.

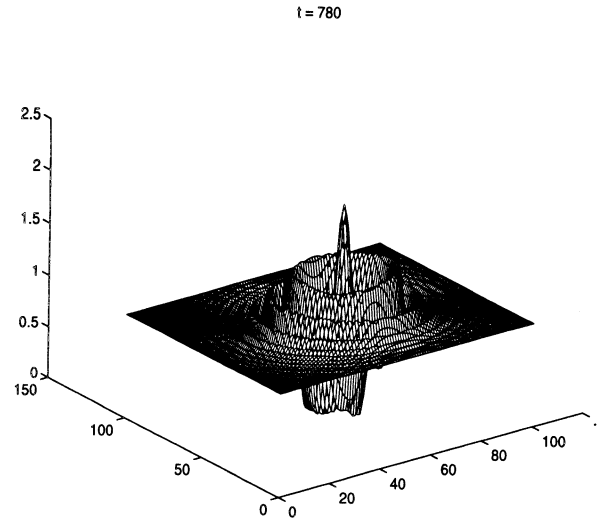


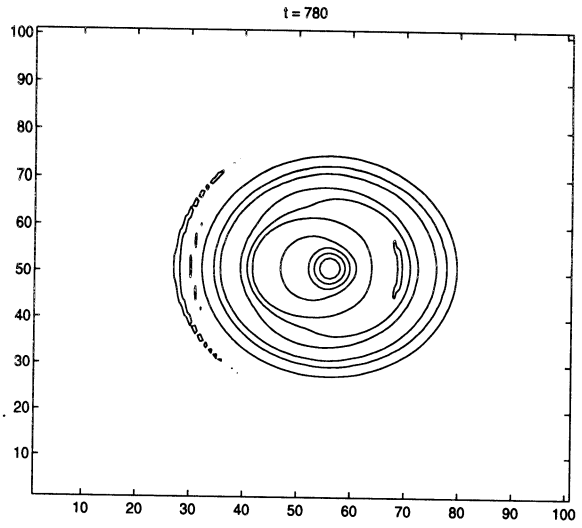

t = 480
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100

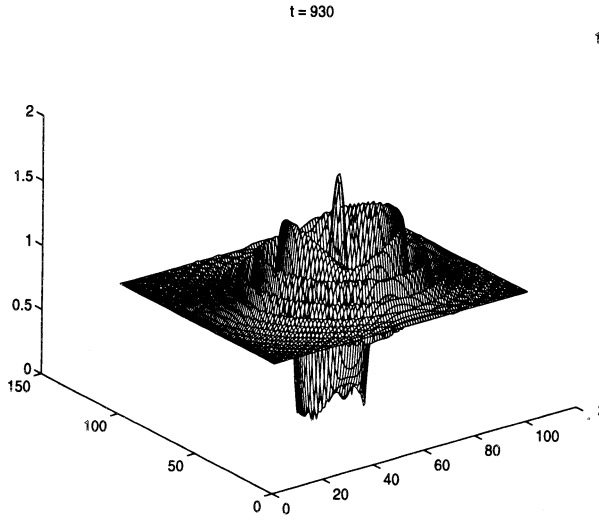

t = 480
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100

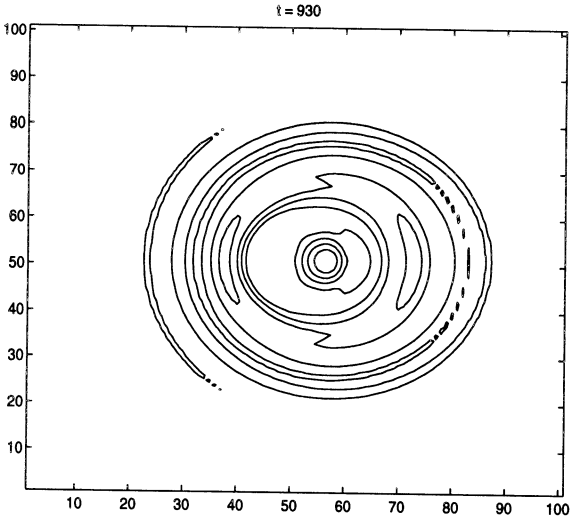

t = 630
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100

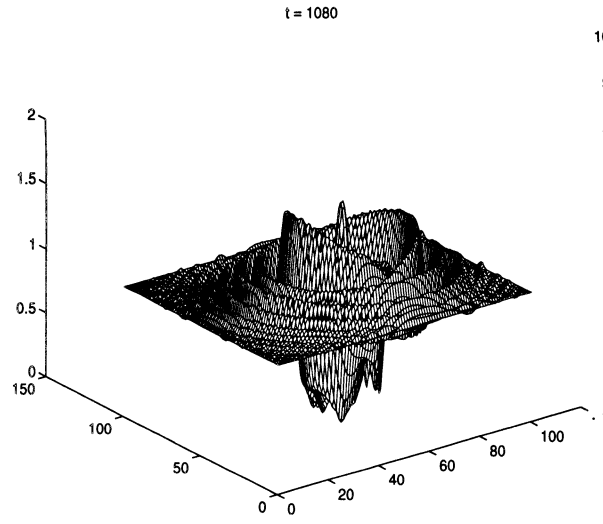

t = 630
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100

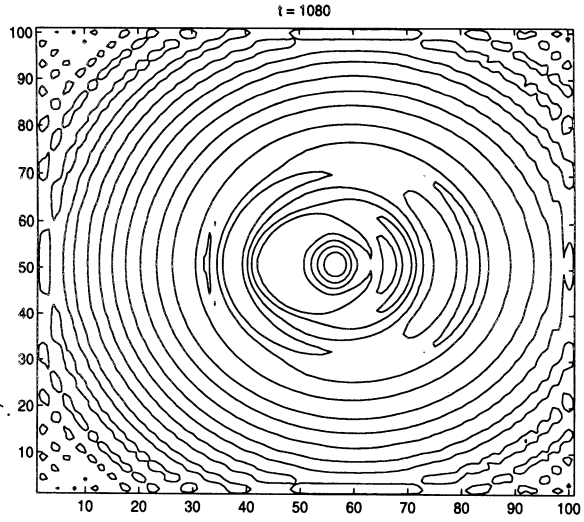

t = 780
2.5
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100

