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Introduction of Elementary Quantum Mechanics Using a Symbolic Manipulation Program

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Abstract

This article discusses a set of symbolic manipulation programs developed to reinforce understanding of basic concepts presented in a introductory quantum mechanics course.

It was designed that the solutions of the problems were analytically tractable as well as numerically obtainable.

We have shown that several examples which are very effective for the constructive reinforce to grasp the basic ideas rather than a complex junk of numerical computational examples.

We derive some guiding principles for the introduction of computational method into the undergraduate course of quantum mechanics.

1. Introduction

Very rapid developments of hardwares and softwares in personal computers enable us to introduce a computer-aided instructions in various field of science and technology.

Even very complicated numerical calculations, which you had to use a main-frame computer a few years ago, can now handle with your personal computer. Various packages for numerical computations are now available [1], and it is very easy for instructors to introduce these packages in their classes. According to my experiences, this type of introduction has never succeeded to extend student's abilities for further understanding of physics. There is always certain barriers between lecturer's analytical descriptions in a blackboard and the output of numerical computations by a computer. Sometimes the destructive interferences have occured in a class, namely, the students understand less physics and get less computational skills. Actually, numerical computations do not teach the students physics.

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On the other hand, it is true that there is a few problem in physics which can be solved analytically. For an example, if you wish to explore a behavior of an electron wave function under a general potential function, suddenly you may encounter severe limitation as long as you stick some analytical solutions. Numerical method can handle much wider and a variety of interesting problems, which can not be solved by analytical method.

The motivation of the present programs is to explore new methods of well-balanced instructions of analytical as well as numerical approaches to the quantum mechanical problems, which may overcome the above mentioned problems.The author selects Mathematica programs for symbolic (analytical) calculations [2]. This is because of its excellent interface with users, and suitable to explore creative programming by students. In the subsequent sections, we treat several elementary quantum mechanical problems with this approach.

2. The One-Dimensional Potential Barrier Problems

The problems of the one-dimensional finite potential barriers and wells are treated universally in introductory quantum mechanics textbooks. There exists a number of ways to attack this problems. In the simple type of potential, the overall wave function is constructed out of pieces having the forms of general wave function by matching wave function and its derivative at the discontinuities of the given potential function. The transfer matrix method is one of commonly used method. The Laplace transformation method is another powerful method for solving the problems. Feynmann's path integral method is also applicable to this type of problems, although it is less merit for simple one-dimensional problems.

The most important point is that the students can understand there exists several different approaches to attack the same problems and the selection of approaches depends on various boundary conditions involved in the problems. As an example, let's consider the finite square barrier as shown in Fig.1.The Schroedinger equation for I, II, and III regions are

$$\frac{d^2\phi}{dx^2}+\alpha^2\phi=0 \quad (x=0, and\ x>a) \tag{2.1a}$$

$$\frac{d^2+\phi}{dx^2}+\beta\phi=0 \quad (0<x<a) \quad V=\varepsilon \tag{2.1b}$$

$$\frac{d^2\phi}{dx^2}+\mu^2\phi=0 \quad (0<x<a) \quad V=\varepsilon \tag{2.1c},$$

where

$$\alpha^2=2m\epsilon/\hbar^2,\ \beta^2=2m(V-\varepsilon)/\hbar^2$$
$$\mu^2=2m(\epsilon-V)/\hbar^2 \tag{2.2}.$$

We take the wave functions in the each region as:

$$\phi_{\rm I}=\exp(i\alpha x)+r\exp(-i\alpha x), \qquad x<0 \tag{2.3a}$$
$$\phi_{\rm II}=a\exp(-\beta x)+b\exp(\beta x), \qquad 0<x<a \tag{2.3b}$$
$$\phi_{\rm III}=t\exp(i\alpha x) \qquad x>a \tag{2.3c}.$$

Example of Mathematica solutions for the above problem:

```
(*Boundary conditions at x=0 and x=a*)
psai1 [x_] :=Exp [I alfa x]  + r Exp [−I alfa x]
psai2 [x_] :=a Exp [−beta x]  + b Exp [beta x]
psai3 [x_] :=t Exp [I alfa x]
boundary=LogicalExpand [(psai1 [x] /.x−>0)==
(psai2 [x] /.x−>0) &&
(psai2 [x] /.x−>a)==(psai3 [x] /.x−>a) &&
(D [psai 1 [x] ,x] /.x−>0)==(D [psai 2 [x] ,x] /.x−>0) &&
(D [psai 2 [x] ,x] /.x−>a)==(D [psai 3 [x] ,x] /.x−>a)]

  a              a  beta        I  a  alfa
-------- + b        ==  E           t  &&
  a beta
E
    a beta                        a  beta                 I  a  alfa
-(--------)  +  b  beta  E           ==  I  alfa  E           t  &&
    a  beta
  E
1 + r == a + b && I alfa − I alfa r ==
−(a  beta)  +  b  beta
```

