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ONE-DIMENSIONAL WAVE PACKET SOLUTIONS OF TIME-DEPENDENT FRICTIONAL OR OPTICAL POTENTIAL SCHRÖDINGER EQUATIONS

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PROGRAM SUMMARY

Title of program: FRICTION

Catalogue number: ACWT

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland (see application form in this issue)

Computers and installations: IBM 360/91-370/145 at IPP Garching, IBM 370/165 at GSI Darmstadt

Operating system: HASP

Program language used: FORTRAN

High speed storage required: 140 K bytes

No. of bits in a byte: 8

Overlay structure: none

No. of magnetic tapes: none

Other peripherals used: card reader, line printer

No. of cards in combined program and test deck: 546

Card punching code: EBCDIC

Keywords: Quantum mechanics, Schrödinger equation, friction, optical potential, atomic, nuclear physics, scattering

Nature of physical problem
Quantum mechanical treatment of classical equation of motion $m\ddot{x} + \gamma m\dot{x} + \mathrm{d}V(x)/\mathrm{d}x = 0$ (incl. $\gamma = 0$), by time dependent nonlinear Schrödinger equations or solution of arbitrary (including optical) hamiltonians.

Method of solution
Finite difference method

Restrictions on the complexity of the program
One-dimensional motion.

Typical running time
Depending on problem 0.5...5 min.

Unusual features of the program
Double precision complex arithmetic (IBM type COMPLEX*16) is used. It should be replaced by single precision complex arithmetic if run on a computer with more than approximately ten digits of accuracy.

LONG WRITE-UP

1. Introduction

Frictional problems occur frequently in various fields of physics, not only in classical mechanics but also in atomic and nuclear physics. A specific example is the so-called deep inelastic reaction, i.e. the scattering of heavy ions with energies well above the Coulomb barrier. At the instant of contact the ions lose their entire kinetic energy and are then repelled by their mutual Coulomb energy. These reactions are well described [1] by classical mechanics with conservative forces and linear frictional forces. The typical equation of motion in one dimension reads

$$\dot{P} + \gamma P + \mathrm{d}V(X)/\mathrm{d}X = 0\,, \tag{1}$$

where X and P are the coordinates of position and momentum, respectively, γ is the frictional constant and $V(X)$ is the conservative potential. If the energy is defined as $E = P^2/2m + V$, the energy dissipation is given by

$$\dot{E} = -(\gamma/m)P^2\,. \tag{2}$$

A classical treatment may not be adequate if the angular momenta, energies, and masses involved are small. However, a full quantum mechanical treatment, for instance by time dependent Hartree–Fock, is immensely complex. Hence, a compromise is to quantize the equation of motion (1). This meets with the problem that frictional forces cannot be derived from a classical hamiltonian which is the connection between classical and quantum mechanics.

The opposite course is to seek quantum frictional potentials $W(x, \partial/\partial x, \psi)$ in the time dependent Schrödinger equation

$$\mathrm{i}\hbar \frac{\partial}{\partial t}\psi = (H_0 + \gamma W)\psi\,, \tag{3}$$

$$H_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\,, \tag{4}$$

which reproduce the classical equations of motion (1) in the Ehrenfest limit $\langle x\rangle = X$, $\langle p\rangle = P$ with $p = -\mathrm{i}\hbar\partial/\partial x$, where the brackets denote expectation values. Three different hermitian, not explicitly time-dependent nonlinear frictional potentials are known which fulfil these requirements,

$$W_{\mathrm{K}} = \hbar(s - \langle s\rangle)\,, \qquad \text{Kostin [2]}, \tag{5a}$$

$$W_{\mathrm{H}} = \tfrac{1}{4}\,[x - \langle x\rangle, p + \langle p\rangle]_+\,, \qquad \text{Hasse [3]}, \tag{5b}$$

$$W_{\mathrm{A}} = \langle p\rangle(x - \langle x\rangle)\,, \qquad \text{Albrecht [4]}, \tag{5c}$$

where $s = -\frac{1}{2}\,\mathrm{i}\ln(\psi/\psi^*)$ is the phase of the wave function and $[,]_+$ denotes the anticommutator.

Analytical wave packet solutions of the Schrödinger equation with the frictional potentials (5) and the trivial conservative potentials (force free motion, free fall, and harmonic oscillator) are given in refs. [2–6]. The present program is primarily intended to provide numerical solutions for nontrivial conservative potentials as they occur for instance in barrier penetration [7]. However, the program is not restricted to solving frictional hamiltonians. It is also capable of computing wave packet solutions of arbitrary nonhermitian optical potentials of the type $V - \mathrm{i}W$ where the real and imaginary parts may depend upon x, $\partial/\partial x$, $\partial^2/\partial x^2$, ψ, etc. In this case, the norm of the wave function may not be conserved.

