PC4230 Project

Wu Yisu

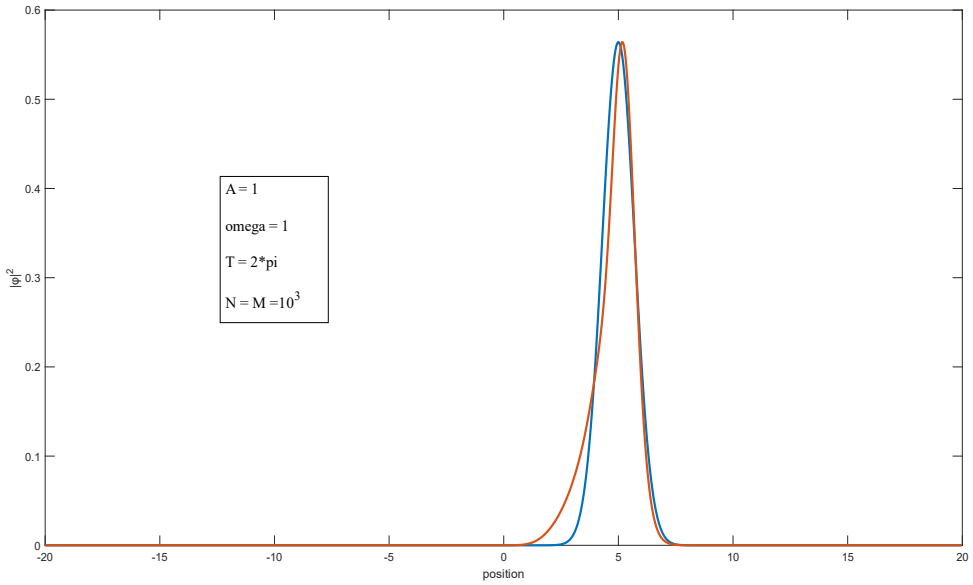
1. Time evolution

For this step I simply adjust the code on Canvas to generate a Gaussian state as initial state with $x_0 = 5$, and plot the square norm of final state after time evolution.

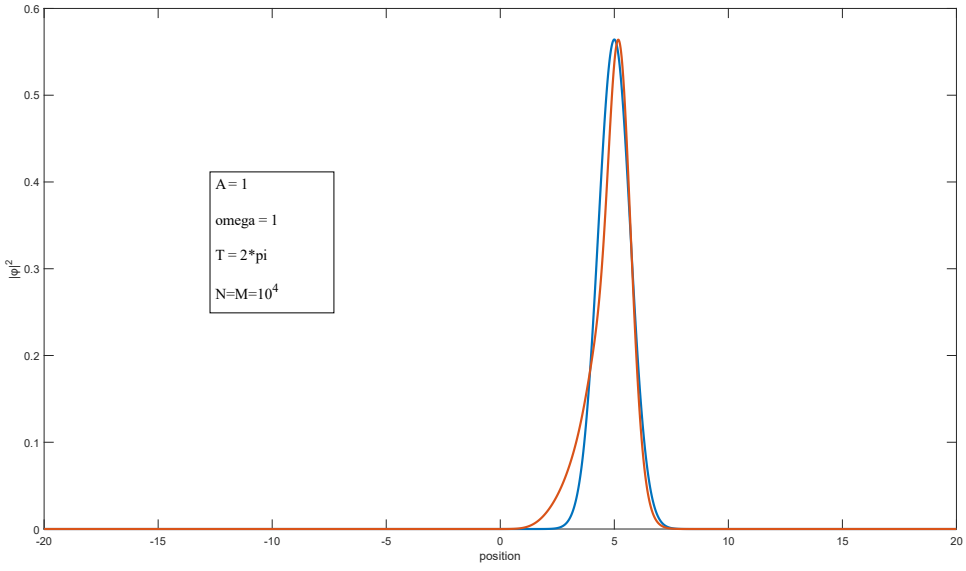
In particular, I use `psi = psiprep/sqrt(sum(abs(psiprep).^2.*dx));` to normalize the probability value, that is, adding a factor of space intervals.

After time duration of 2π, the final state is supposed to evolve back to x_0 with a same shape if it's a harmonic oscillator. Here we have time-periodic perturbation, so I'll tune the driving amplitude A and frequency ω to see how the final state change correspondingly.