From the above Mathematica procedures, we obtain the following relations between r and t;

$$(\beta - i\alpha)\, r - \exp(i\alpha a - \beta a)\,(\beta + i\alpha)\, t + (\beta + i\alpha) = 0 \qquad (2.4a),$$

$$(\beta + i\alpha)\, r - \exp(i\alpha a + \beta a)\,(\beta - i\alpha)\, t + (\beta - i\alpha) = 0 \qquad (2.4b).$$

From Eqs.(2.4a) and (2.4b), we can derive the transmission coefficient of a particle which tunnels through the potential barrier;

```
(*Calculation of the Transmission Coefficient*)
t1:= 2  I alfa beta Exp  [−I alfa a]
t2:=alfa^ 2  Sinh  [beta a]  −
beta^ 2  Sinh  [beta a]  + 2  I alfa beta Cosh  [beta a]
t:=t1/t2
tc:=−2 I alfa beta Exp[I alfa a] /
((alfa^ 2 −beta^ 2 ) Sinh  [beta a]  − 2 I alfa beta Cosh  [beta a])
d=ExpandAll  [t*tc]
```

Fig. 1 A finite square potential barrier.

```
        2    2
(4 alfa  beta ) /

         2       2                2        4                2
(4  alfa  beta  Cosh [a beta]  + alfa  Sinh [a beta]  -

          2       2                2        4                2
   2 alfa  beta  Sinh [a beta]  +  beta  Sinh [a beta]  )
```

We have the final result for the transmission coefficient D as

$$D=\frac{4\alpha^2\beta^2}{4\alpha^2\beta^2+(\alpha^2+\beta^2)^2\sinh^2(\beta a)} \tag{2.5}$$

Now, let us perform the numerical calculations of D for a free electron;

```
(*Physical parameters*)
m=9.01 10^(-31);
hbar=1.0546 10^(-34);
v=0.5 1.602 10^(-19);
en=ep 1.602 10^(-19);
alfa=Sqrt [2 m en] /hbar;
beta=Sqrt [2 m ( v -en)] /hbar;
a= 10 10^(-10);
(* D as a function of electron energy *)
d:=4 alfa^2 beta^2/
(4 alfa^2 beta^2 + (alfa^2 + beta^2)^2 (Sinh [beta a])^2);
l1=Table [{ep, Log [d]} , {ep, 0.01, 0.48, 0.001}] ;
g1=ListPlot [l1, PlotRange-> {{0,0.48} , {-9,-1}} ,
Frame->True]
```

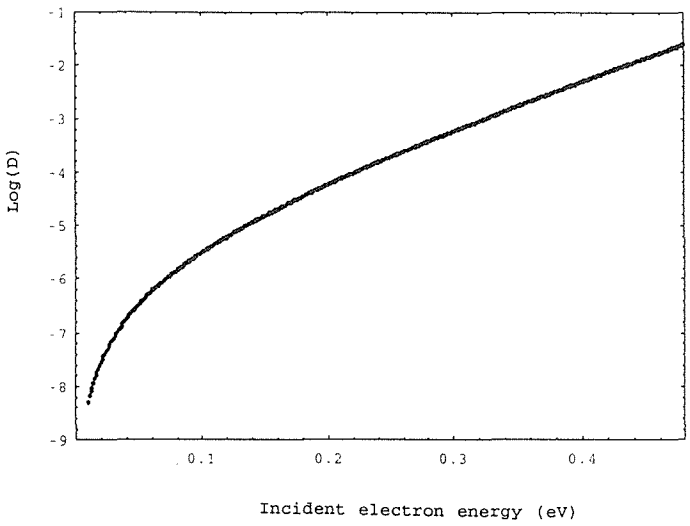


Fig. 2 Transmission coefficient as a function of electron energy. Barrier height; 0.5 eV. Barrier width: 10 angstroms.

```
m=9.01 10^(-31);
hbar=1.0546 10(-34);
v=0.5 1.602 10^(-19);
en=ep 1.602 10^(-19);
beta=Sqrt [2 m ( v -en)] /hbar;
a= 10 10^(-10);
p=en/v;
d=16 p (1-p) Exp [-2 beta a] ;
l2=Table [{ep, Log [d]} , {ep, 0.01,0.48, 0.01}] ;
g2=ListPlot [l2, Frame->True]
```