2. Method of solution

The numerical method for the solution of the partial differential equation (3) follows closely Goldberg et al. [8] but is here generalized for arbitrary, not necessarily hermitian, potentials.

If H does not depend explicitly on time, eq. (3) has the formal solution (with $\hbar = m = 1$)

$$\psi(x, t + \delta) = \mathrm{e}^{-\mathrm{i}\delta H}\,\psi(x, t)\,, \tag{6}$$

which is approximated by the Cayley expression

$$\psi(x, t + \delta) = \frac{1 - \frac{1}{2}\,\mathrm{i}\delta H}{1 + \frac{1}{2}\,\mathrm{i}\delta H}\psi(x, t)\,. \tag{7}$$

This is unitary if H is hermitian and the error involved is $O(\delta^3)$. If we consider a one-dimensional box of length L with infinitely high walls which is divided into J equal parts of length ϵ, then the mesh points are denoted by x_j, $j = 0, 1, \ldots, J$. The initial time is $t = 0$, the final time is $t = T$ and constant time increments are denoted by δ so that the running time is $t_n = n\delta$, and a wave function $\psi(x, t)$ is characterized by ψ_j^n. The box boundary condition demands $\psi_0^n = \psi_J^n = 0$. Hence the finite difference approximation of eq. (7) is

$$(1+\tfrac{1}{2}\,\mathrm{i}\delta H)\,\psi_j^{n+1} = (1-\tfrac{1}{2}\,\mathrm{i}\delta H)\,\psi_j^n\,. \tag{8}$$

In addition, one has to specify the finite difference approximation of $H\psi$. If H contains at most second derivatives but is otherwise arbitrary in the sense that it may depend upon x and ψ (and functions of x and ψ) then the most general form is

$$H\psi_j^n = \frac{1}{2\epsilon^2}\,(-a_j^n\psi_{j-1}^n + b_j^n\psi_j^n - c_j^n\psi_{j+1}^n)\,. \tag{9}$$

If H is hermitian, the coefficients are restricted to $b_j^n = (b_j^n)^*$ and $c_j^n = (a_{j+1}^n)^*$. The finite difference approximation for the second derivative is

$$\psi_j'' = \frac{1}{\epsilon^2}\,(\psi_{j-1} - 2\psi_j + \psi_{j+1})\,, \tag{10}$$

and hence the coefficients a_j, b_j, c_j of H_0 read

$$a_j = c_j = 1\,, \qquad b_j = 2(1+\epsilon^2 V_j)\,, \tag{11}$$

where $V_j = V(x_j)$.

Eq. (8) is an implicit equation for ψ_j^{n+1} because it contains also the quantities ψ_{j-1}^{n+1} and ψ_{j+1}^{n+1}. Its solution proceeds according to ref. [8] as follows. Under the assumption

$$a_j^{n+1} \approx a_j^n\,, \qquad b_j^{n+1} \approx b_j^n\,, \qquad c_j^{n+1} \approx c_j^n\,, \tag{12}$$

and with the definitions

$$A_j^n = \frac{a_j^n}{c_j^n}, \qquad B_j^n = \frac{b_j^n - \mathrm{i}\lambda}{c_j^{n+1}},$$

$$C_j^n = (b_j^n + \mathrm{i}\lambda)/c_j^{n+1}\,, \tag{13}$$

where $\lambda = 4\epsilon^2/\delta$, eq. (8) becomes

$$\psi_{j+1}^{n+1} - B_j^n\psi_j^{n+1} + A_j^n\psi_{j-1}^{n+1} = -\psi_{i+1}^n + C_j^n\psi_j^n - A_j^n\psi_{j-1}^n\,,$$

$$= \Omega_j^n\,. \tag{14}$$

The right-hand side of eq. (14) is known at $t = t_n$ and is therefore abbreviated by Ω_j^n. On the other hand, if one defines