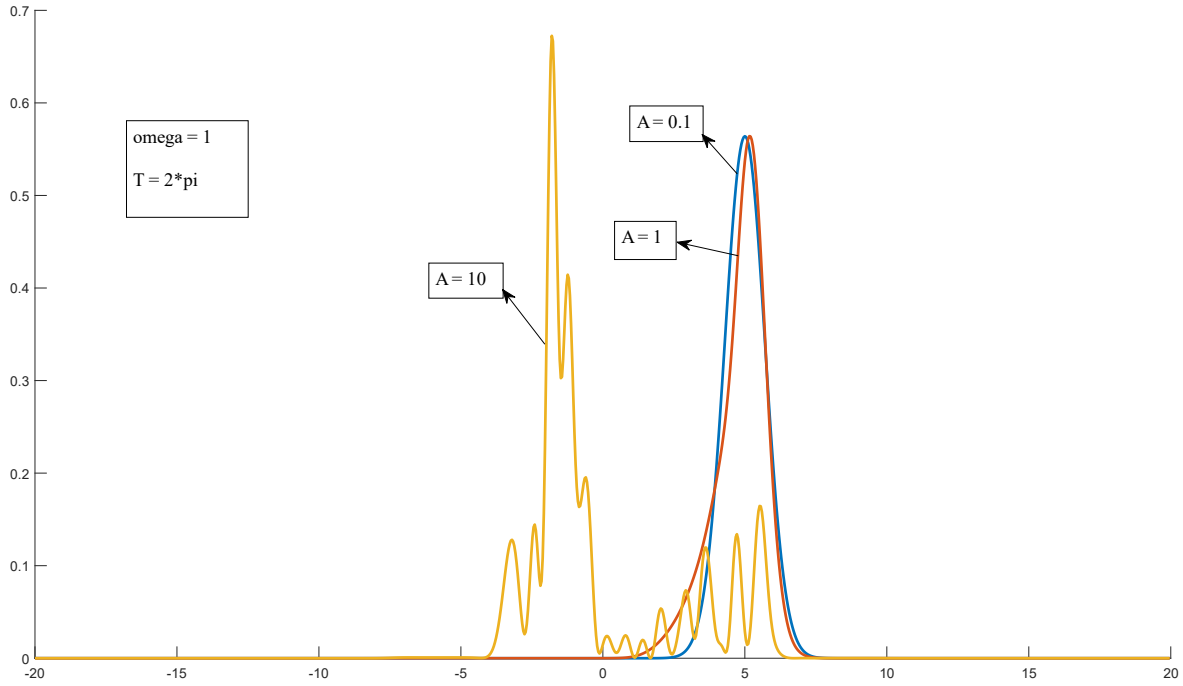
I. Checking convergence



Originally, the position step number is 10^3 & time step number 10^3. I change them to be $5 * 10^3$, and the plot doesn't make much difference, except the computation time takes longer. To save time, I just keep them to be 10^3.

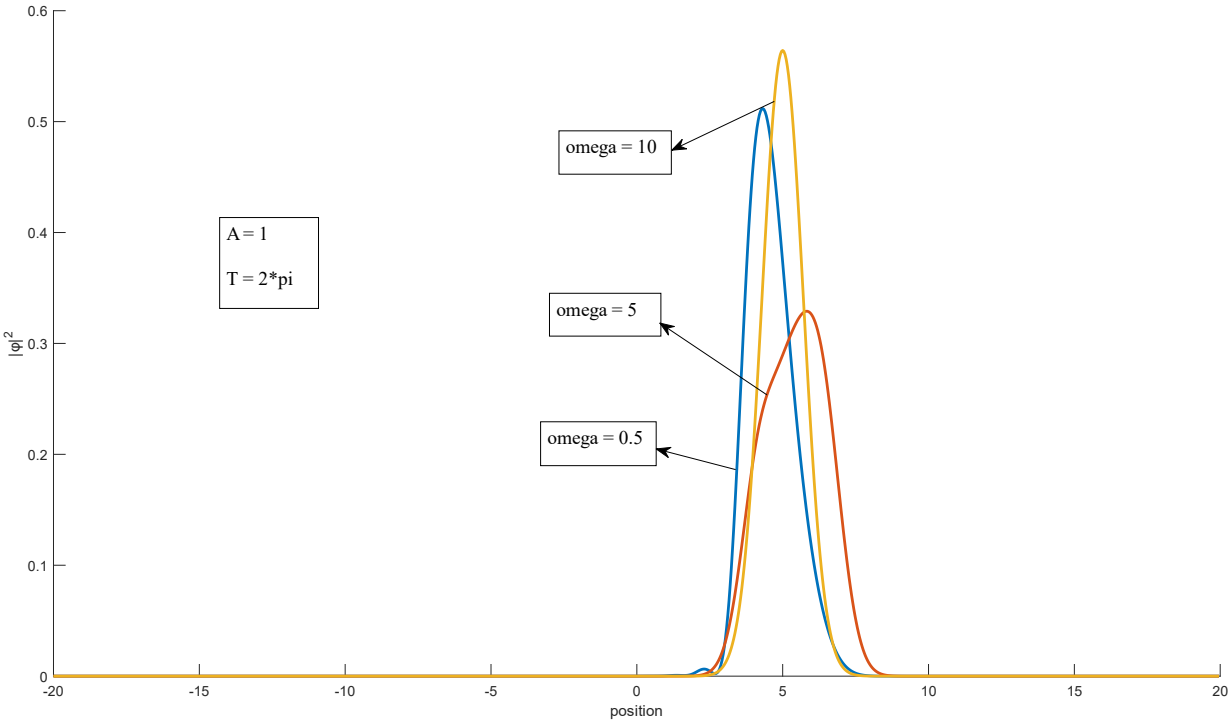


II. Tuning A



When driving amplitude is small, the wave function doesn't change too much, or just shift a little. When A is large, the final state has a more chaotic behavior, may have introduced some nonlinear effects.

III. Tuning omega



When the driving frequency is much bigger than the system's natural frequency, it may not respond to the perturbation in a timely manner. So the final state is almost like initial state (omega=10 in the plot).

2. DVR method

I. To generate initial state & boundary conditions

In this step, I use DVR method to generate the unperturbed eigenstates. Comparing to FFT method which use periodic boundary conditions, DVR use rigid boundary conditions, so only N-1 grid points will be useful.