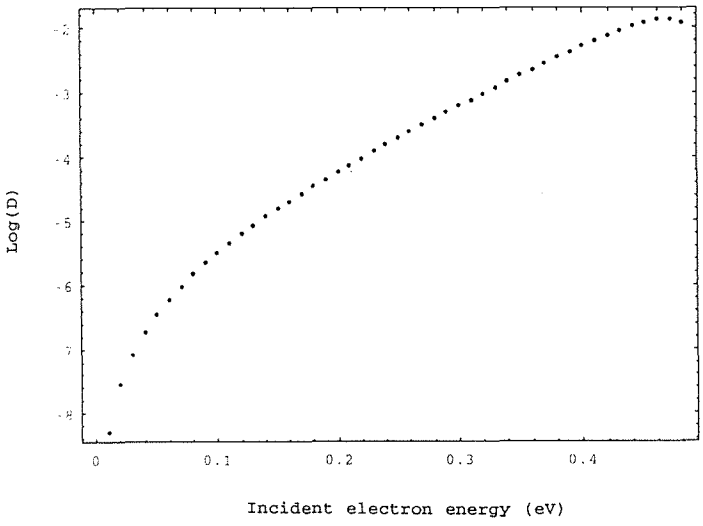


Fig. 3 Approximate solution of the transmission coefficient.

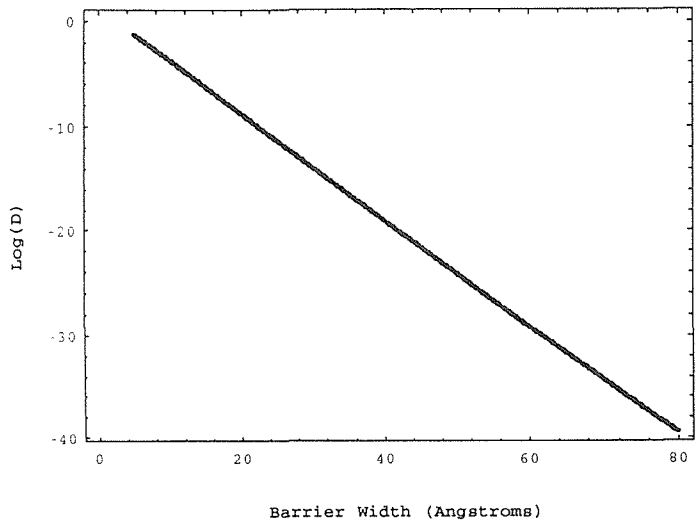


Fig. 4 Transmission coefficient as a function of the barrier width. electron energy: 0.35 eV, Barrier height: 0.5eV.

We have illustrated quantum mechanical tunneling phenomena using the symbolic manipulation program. It is seen that we can easily established a well-balanced instructions using analytical as well as numerical approaches to this elementary problem. From Fig. 3, the current transmission factor is determined by the exponentially damped factor exp [-2qw] inside the potential barrier, and other phase factor do not play any appreciable contribution to the transmission. Let us consider the actual behavior of the wave functions in the each region in this tunneling phenomena;

```
m=9.01 10^(-31);
h bar=1.0546 10^(-34);
v 1 =0.5 1.602 10^(-19);
v 2 =0.1 1.602 10^(-19);
en=0.35 1.602 10^(-19);
k 1 =Sqrt [2 m en] /hbar;
k 3 =Sqrt [2 m (en -v2)] /hbar;
q 2 =Sqrt [2 m ( v1 -en)] /hbar;
w= 10 10^(-10);
(* Wave functions and Boundary Conditions*)
psiL [x_] :=Exp [I k1 x] + r Exp [-I k1 x] ;
psi I [x_] :=a Exp [q2 x] + b Exp [-q2 x] ;
psiR [x_] :=t Exp [I k3 x] ;
set = LogicalExpand [ (psiL [x] /.x->0)==
(psi I [x] /.x-> 0 ) &&
(psi I [x] /.x->w)==(psiR [x] /.x->w) &&
(D [psiL [x] ,x] /.x-> 0 )==(D [psiI [x] ,x] /.x-> 0 ) &&
```

```
(D [psiI [x] ,x] /.x->w)==(D [psiR [x] ,x] /.x->w)] ;
sol=Solve [%, {r,t,a,b}]
psi [x_] :=Exp [I k1 x]  + (0.378817 - 0.88792 I)*
Exp [-I k1 x] /;x< 0;
psi [x_] :=(-0.0105823 + 0.0300405 I) Exp [q2 w] +
(1.36823 - 0.918833 I) Exp [-q2 x] /;(x> 0) && (x<w)
psi [x_] :=(-0.1712 -0.222328 I) Exp [I k3 x] /;x>=w

(* Plotting of real part of the wave functions *)
Plot [Re [psi [x]] ,
 {x, -50 10^(-10), 50 10^(-10)} , AspectRatio->0.7,
Epilog-> {Line [{{0,0} , {0,1.7} , {1 10^(-9), 1.7} ,
 {1 10^(-9), 0.34} , {7 10^(-9), 0.34}}]} ,
Frame->True]
 {{r -> 0.378817 - 0.888792 I,
 t -> -0.1712 - 0.222328 I,
 a -> 0.0105823 + 0.0300405 I,
 b -> 1.36823 - 0.918833 I}
```