$$\psi_{j+1}^{n+1} = e_j^n\psi_j^{n+1} + f_j^n\,, \tag{15}$$

one obtains three relations by a comparison of eq. (14) with eq. (15),

$$\psi_j^{n+1} = (\psi_{j+1}^{n+1} - f_j^n)/e_j^n\,, \tag{16}$$

$$e_j^n = B_j^n - A_j^n/e_{j-1}^n\,, \tag{17}$$

$$f_j^n = \Omega_j^n + A_j^n f_{j-1}^n/e_{j-1}^n\,. \tag{18}$$

Eqs. (16–18) provide a numerically stable scheme for the computation of the wave function at time t_{n+1} if ψ_j^n is given. Initially, the coefficients a_j^n, b_j^n, c_j^n and A_j^n, B_j^n, C_j^n are computed from eq. (13) for $j = 1, \ldots, J-1$; then the coefficients e_j^n and f_j^n are computed upwards from the recursion relations (17, 18). The starting values are obtained from the box boundary condition, $e_1^n = B_1^n$ and $f_1^n = \Omega_1^n = -\psi_2^n + C_1^n\psi_1^n$. Once these quantities are calculated the wave function at time t_{n-1} is iterated downwards with the recursion relation (16). Its starting value is $\psi_{J-1}^{n+1} = -f_{J-1}^n/e_{J-1}^n$ by virtue of $\psi_J^{n+1} = 0$. By this procedure the accumulation of rounding errors is avoided.

A simplification arises which leads to a saving in computation time if the coefficients a_j, b_j, c_j do not depend on time. Then also A_j, B_j, C_j do not depend on time and the coefficients e_j are only calculated once. The f_j^n, however, do depend on time via the Ω_j^n.

3. The coefficients a_j^n, b_j^n, c_j^n

The different frictional potentials (5) contain the first derivative and the phase of the wave function and the expectation values of position $\langle x\rangle = X$, momentum $\langle p\rangle = P$ and phase $\langle s\rangle = S$. The corresponding finite difference approximation for $\partial\psi/\partial x$ is

$$\psi_j' = \frac{1}{2\epsilon}\,(\psi_{j+1} - \psi_{j-1})\,. \tag{19}$$

To avoid the multivalued behavior of the complex logarithm, the phase is computed by a recursion relation similar to ref. [6],

$$s_j = s_{j-1} - \mathrm{Im}\left[\frac{\psi_{j-1}}{\psi_j} - \frac{1}{8}\left(\frac{\psi_{j+1} - \psi_{j-1}}{\psi_j}\right)^2\right], \tag{20}$$

with the starting value $s_1 = \mathrm{Im}(\ln\psi_1)$ and the final value

$$s_{J-1} = s_{J-2} + \mathrm{Im}\,[\psi_{J-1}/\psi_{J-2} - (\psi_{J-1} - \psi_{J-3})^2/8\psi_{J-2}^2]\,.$$

Expectation values are computed using the trapezoidal rule

$$X^n = \epsilon \sum_{j=1}^{J-1} x_j |\psi_j^n|^2 , \tag{21}$$

$$P^n = \mathrm{Im} \sum_{j=1}^{J-2} (\psi_j^n)^* \psi_{j+1}^n , \tag{22}$$

and S^n similar to eq. (21). In evaluating eq. (5b) no use should be made of the commutator relation $px = xp - \mathrm{i}$ because this gives rise to an imaginary contribution to the coefficient b_j^n which makes the finite difference approximation nonhermitian. With eqs. (19–22) the coefficients become

W_K:

$$a_j = c_j = 1 ,$$
$$b_j^n = 2[1 + \epsilon^2 V_j + \epsilon^2 \gamma (s_j - S^n)] , \tag{23a}$$

W_H:

$$a_j^n = 1 - \tfrac{1}{2} \mathrm{i}\epsilon\gamma (x_j - X^n - \tfrac{1}{2}\epsilon) ,$$
$$b_j^n = 2[1 + \epsilon^2 V_j + \tfrac{1}{2}\epsilon^2 \gamma P^n (x_j - X^n)] ,$$
$$c_j^n = 1 + \tfrac{1}{2} \mathrm{i}\epsilon\gamma (x_j - X^n + \tfrac{1}{2}\epsilon) , \tag{23b}$$

W_A:

$$a_j = c_j = 1 ,$$
$$b_j^n = 2[1 + \epsilon^2 V_j + \epsilon^2 \gamma P^n (x_j - X^n)] . \tag{23c}$$

4. Error analysis

The error associated with eq. (14) is threefold: (i) from the approximation (8); (ii) from the finite difference approximation of the hamiltonian, i.e. the error in the coefficients a_j^n, b_j^n, c_j^n; and (iii) from the approximation (12). By multiplication with λ the error (i) in eq. (14) is $O(\epsilon^2\delta^2)$. Taking into account that the first, eq. (19), and second derivatives, eq. (10), have errors $O(\epsilon^4)$ and the expectation values errors of $O(\epsilon^2)$ using the trapezoidal rule (Simpson's rule gives no improvement) the coefficients b_j^n have errors $O(\epsilon^4)$. Similarly, the a_j^n and c_j^n have errors $O(\epsilon^4)$ if no potential or W_K or W_A is employed but $O(\epsilon^3)$ if W_H is used. With respect to contribution (iii) the differences $b_j^{n+1} - b_j^n = \delta \dot{b}_j^n$ are of the order $O(\epsilon^2\delta)$ whereas the coefficients a_j^n and c_j^n contribute nothing except in W_H where the error is $O(\epsilon\delta)$.