To joint these two methods together, I define two sets of position points:

```
X1 = a+L*(0:N-1)/N;          %N grid points for FFT
X2 = a+L*(1:N-1)/N;          %N-1 for DVR
```

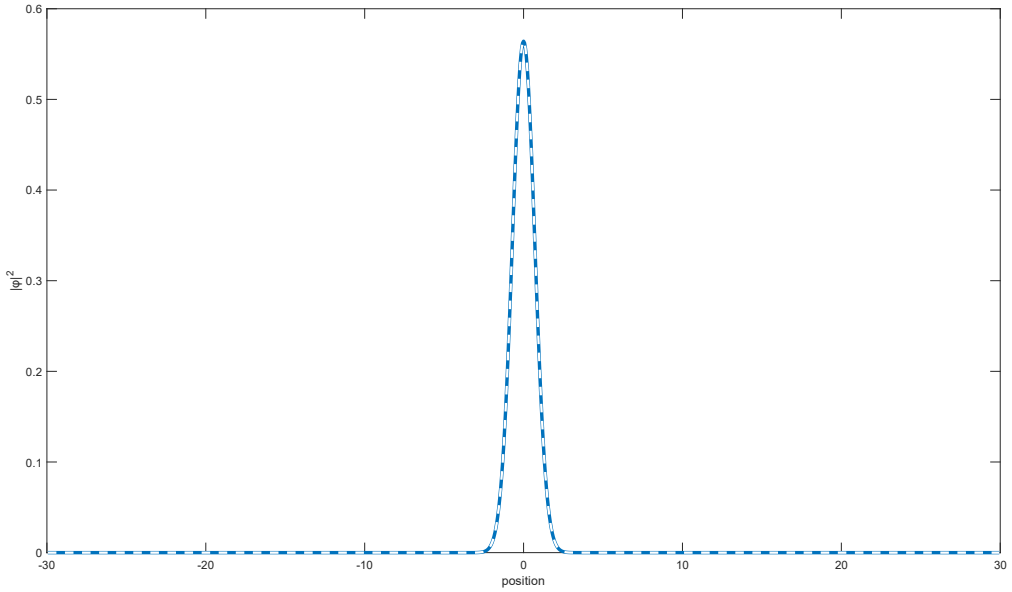
After generating these states, I extend them to N dimension for calculating inner products later.

```
vec0 = vec(1:N-1,1)./sqrt(sum(abs(vec(1:N-1,1)).^2*dx));  %ground state
psi0 = [0;vec0];      %extend to N dimension
```

II. Comparing to theoretical results

I also use Hermite polynomials to generate eigenstates in an analytical form, and compare it with the states get by DVR methods to justify the accuracy.

```
% theory
%n=0;
%Hn = hermiteH(n, X1);
%psi00 = (1/sqrt(2^n*factorial(n)*sqrt(pi)))*exp(-X1.^2/2).*Hn;
%plot (X1(1:N),abs(psi00(1:N)).^2,'LineWidth',3,'LineStyle',':')
%hold on
```



The dotted line is computed by DVR, and the blue line is the theoretical results. They match very well.

3. Transition probabilities

I. Projecting to the first excited state

This step aims to compute transition probabilities. The final state can be written into the superposition of all eigenstates, $|\psi\rangle = \sum_n C_n|\psi_n\rangle$, where $C_n = \langle\psi_n|\psi\rangle$. The transition probability is defined as $|C_n|^2$.

To calculate the transition probabilities from the ground state to the first excited state, I use `P_1=abs(psi1(1:N)'*psi(1:N)*L/N)^2;` in MATLAB code.

II. Driving frequency

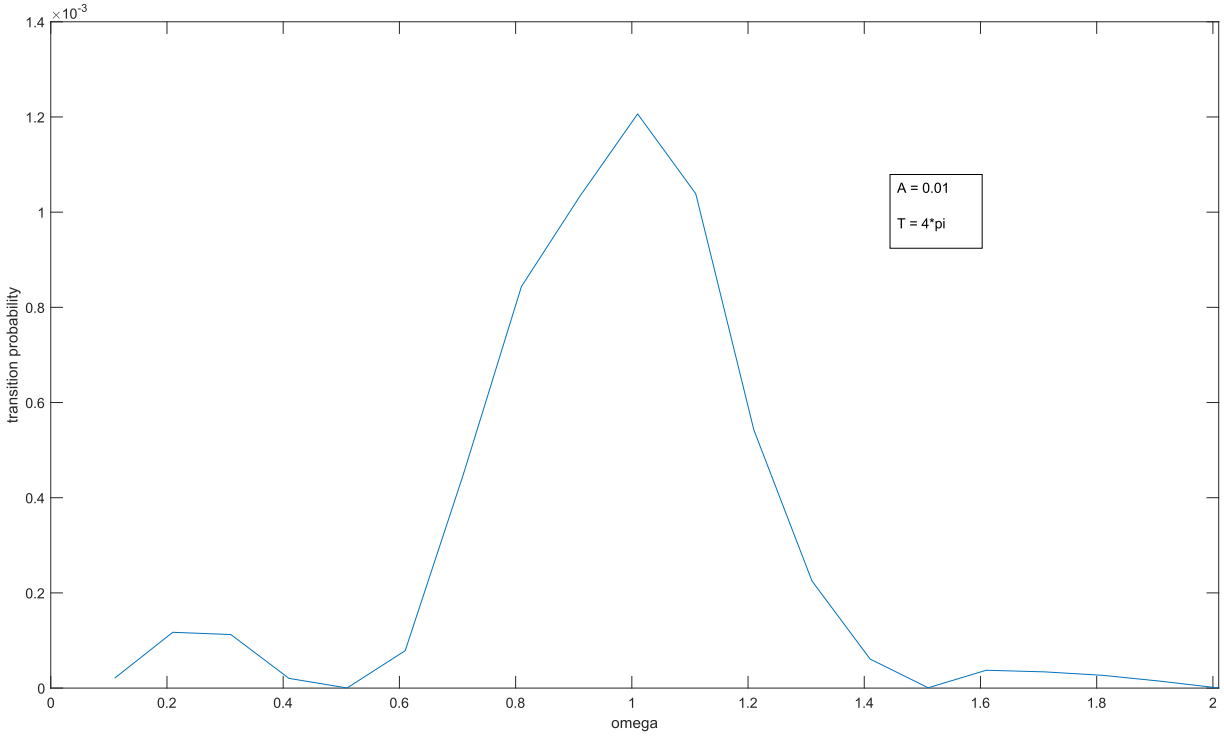
In this dimensionless form,

$$\tilde{t} = \omega_0 t$$

$$\cos\tilde{\omega}\tilde{t} = cos\tilde{\omega}\omega_0 t = cos\omega t$$

The omega defined in the code is $\frac{\omega}{\omega_0}$, which is the actual driving frequency over the system's characteristic frequency. When these are on-resonance, omega = 1.