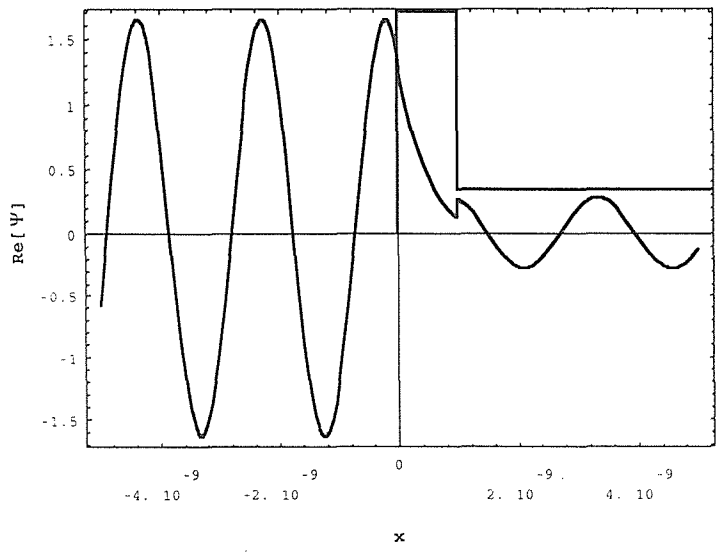


Fig. 5 Real part of the wave function amplitudes around a one-dimensional square potential.

Here, we put some modification on the one-dimensional potential form as illustrate in Fig. 5. This is very intuitive illustration on quantum mechanical tunneling through a simple potential barrier, and very effective for the student to understand the actual wave function penetration through a potential barrier.

Let us now study the situation where the incident electron energy is much larger than the potential energy.

The wave function in region II in this case is determined by

$$\phi_{II} = p\cos(\beta x) + (q\sin(\beta x) \tag{2.6}.$$

By the similar calculation procedures as in the case of $v > \varepsilon$, we obtain the following relations;

$$r = \frac{(\alpha^2-\beta^2)\sin(\beta a)}{(\alpha^2+\beta^2)\sin(\beta a)+2i\alpha\beta\cos(\beta a)} \tag{2.7a},$$

$$t = \frac{2i\alpha\beta\exp(-i\alpha a)}{(\alpha^2+\beta^2)\sin(\beta a)+2i\alpha\beta\cos(\beta a)} \tag{2.7b}.$$

It is considered that the above solutions describe the scattering of electrons due to one-dimensional potential barrier, although there exists very limited spatial variable in the one-dimensional case, and therefore the physical meaning of scattering in this case is different from the general scattering theory in three-dimensional cases.

The reflection coefficient R is given by r. r^* and

$$R = \frac{V^2\sin^2(\beta a)}{V^2\sin^2(\beta a)+4\varepsilon(\varepsilon - V)} \tag{2.8}.$$

From Eq.(2.8) it is easily verified that R approaches to zero when the electron energy is large enough compare with V. However, due to $\sin^2(\beta a)$ factor involved in Eq.(2.8), there is the resonant scattering of electrons from the potential barrier.

Let us estimate this resonant phenomena using numerical calculation:

```
m=9.01 10^(-31);
h bar=1.0546 10^(-34);
v=0.5 1.602 10^(-19);
en= ep 1.602 10^(-19);
beta=Sqrt [2 m(en-v)] /hbar;
a=10 10^(-10);
p1=v^2 (Sin [beta a])^2;
p2=v^2 (Sin [beta a])^2 + 4 en(en - v);
r=p1/p2;
l1=Table [{ep, Log [r]} , {ep, 0.7, 20, 0.005}] ;
ListPlot [l1, PlotJoined->True, Frame->True,
AspectRatio->0.7]
```

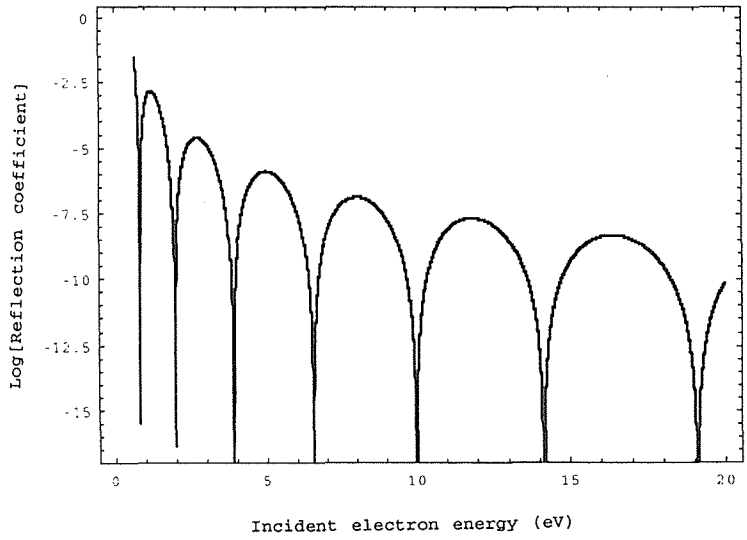


Fig. 6 Resonant scattering in a one-dimensional potential well.