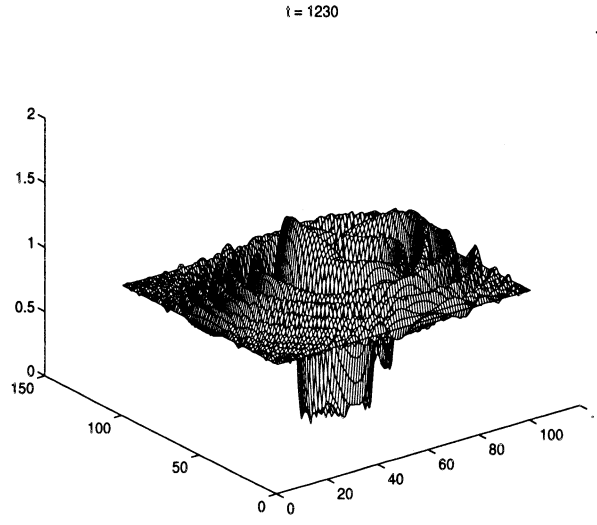

t = 780
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100

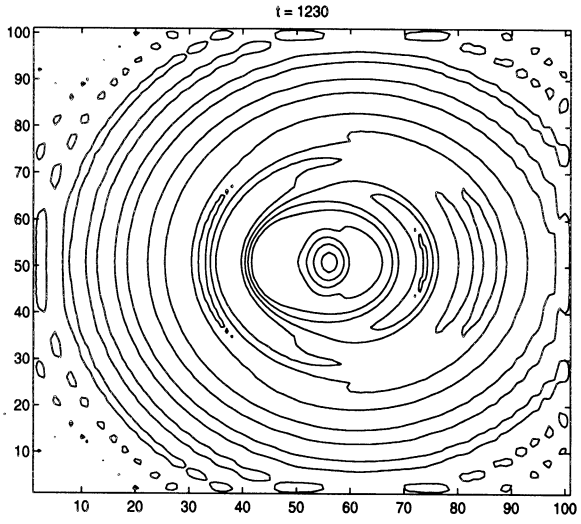

t = 930
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100


t = 930
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100


t = 1080
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100


t = 1080
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100


t = 1230
2
1.5
1
0.5
0
150
100
50
0
0
20
40
60
80
100


t = 1230
100
90
80
70
60
50
40
30
20
10
10
20
30
40
50
60
70
80
90
100