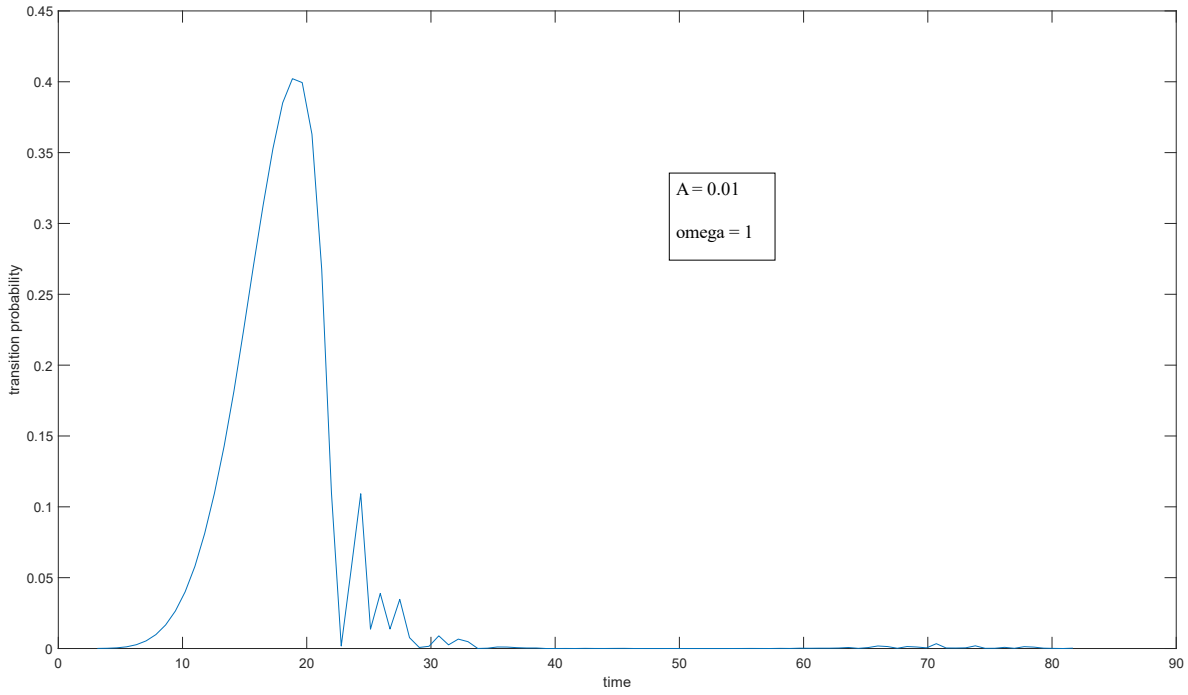
I set A=0.01, T=4π, and plot the transition probability to the change of driving frequency. The plot shows a reasonable behavior of transition probability:



When omega approaches to 1, the transition probability grows much bigger, which is corresponding to one-photon transition probability.