It is seen from Fig.6 that there are the resonant transmission of incident electron when $\beta a = n\pi$. We can expect that the similar resonant transmission can be observed in a one-dimensional square well potential.

3.A Coupled Harmonic Oscillator

The problems of the one-dimensional simple harmonic oscillator are also treated universally in introductory quantum mechanics textbooks. The eigen function of a simple one-dimensional harmonic oscillator with the potential energy v(x) = m $\omega^2 x^2/2$ is given by [3]

$$\phi_n = c_n H_n(x/\sigma)\exp(-x^2/2\sigma^2) \tag{3.1a}$$

where

$$c_n = (\pi 2^n n!\sigma)^{-1/2}, \quad \sigma = \hbar/m\omega \tag{3.1b},$$

and H_n is the Hermite polynomial of order n. The corresponding eigenvalues are

$$E_n = \left((n+\frac{1}{2})\right)\hbar\omega \tag{3.2}.$$

```
m=9.01 10^(-31);
h bar=1.0546 10^(-34);
en= ep 1.602 10^(-19);
w=0.1 1.602 10^(-19)/h bar;
s 0=Sqrt [hbar/(m 1.51906 10^14)]
c [n_] :=(Sqrt [Pi] 2n n ! s0)^(-1/2)
psai [n_,x_] :=c [n] HermiteH [n, x/s0] Exp [-x^2/(2 s0^2)]
```

In Fig. 7, the first few eigen functions are plotted. All the eigen functions are normalized .

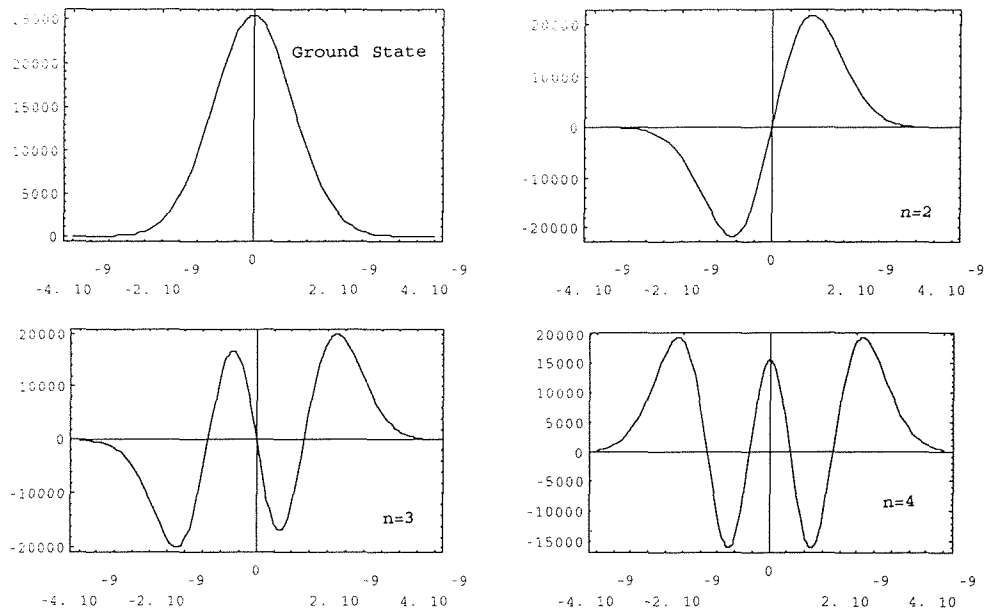


Fig. 7 Eigen functions of a simple harmonic oscillator.

```
(*Normalization*)
m=9.01 10(-31);
hbar=1.0546 10(-34);
en= ep 1.602 10^(-19);
w=0.1 1.602 10^(-19)/hbar;
s 0=Sqrt [hbar/(m 1.51906 10^14)] ;
c [n_] :=(Sqrt [Pi] 2n n ! s 0)^(-1/2)
psai [n_,x_] :=c [n] HermiteH [n, x/s 0 ] Exp [-x^ 2 /( 2 s0^ 2 )]
NIntegrate [(psai [0,x])^2, {x, -100 10^(-10), 100 10^(-10)}]
NIntegrate [(psai [1,x])^2, {x, -100 10^(-10), 100 10^(-10)}]
NIntegrate [(psai [2,x])^2, {x, -100 10^(-10), 100 10^(-10)}]
NIntegrate [(psai [3,x])^2, {x, -100 10^(-10), 100 10^(-10)}]
NIntegrate [(psai [4,x])^2, {x, -100 10^(-10), 100 10^(-10)}]
1.
1.
1.
1.

1.
```

The width of the ground-state function is given by σ, and in the case of $h\omega/2\pi$=0.1 eV, the width becomes 8.78 A. The actual spreading of the ground-state wave function is around 20 A

as can be seen from Fig.8. As $h\omega/2\pi$ becomes smaller, the spreading of the wave functions becomes larger, and this is easily verified by a simple numerical calculations of the actual eigen functions. The author used to ask the following question to my colleague;

"How long the ground-state wave function of simple harmonic oscillator extends when $h\omega/2\pi$ is equal to 0.1 eV ?"