Maximum performance is achieved if all terms in eq. (14) have the same order of magnitude. Eq. (13) therefore demands $\lambda \approx 2$, or, $\delta \approx 2\epsilon^2$. Consequently, the maximum error in H_0, W_K and W_A is $O(\epsilon^2\delta) = O(\epsilon^4)$ and in W_H is $O(\epsilon\delta) = O(\epsilon^3)$. With $\epsilon = 10^{-3}$ and $\delta = 5 \times 10^{-6}$ and 1000 time steps the accuracy is still about 10^{-3} which, however, in actual computations depends very much on how sharply peaked the wave packet is. Double precision complex arithmetic should not give rise to serious rounding errors.

5. Physical units

The basic unit is L, the length of the box, chosen as $L = 1$ in the program. From this the following physical units are derived:

$$\begin{aligned} &\{x\}, \text{ position} = L , \\ &\{p\}, \text{ momentum} = \hbar/L , \\ &\{t\}, \text{ time} = mL^2/\hbar , \\ &\{\gamma\}, \text{ frictional constant} = \{t^{-1}\} = \hbar/mL^2 , \\ &\{E\}, \text{ energy} = \hbar^2/mL^2 . \end{aligned} \tag{24}$$

6. Program options

To make the program as versatile as possible, several options have been built in. The integer IFRI = 1, 2, 3, 4, 5 determines whether no friction, Hasse, Kostin, or Albrecht friction, or a user-supplied optical potential is used. In the latter case the appropriate coefficients a_j^n, b_j^n and c_j^n have to be computed and inserted into the subprogram OPT. The integer IPAC determines the initial wave packet $\psi(x, t = 0)$. IPAC = 1 uses one initial gaussian wave packet

$$\psi = \exp\left(-\frac{(x-x_0)^2}{2\sigma_0^2} + \mathrm{i}p_0 x\right) \tag{25}$$

with initial position x_0, momentum p_0, and width σ_0, IPAC = 2 gives two countermoving initial gaussian wave packets

$$\psi = \exp\left(-\frac{(x-x_0)^2}{2\sigma_0^2} + \mathrm{i}p_0 x\right) + \exp\left(-\frac{(x+x_0)^2}{2\sigma_0^2} - \mathrm{i}p_0 x\right) , \tag{26}$$

and IPAC = 3 selects a user-supplied, not necessarily normalized, initial wave packet to be inserted into the function PSI.

IPOT = 1, 2, 3 chooses the conservative potential, ie. no potential, a square well potential of height VBAR (or depth −VBAR) positioned between $-0.05 \leqslant x \leqslant 0.05$ and a user-supplied conservative potential to be inserted into the function POT. Finally, the integer IPRI = 1, 2 selects between the options of print and plot on the printer of the wave function or suppression of the plot, respectively.

7. Input

There is only one input card in the FORMAT (9D7.1, 3X, 4I1) for each run. The number of runs, however, is unlimited and termination of the computation is achieved by adding a blank card.

The nine data fields correspond to the following nine quantities:

(i) TIME: T, total running time of the wave packet as defined below eq. (7);

(ii) DTIME: printing time interval; if for instance 20 printouts are requested during TIME, then DTIME=TIME/20;

(iii) PIN: p_0, initial momentum;

(iv) SIN: σ_0, initial width, and

(v) AIN: x_0, initial position of the wave packet, as defined in eqs. (25, 26).

They should be chosen in such a way that the initial wave packet is essentially zero at $x = \pm 0.5$. For instance if AIN = −0.25 and PIN = 150, the centre of the wave packet travels from $x = -0.25$ to larger x-values, i.e. from left to right in the plot.

(vi) GAM: γ, frictional constant from eq. (7). If the optical potential option (IFRI = 5) is used GAM may be employed in OPT for other purposes.

(vii) VBAR: height (if positive) or depth (if negative) of the square well potential. If the user-supplied conservative potential option (IPOT = 3) is used it may be employed in POT for other purposes or in the optical potential version in OPT.

(viii) EPS: ϵ, the mesh size, and

(ix) DEL: δ, the time increment. The four integers IFRI, IPAC, IPOT, IPRI complete the data card.