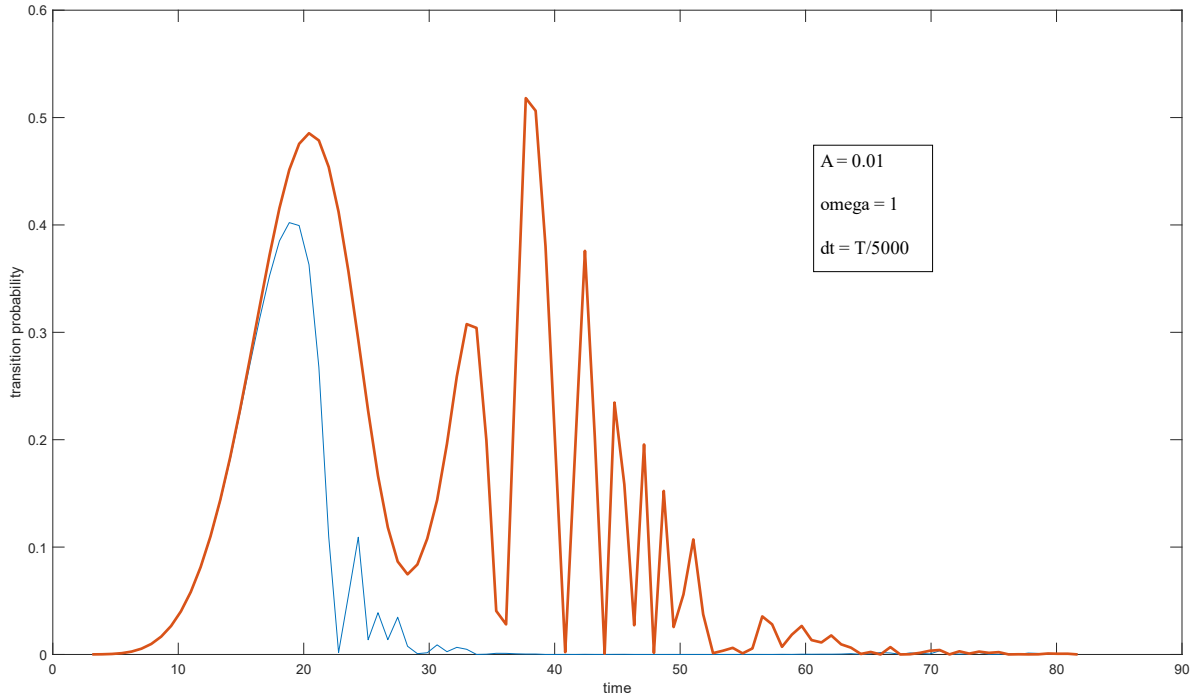
III. Time

Due to the time-periodic perturbation, the transition probability is also supposed to be time-periodic. Here I plot the time dependence of transition probability, with A=0.01, omega=1.



Near the point of on-resonance, the probability seems not be oscillating perfectly, but still have a tendency to oscillate. I assume this is because when total time increases, the time step taken in FFT method is not small enough to calculate time evolution accurately.

To justify this claim, I change the time step number 1000 into 5000, and make this plot again.



So it's indeed oscillating. In most cases to save the time for computing, I set total time to be around 4π.

4. Comparing to perturbation theory

We have calculated the transition probability using first-order perturbation theory in lecture:

$$
\begin{aligned}
P_{n\leftarrow m} &= \left(\frac{1}{\hbar}\right)^2 \left| \int_{t_0}^{t} \langle \psi_n^0 | \hat{V}(t_1) | \psi_m^0 \rangle e^{\frac{i(E_n^0 - E_m^0)(t_1 - t_0)}{\hbar}} dt_1 \right|^2 \\
&= \left| \int_0^t \langle \psi_n^0 | A \sin(\hat{x}) \cos(\omega t_1) | \psi_m^0 \rangle e^{i(E_n^0 - E_m^0)t_1} dt_1 \right|^2 \\
&= \left| A \int_{-\infty}^{\infty} \psi_n^0(x)^* \cdot \sin x \cdot \psi_m^0(x) \mathrm{d}x \int_0^t \cos(\omega t_1) e^{i(E_n^0 - E_m^0)t_1} dt_1 \right|^2
\end{aligned}
$$

I insert this computation into the FFT process:
(without and with RWA)

```
for m = 1:M
    t = m*dt;
    V_t = A * sin(X1).* cos(omega * t);
    %transition probability (1st perturbation)
    p_1=sum(psi1(1:N)'*diag(V_t(1:N))*psi0(1:N).*(L/N));
    pt=p_1*exp(1i*t)*dt;
    P1_p= P1_p+pt;
P1_perturbation_rwa=abs(P1_p)^2

%%with RWA
%V_rwa=A*sin(X1)
%p_1rwa=sum(phi1(1:N)'*diag(V_rwa(1:N))*phi0(1:N).*L/N);
%P1_rwa=p_1rwa*(exp(1i*(omega-1))-1)/(omega-1)
%P1_perturbation_rwa=abs(P1_rwa)^2
```

I. Results

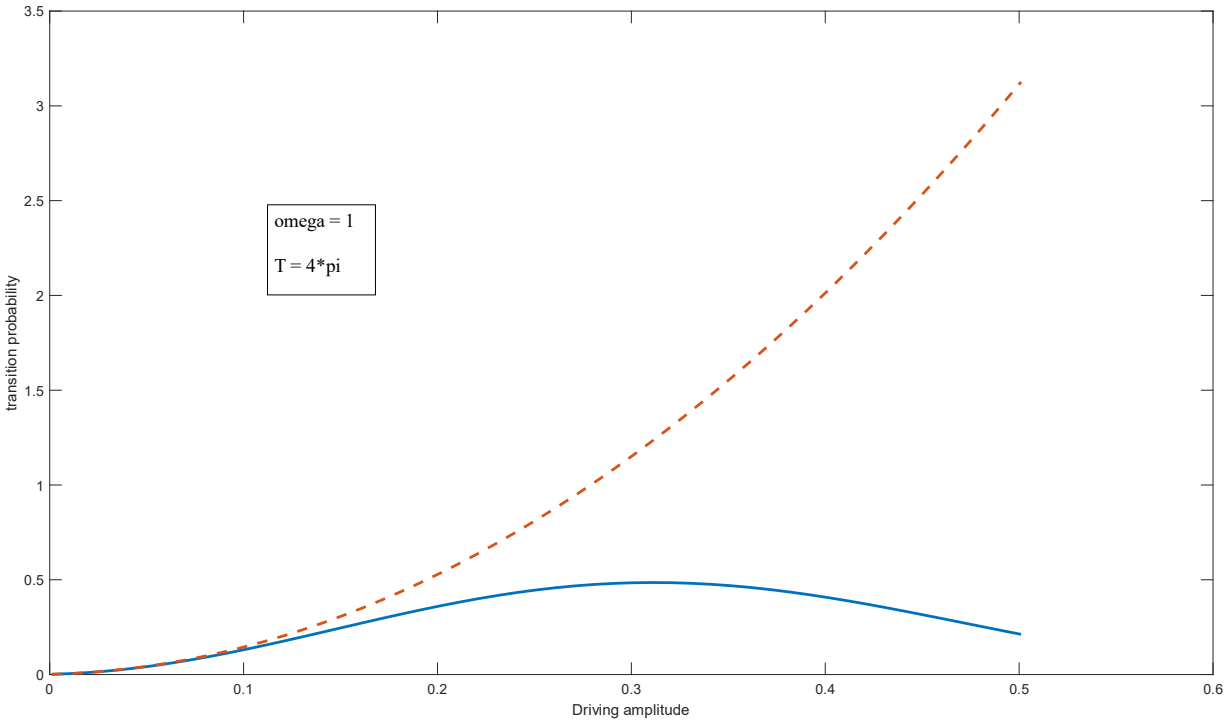
When the driving amplitude is small, which is suitable for applying perturbation theory, the transition probability is almost the same to the one we get by projecting the final state to the first excited state.