Usually nobody can answer the correct order of the actual wave function spread.

Now, let us consider a coupled harmonic oscillator as an example of the wave function of a two-particle system.

The Hamiltonian of the system is

$$H=-\left(\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x_1}+\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x_2}\right) \tag{3.3a},$$

$$V(x_2,x_2)=\frac{k}{2}(x_1^2+x_2^2)+\frac{\delta}{2}(x_1-x_2)^2 \tag{3.3b}.$$

The last term inv Eq.(3.3b) describes the coupling between the two harmonic oscillators. In classical mechanics, the equation for a coupled harmonic oscillator can be decoupled into tow independent oscillators using center-of mass coordinate and relative coordinate. The same procedures can applied for this quantum system. Using $R=(x_1+x_2)/2$ and $r=x_2-x_1$ with $M=2$ m and $\mu=m/2$, we obtain

$$H=H_R+H_r$$

$$H=-\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2}+kR^2,\qquad H_r=-\frac{\hbar^2}{2}\frac{d^2}{dr^2}\frac{1}{2}\left(\frac{k}{2}+\delta\right)r^2 \tag{3.4}.$$

The eigen function and the corresponding eigenvalues are

$$\psi(x)=\varphi_N(R)\,\phi_n(r) \tag{3.5a},$$

$$\varepsilon=(N+1/2)\,\hbar\,\omega_R+(n+1/2)\,\hbar\,\omega_r \tag{3.5b},$$

where

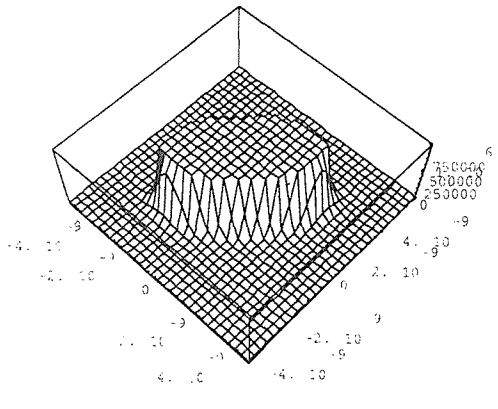
$$\omega_R=k/m,\quad \omega_R=(k+2\delta)/m \tag{3.5c}.$$

Some numerical examples of the coupled oscillator are shown in Fig.8a and 8b.

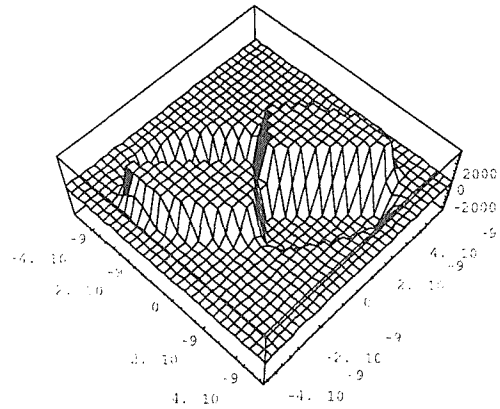
(*Numerical Examples of the Coupled Oscillator*)

```
m= 9.01  10^(-31);
h bar=1.0546  10^(−34);
w1=0.1  1.602  10^(−19)/hbar;
w2=0.12  1.602  10^(−19)/hbar;
k1=m  w1^2;
k2=m  w2^2;
```

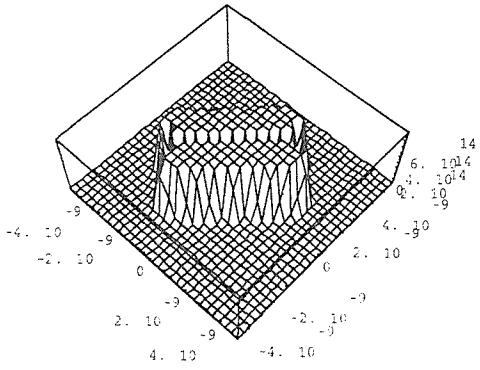
```
s1=Sqrt [hbar/(2 m 1.51906 10^14)] ;
s2=Sqrt [hbar/((m/2) 1.82287 10^14)] ;
r:=(x1 + x2)/2
t:=x2−x1
c [q_] :=(Sqrt [Pi] 2^q q! s1)^(−1/2)
psai [q_,r_] :=c [q] HermiteH [q, r/s1]*
 Exp [−r^2/(2 s1^2)]
c [s_] :=(Sqrt [Pi] 2^s s! s2)^(−1/2)
psai [s_, t_] :=c [s] HermiteH [s, t/s2] *
 Exp [−t^2/(2 s2^2)]
```