There are several restrictions on the magnitude of the input quantities [8]. As already mentioned $\delta \approx 2\epsilon^2$ is optimal. To keep the wave function away from the wall, $|x_0| \lesssim 0.25$ and $\sigma_0 \lesssim 0.05$ are necessary. Since $J = 1/\epsilon$ and the dimensions are limited to 1000 (may be easily removed), we have $\epsilon \geqslant 10^{-3}$, but $1/\epsilon$ must be a multiple of 100. The finite resolution of energy requires $|p_0|\epsilon \lesssim 0.15$ and $|V|\epsilon^2 \lesssim 0.02$. Finally, the wave packet should not travel too close to the wall and frictional effects should come out clearly. Since friction damps momenta by $e^{-\gamma t}$ and the motion by $1-e^{-\gamma t}$, optimum results are obtained if $\gamma T \approx 1$ and $|p_0|T \approx 0.7$. The latter two conditions are only valid for free running wave packets, in other cases γ and T should be estimated by similar arguments.

8. Output

The output consists of as many double (IPRI = 1) or single (IPRI = 2) pages as specified by TIME and DTIME. The first page contains in the heading what kind of friction, initial wave packet and conservative potential is chosen and the input parameters. The next block on the first page lists the running time, the reflection and transmission coefficients, i.e. the fraction of the norm of the wave packet located at $-0.5 \leqslant x \leqslant 0$ and $0 \leqslant x \leqslant 0.5$, respectively and the norm. The latter should be equal to one if H is hermitian. Then the expectation values of position, momentum, kinetic, potential, and total energy are printed. In the last block the absolute value of the wave function is printed at the 99 mesh points $x_1 = -0.49, x_2 = -0.48, \ldots, x_{49} = -0.01, x_{50} = 0, x_{51} = 0.01, \ldots, x_{98} = 0.48, x_{99} = 0.49$.

The second page, if requested, gives a plot of the absolute value of the wave function at these 99 mesh points. The abscissa is fixed but the ordinate is compiled automatically in such a way that twice the initial height can be accomodated in the plot. This scale is also printed out.

4. Comments on the program

(i) Due to the fact that a second order partial differential equation is solved and that IBM computers have a single precision accuracy of less than seven digits, the program employs double precision complex arithmetic (IBM type COMPLEX*16). If run on a computer with

more than approximately ten digits of accuracy in a real word, it should be replaced by the usual single precision complex arithmetic.

(ii) The plots on the printer have a resolution of $\Delta x = 0.01$. Therefore interference of two counter-moving wave packets with an approximate wavelength of $\Delta x = \pi/p$ (p is the momentum of each wave) cannot be resolved in this plot if $p \geqslant 2\pi$. If high resolution is required a plotter or movie camera should be used.

10. Test run output

A data card is supplied with the program which treats the problem of barrier penetration of a wave packet with Albrecht-friction. With TIME = 3.7×10^{-3}, DTIME = 1.2×10^{-3}, PIN = 150, SIN = 0.05, AIN = -0.25, GAM = 150, VBAR = 10^4, EPS = 10^{-3}, DEL = 5×10^{-6}, IFRI = 4, IPAC = 1, IPOT = 2, IPRI = 1, the following four double pages of output are printed at the wave packets running times of 0, 0.0012, 0.0024 and 0.0036, respectively.