Some of the output:

```
>> transition_probability(0.001,1,pi)

ans =

   1.0e-06 *

    0.7483    0.7483

fx >>
```

```
>> transition_probability(0.01,1,2*pi)

ans =

   1.0e-03 *

    0.2992    0.2993

fx >>
```

When A is increasing, the perturbation theory is no longer work. Here I plot the change of transition probability with respect to A.



The dotted line is the probability calculated by perturbation theory. When A is large, it grows bigger than 1, which is not physical, thus the perturbation theory breaks down.

Moreover, the real transition probability seems to decrease when A is around 0.3~0.5. I have 2 assumptions:

A. When the driving amplitude is large, the system evolves easier and faster. At this point, the system has stepped over the maximum of transition probability and keeps on oscillating, so it seems decrease than before.

To justify this, I calculate the transition probability where A=0.5, but T=5π.

```
>> transition_probability(0.5,1,4*pi)

ans =

    0.2344    2.9931

>> transition_probability(0.5,1,5*pi)

ans =

    0.0389    4.6767
```

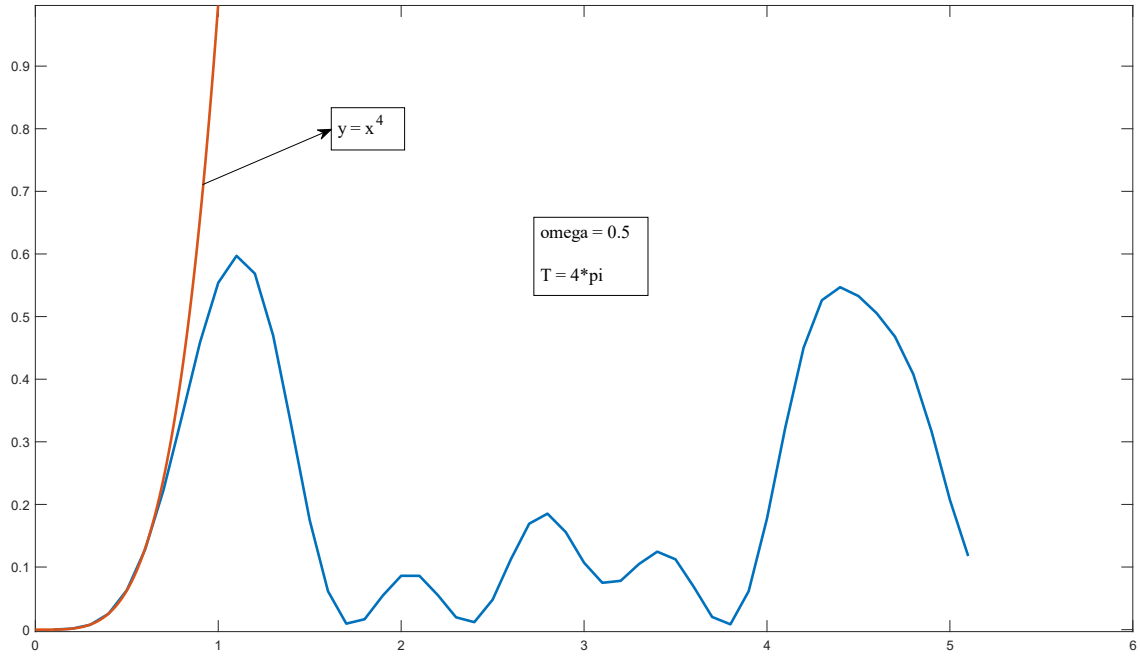
B. The large driving amplitude brings in other transition process, like many-photon process and transition between more levels, so the transition between ground state and first excited state will decrease correspondingly.

4. Two-photon process

In lecture we discussed about two-photon process. After RWA, the transition probability has a form of $\left| \sum_k \langle \psi_n{}^0 | \hat{V} | \psi_k{}^0 \rangle \langle \psi_k{}^0 | \hat{V} | \psi_m{}^0 \rangle \int_0^t dt_1 (\ldots) \right|^2$.

For fixed ω and T, the probability is proportional to A^4 (when A is small, otherwise may introduce nonlinear processes). When it's a one-photon process, this probability is proportional to A^2.

I plot the change of transition probability with respect to A when omega ≈ 0.5:



The red line is a curve fitting for the small part of A, and it fits A^4 very well.

Additionally, when omega=1, the one-photon effect is supposed to reach the maximum because of on-resonance. That is, the off-resonance one-photon transition probability is less than 0.0224 (see below, when A=1.2, T=4π). Comparing to the transition probability when omega=0.5, the much bigger probability may due to two-photon processes, instead of off-resonance one-photon process.

```
>> transition_probability(1.2,0.5,4*pi)

ans =

    0.5970    0.0000

>> transition_probability(1.2,1,4*pi)

ans =

    0.0224   17.2403
```

As the two reasonings above, the transitions are due to two-photon processes.

6. Higher excited states

In the first perturbation theory, the transition probability has a term of:

$\int_{-\infty}^{\infty} {\psi_n}^0(x)^* \cdot \sin x \cdot {\psi_m}^0(x)\,dx$. When n=2 & m=0, the two states both have an even parity.