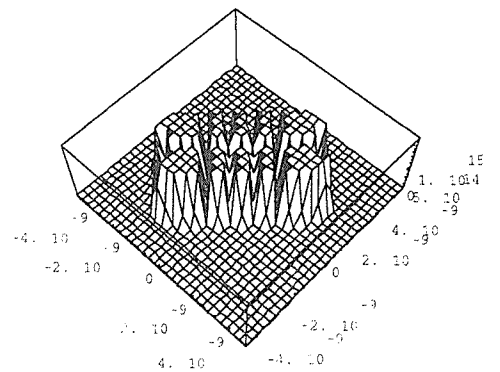
(a) $\delta=0$.



(b) N=1, n=1.



(c) N=1, n=2



(d) N=2, n=1.

Fig. 8 Numerical examples of the coupled harmonic oscillator. $\hbar\omega R=0.1\,eV$ $\hbar\omega r=0.12\,eV$

In Fig.8a and Fig 8b, it is seen that a variety of mixture of the eigenfunctions occurs due to the coupling constant d.

This fact corresponds to the normal mode mixing in classical coupled harmonic oscillators. It might be a good exercise for the students to explore the variation of the wave functions as a function of the coupling constant.

4. Time-Dependent Solutions of Wave Packets

We have shown several typical examples of stationary state wave functions in simple potentials in the previous sections. The time-dependent behaviors of the wave functions are one of the most difficult problems for the undergraduate students to grasp their physical meaning. Here, we illustrate some of the visualized instruction for this kind of problems.

In order to describe a particle at a local position in quantum mechanics, it is necessary to construct a wave packet. A free electron wave function with momentum p is

$$\phi_e = (2\pi\hbar)^{-1/2}\exp\left[-\frac{i}{\hbar}(\varepsilon t - px)\right] \tag{4.1a},$$

which satisfy the time-dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\phi_e = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi_e \tag{4.1b}.$$

Since the Eq.(4.1b) is linear, the superposition

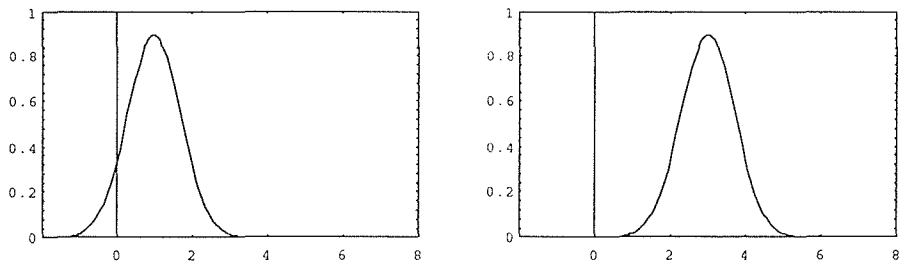
$$\psi(x,t) = \sum_{n=1}^{N} a_n\phi_{pn}(x,t) \tag{4.2a}$$

is also the solution of the wave equation, where pn corresponds to different momenta pn. Replacing the sum by an integral, we have

$$\psi(x,t) = \int_{-\infty}^{\infty} f(p)\,\phi_{pn}(x-x_0,t)\,dp \tag{4.2b},$$

where f(p) is the weighting function for the different momenta p. Let us consider the case where f(p) is given by a Gaussian distribution function;

$$f(p) = \frac{1}{(2\pi)^{1/4}\sigma_p}\exp\left[-\frac{(p-p_0)^2}{4\sigma_p^2}\right] \tag{4.3}.$$



(a) Normal distribution. (b) Displaced Gaussian.

Fig. 9 Examples of Gaussian distribution functions.

Substituting (4.1a) and (4.3) into (4.2b), we have the Fourier transform of function f(p) from momentum space into coordinate space.

```
(*Fourier Transform*)

<<Calculus'FourierTransform'
FourierTransform [Exp [-a^2 r^2/(4s^2)], r, x]
```

```
                  2
           Pi s
2 Sqrt [-----]
           2
           a
-------------
    2  2    2
  (s  x )/a
```