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References

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TEST RUN OUTPUT

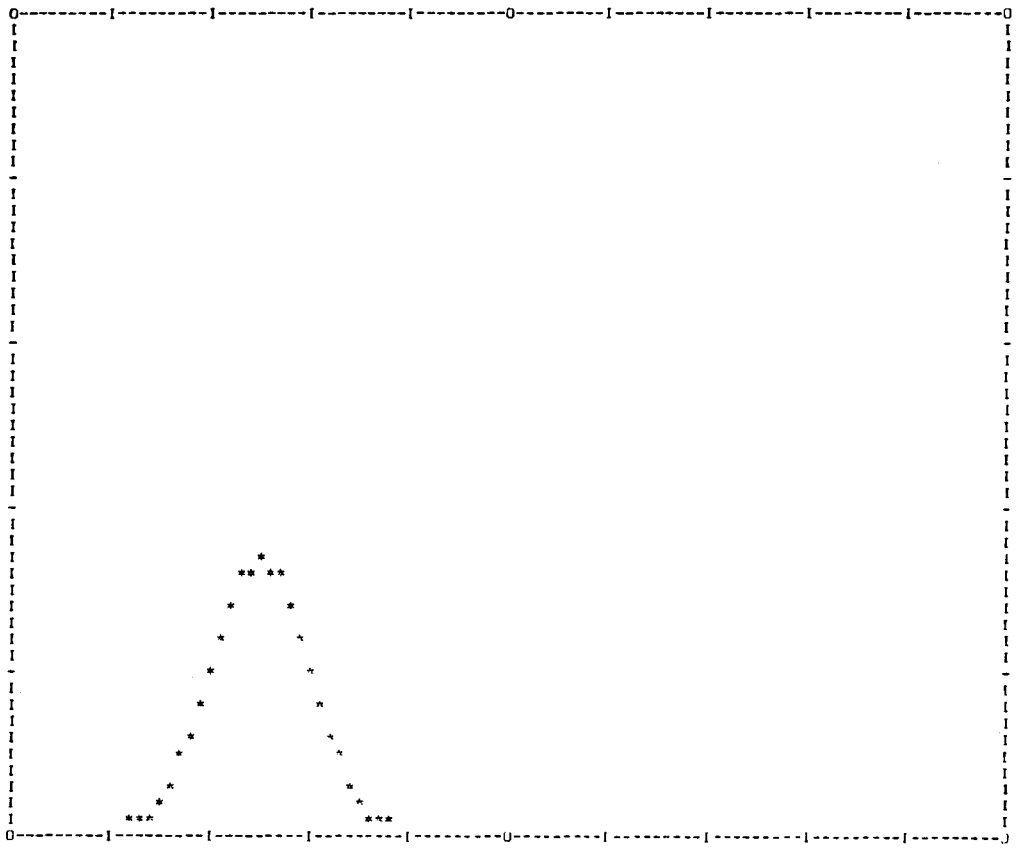
```
ALBRECHT FRICTION   ONE WAVE PACKET     SQUARE POTENTIAL        V=  10000.00
EPS=1.000-03   DEL=5.00D-06
P IN=  150.00   S IN= 0.0500   A IN=-0.2500
GAMMA=  150.00

TIME= 0.0
LEFT= 0.1000D 01   RIGHT= 0.7713D-12   NORM= 1.0000D 00
(X)= -0.2500   (P)=  149.4231   (T)=  11261.3925   (V)=       0.0001   (E)=  11261.3926
```

ABSOLUTE VALUE OF WAVE FUNCTION

0.000033	0.000085	0.000210	0.000496	0.001127	0.002458	0.005152	0.010375	0.020074	0.037317
0.066649	0.114373	0.188564	0.298699	0.454609	0.664768	0.933965	1.260720	1.635066	2.037418
2.439233	2.805785	3.100873	3.292620	3.359136	3.292620	3.100873	2.805785	2.439233	2.037418
1.635066	1.260720	0.933965	0.664768	0.454609	0.298700	0.188564	0.114370	0.066649	0.037317
0.020074	0.010375	0.005152	0.002458	0.001127	0.000496	0.000210	0.000085	0.000033	0.000013
0.000005	0.000002	0.000001	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	

Y-SCALE= 10.000

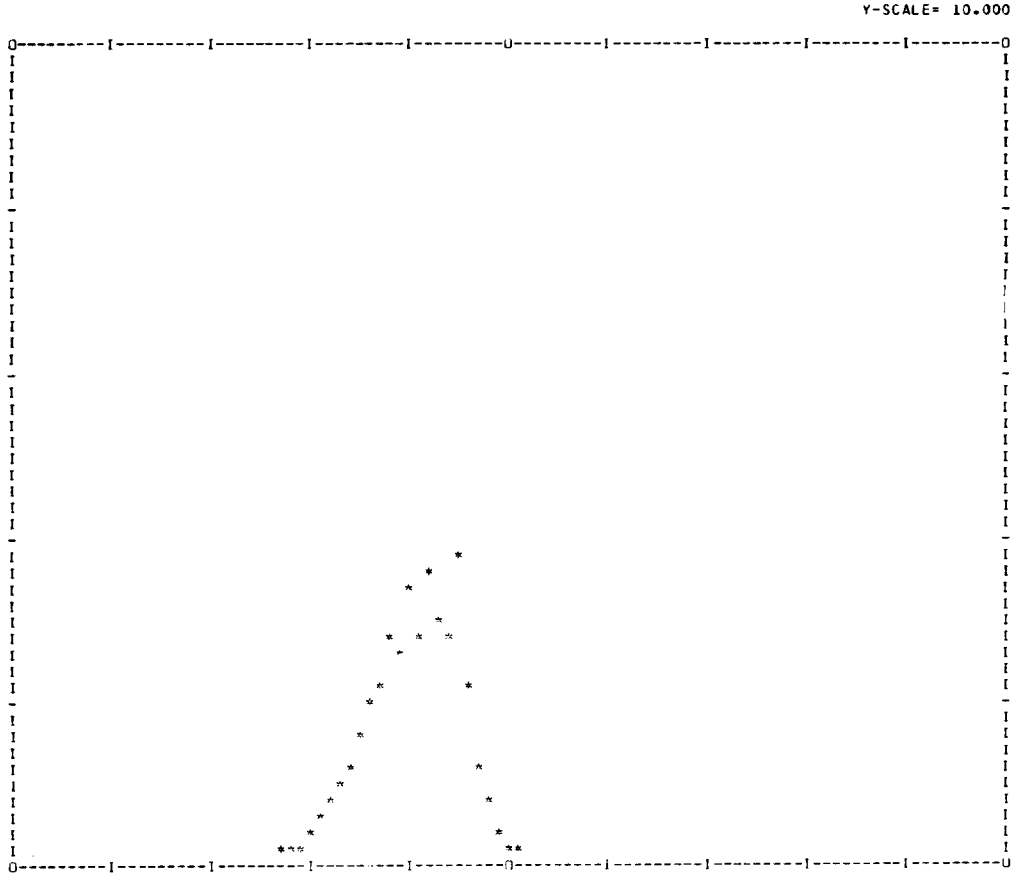


```
ALBRECHT FRICTION   ONE WAVE PACKET     SQUARE POTENTIAL        V=  10000.00
EPS=1.000-03   DEL=5.000-06
P IN=  150.00   S IN= 0.0500   A IN=-0.2500
GAMMA=  150.00

TIME= 0.00120000
LEFT= 0.9995D 00   RIGHT= 0.5135D-03   NORM= 1.00000 00
(X)= -0.0890   (P)=  102.6700   (T)=   6849.6190   (V)=   1182.9538   (E)=   8032.5728
```