So, the whole integrand has an odd parity, causing the transition probability from ground state to second excited state to be 0.

I check the numerical simulations:

```
>> transition_probability2(0.01,2,4*pi)

ans =

   7.6282e-21

fx >>
```

The result turned out to be close to 0, which is our expectation.

For the fourth excited state:

```
>> transition_probability4(0.01,2,4*pi)

ans =

   4.0172e-10

fx >>
```

The transition probability is much bigger than the one from ground state to second excited state.

I think this is because omega=2 satisfies the condition of two-photon transition $|0\rangle \to |4\rangle$, just like the situation in step 5.

7. Multiple driving frequencies

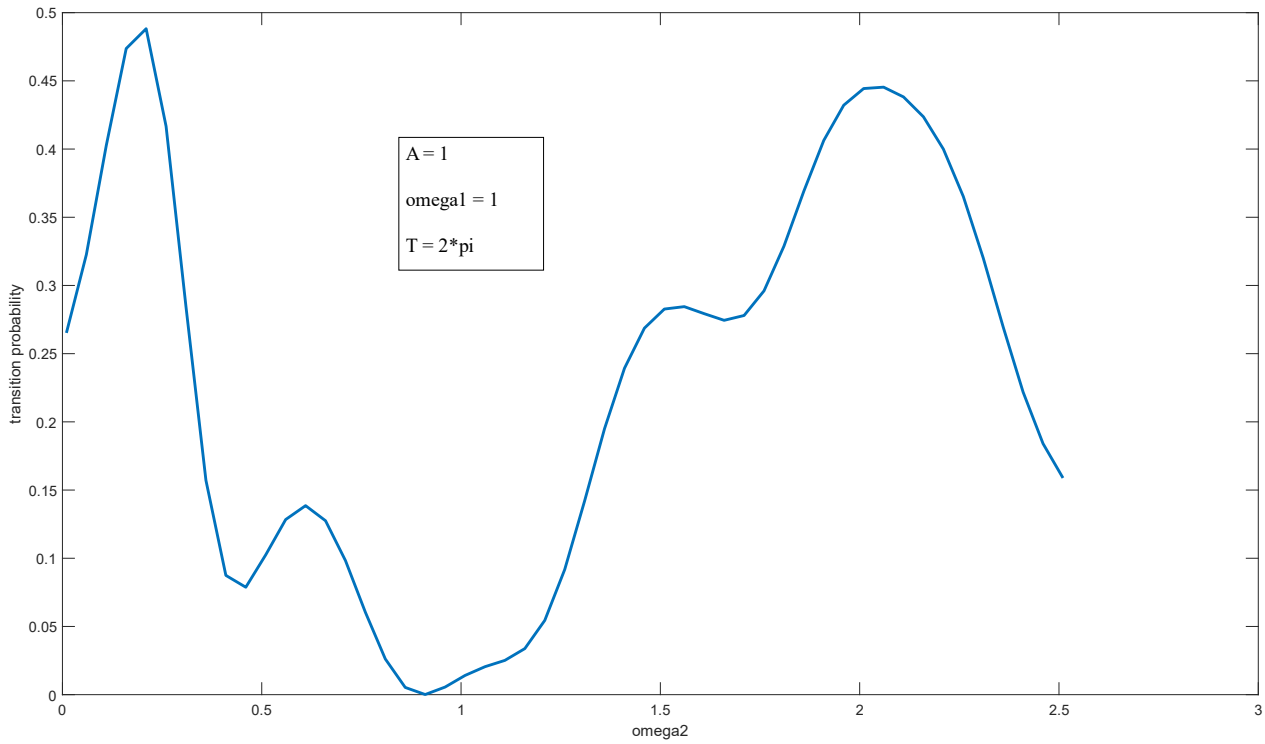
In this section I explored the situation that there are 2 driving frequencies, ω_1 and ω_2.

$$\hat{V} = A\sin(\hat{x})\cos(\omega_1 t)\cos(\omega_2 t)$$

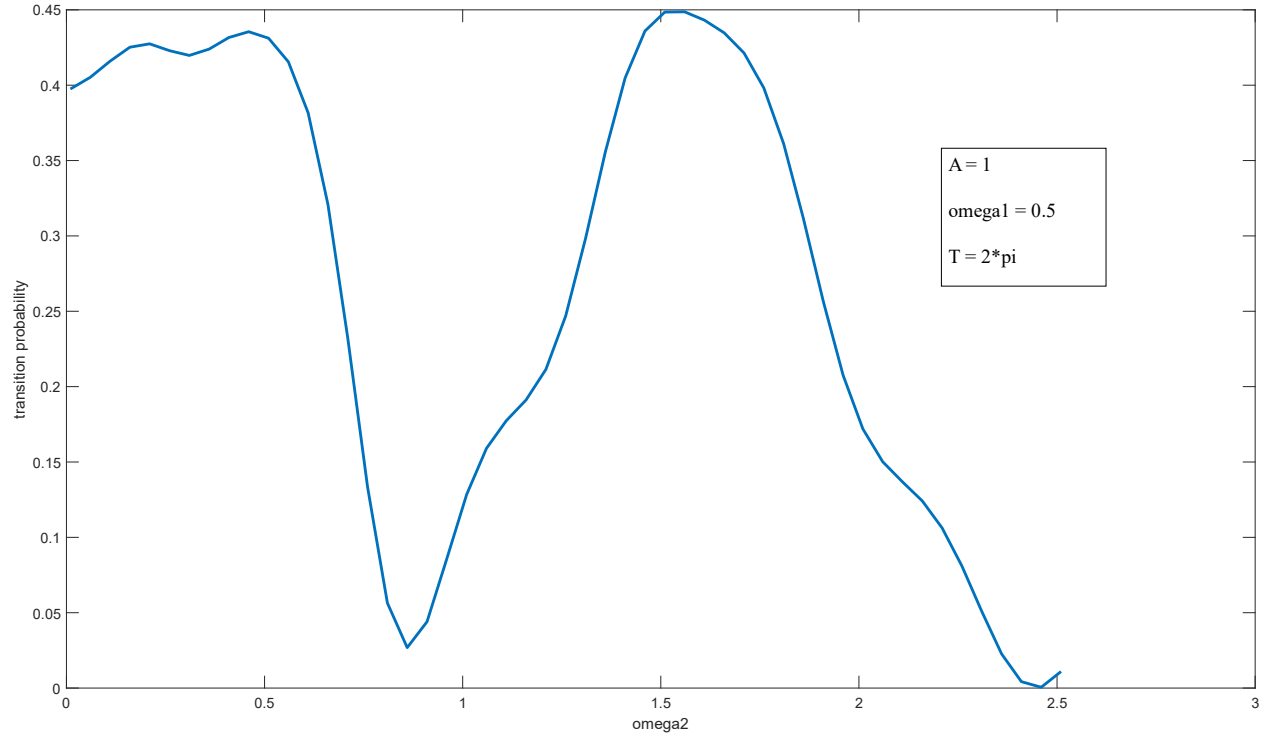
$$= \frac{1}{2}A\sin(\hat{x})\left[\cos\left((\omega_1+\omega_2)t\right)+\cos\left((\omega_1-\omega_2)t\right)\right]$$