E

Using the above Fourier transformation, the probability density for observing the free particle at position x and time t is given by

$$|\psi(x,t)|^2=\frac{1}{2\pi\sigma_x}\,exp\left(\frac{[x-(x_0+vt)^2}{2\sigma_x^2}\right) \tag{4.4a},$$

where

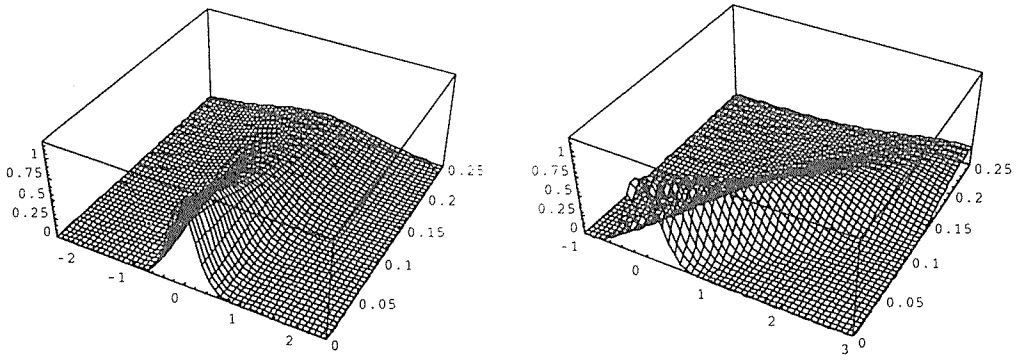
$$\sigma_x^2=\sigma_{x0}^2+\frac{\hbar^2t^2}{4\sigma_{x0}^2},\qquad \sigma_{x0}=\frac{\hbar}{2\sigma_p} \tag{4.4b}.$$

The very important point on the wavepacket is the fact that it must satisfy *Heisenberg's Uncertain Principle*. In fact,
the widths σ_x and σ_p satisfy the relation

$$\sigma_x\sigma_p\geq\hbar/2$$

Examples of the wave packet dispersion and and the propagation of the wave packet are illustrated in Fig. 10a and 10b.

```
b:= a^2 + 4 h bar^2 t^2/(m^2 a^2)
h bar=1;
m=1/2;
a =0.5;
r =(a/Sqrt [b]) Exp [-2 x^2/b] ;
g1=Plot3D [r, {x, -2.5, 2.5}, {t, 0, 0.25} , PlotPoints->50,
PlotRange-> {0, 1.2}] ;
b:= a^2 + 4 hbar^2 t^2/(m^2 a^2)
h bar=1;
m=1/2;
a =0.5;
v =12;
r =(a/Sqrt [b]) Exp [-2 (x-v t)^2/b] ;
g2=Plot3D [r, {x, -1, 3} , {t, 0, 0.25} , PlotPoints->50,
PlotRange-> {0, 1.2}] ;
```



(a) diffusion of wavepacket. (b) diffusion and propagation of wavepacket.

Fig. 10 Motions of Gaussian wavepacket.

It is easily realized from Fig.10a and 10b that the wave packet behaves as a probability density in a diffusion process. Actually if we put τ =it/h in the time-dependent Schroedinger equation, we have

$$\frac{\partial \psi(x,\tau)}{\partial \tau} = \frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,\tau)}{\partial x^2} \qquad (4.5a),$$

and this is a typical diffusion equation with a diffusion constant D, where

$$D = \frac{\hbar^2}{2m} \qquad (4.5b).$$

It is rather easy to extend the above discussion into the into the problems of wavepacket propagation through a simple potential barrier or well, and this offers very good exercise for the students. The most simple computational technique for this problem is the the finite difference method, and the wave equation is replaced by the corresponding difference equation;

$$i\hbar \frac{\partial \psi(x_i,t)}{\partial t} \approx$$
$$-\frac{\hbar^2}{2m} \frac{\psi(x_{i+1},t) - 2\psi(x_i,t) + \psi(x_{i-1},t)}{\delta x^2} + V(x_i,t)\psi(x_i,t) \qquad (4.6).$$

By performing the actual computational procedures, the students will realize the precision and the limitation of the finite difference method as well as the actual dynamical behaviors the wave packet, namely the transmission and the reflection of the wave packet.

5. Concluding Remarks

We have shown several well-balanced computing programs for elementary quantum mechanics which involve analytical as well as numerical calculations using a symbolic manipulation programs. We would like to point out the following remarks for this program;

1) It is not necessary to provide all the topics which usually described in the standard textbooks.

A few basic problem is enough for the students to grasp the basic ideas involved in quantum mechanics. The most important point for the success of the program is to illustrate to the students that there exist various approaches to the same problem, rather than just to show a junk of numerical examples.

2) The instructors should endeavor to seek creative Mathematica procedures which may continue to keep the student's interests. Concrete examples of this type of procedure were described in some details.

3) The instructors should illustrate the fact that there exists basic principle which can applied for wide variety of the problems. For examples, the treatments of one-dimensional potential barrier problem can easily extend to the problems of an one-dimensional periodic potential, and the concept of classical particle diffusion can apply for the Schroedinger wave equation using the imaginary time-domain.