ABSOLUTE VALUE OF WAVE FUNCTION

0.000007	0.000008	0.000002	0.000007	0.000009	0.000005	0.000007	0.000010	0.000008	0.000010
0.000014	0.000009	0.000020	0.000017	0.000038	0.000093	0.000176	0.000431	0.000847	0.001807
0.003493	0.006771	0.012504	0.022430	0.039177	0.065320	0.107658	0.166937	0.259696	0.374472
0.549337	0.738613	1.016026	1.287190	1.632667	1.993008	2.256723	2.779495	2.665848	3.428967
2.796444	3.565979	3.062735	2.717134	3.701542	2.129697	1.252750	0.738529	0.430528	0.246282
0.137525	0.074636	0.039953	0.020104	0.008670	0.005596	0.003499	0.002121	0.001244	0.000709
0.000396	0.000222	0.000132	0.000093	0.000079	0.000075	0.000074	0.000072	0.000070	0.000067
0.000062	0.000057	0.000052	0.000046	0.000041	0.000036	0.000031	0.000027	0.000024	0.000021
0.000019	0.000017	0.000015	0.000013	0.000012	0.000011	0.000010	0.000009	0.000008	0.000007
0.000006	0.000006	0.000006	0.000005	0.000004	0.000005	0.000005	0.000006	0.000003	

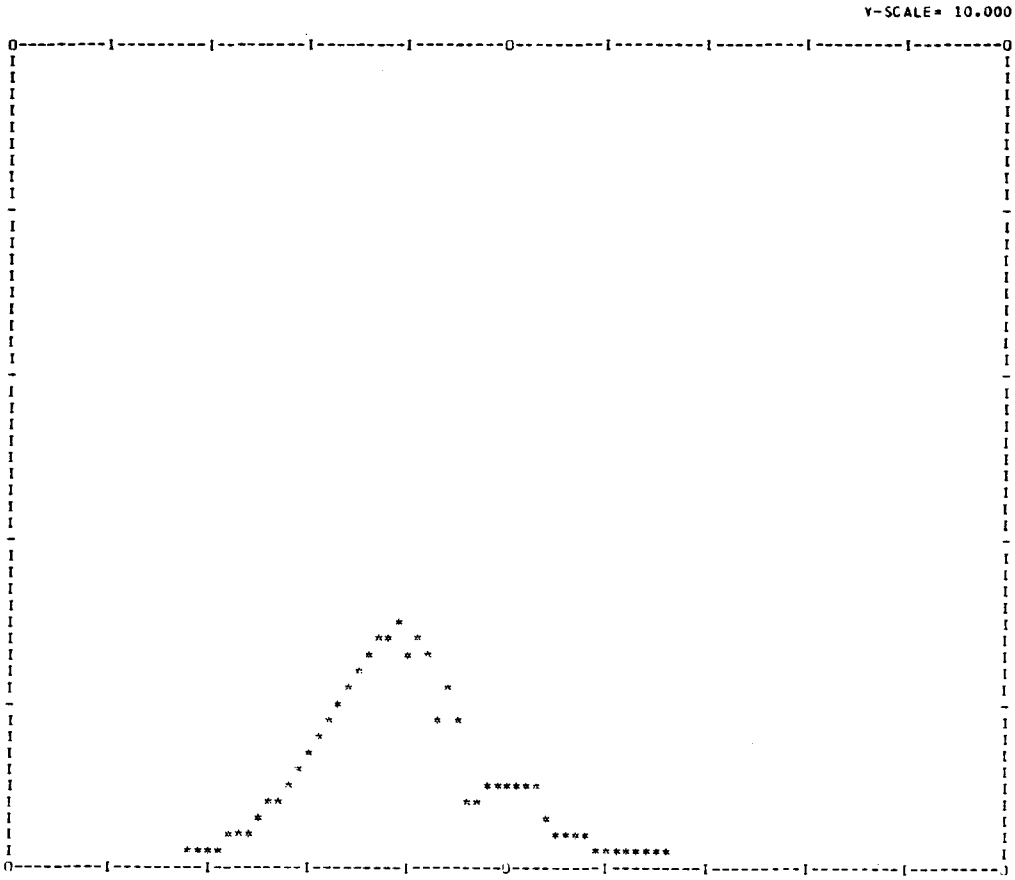


```
ALBRECHT FRICTION   ONE WAVE PACKET     SQUARE POTENTIAL        V=  10000.00
EPS=1.00D-03   DEL=5.00D-06
P IN=  150.00   S IN= 0.0500   A IN=-0.2500
GAMMA=  150.00

TIME= 0.00240000
LEFT= 0.9548D 00   RIGHT= 0.4520D-01   NORM= 1.0000D 00
(X)= -0.1138   (P)= -100.0651   (T)=   6314.0513   (V)=    845.9126   (E)=   7159.9639
```

ABSOLUTE VALUE OF WAVE FUNCTION

0.000249	0.000325	0.000543	0.000867	0.001327	0.002065	0.003076	0.004585	0.006756	0.009747
0.013943	0.019708	0.027452	0.037819	0.051504	0.069251	0.092072	0.121024	0.157238	0.202000
0.256678	0.322622	0.401246	0.493793	0.601466	0.725630	0.866200	1.023488	1.199634	1.388883
1.589074	1.810192	2.024798	2.223289	2.458362	2.630112	2.702168	2.899676	2.915937	2.629265
2.810188	2.598619	1.716585	2.276249	1.834086	0.830490	0.791384	0.936433	0.994964	0.976100
0.968079	0.995783	0.927957	0.656666	0.375726	0.355238	0.332870	0.308964	0.283908	0.258108
0.231987	0.205959	0.180450	0.155853	0.132557	0.110901	0.091172	0.073588	0.058265	0.045223
0.034396	0.025623	0.018686	0.013334	0.009311	0.005358	0.004277	0.002823	0.001827	0.001154
0.000721	0.000461	0.000300	0.000184	0.000108	0.000089	0.000085	0.000057	0.000046	0.000070
0.000071	0.000038	0.000045	0.000074	0.000063	0.000019	0.000050	0.000074	0.000053	



```
ALBRECHT FRICTION   ONE WAVE PACKET     SQUARE POTENTIAL        V=  10000.00
EPS=1.000-03   DEL=5.000-06
P IN=  150.00   S IN= 0.0500   A IN=-0.2500
GAMMA=  150.00

TIME= 0.00360000
LEFT= 0.93380 00   RIGHT= 0.66190-01   NORM= 1.00000 00
(X)= -0.2270   (P)=  -85.6952   (T)=   5261.9880   (V)=    297.0225   (E)=   5559.0104
```

ABSOLUTE VALUE OF WAVE FUNCTION

0.227380	0.103310	0.250810	0.207735	0.307230	0.321757	0.401207	0.454239	0.533200	0.613190
0.703265	0.804899	0.912110	1.033450	1.160122	1.299944	1.445230	1.600490	1.759251	1.922074
2.082508	2.237195	2.378641	2.500299	2.593631	2.650487	2.662504	2.622222	2.523663	2.363232
2.141332	1.863879	1.544158	1.203254	0.869926	0.578020	0.360446	0.238061	0.193402	0.180919
0.178626	0.164969	0.142168	0.121003	0.102043	0.083736	0.069175	0.063737	0.273565	0.545344
0.790668	0.913421	0.844249	0.586993	0.348812	0.358153	0.367222	0.375945	0.384279	0.391991
0.398965	0.405127	0.410229	0.414173	0.416833	0.417985	0.417623	0.415569	0.411689	0.406086
0.398566	0.389172	0.378065	0.365101	0.350544	0.334473	0.316923	0.298261	0.278460	0.2578+9
0.236724	0.215143	0.193699	0.172466	0.151802	0.132169	0.113530	0.096377	0.080740	0.066747
0.054387	0.043723	0.034943	0.026771	0.021050	0.016554	0.013397	0.009973	0.008619