I suppose this means two coupling photons are driving the system, so it will have many nonlinear effects. There is a high frequency part $(\omega_1+\omega_2)$ and a low frequency part $(\omega_1-\omega_2)$.

Firstly, I set one frequency to match the resonance condition, and the other frequency is used for modulation.



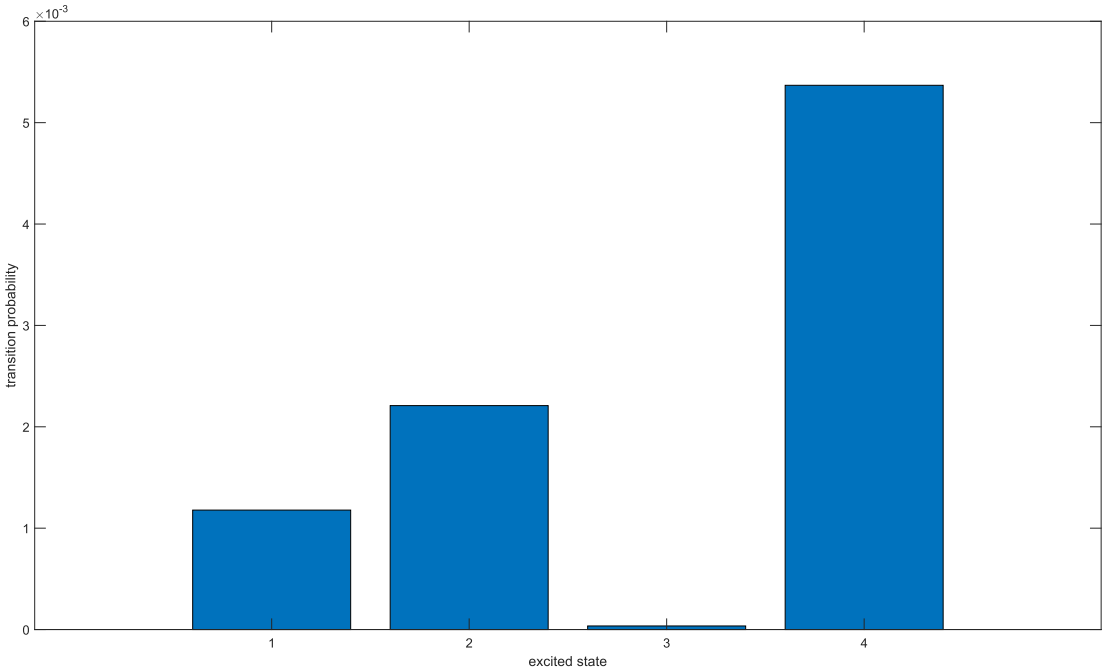
When ω_1 is already on-resonance with $|0\rangle \rightarrow |1\rangle$, the change of ω_2 may speed up evolution or cause off-resonance. There are several maximums and minimums, some are hard to tell physical meaning, but the following example is much simpler.



This plot showed roughly 2 maximum of transition probabilities, $\omega_2 = 0.5$ & 1.5, which simply is when $(\omega_1 + \omega_2)$ and $(\omega_1 - \omega_2)$ reaches on-resonance with $|0\rangle \rightarrow |1\rangle$.

Secondly, I want to check if the coupling frequency will cause multiple transition paths at same time. In particular, the high frequency part $(\omega_1 + \omega_2)$ and the low frequency part $(\omega_1 - \omega_2)$ are both on-resonance with some natural frequencies.

Here I set $\omega_1 = 1, \omega_2 = 3$, and plot the transition probabilities of 4 excited states. (A=1, T=6π)



First of all, the transition probability has an order of 10^{-3}, which is much smaller than single-frequency case (with same A and T). This means the system prefers to stay in ground state. (or have emitted photons?)

The interesting thing is, $|0\rangle \to |4\rangle$ and $|0\rangle \to |2\rangle$ seems to be the most possible paths, which is on-resonance with $(\omega_1 + \omega_2)$ and $(\omega_1 - \omega_2)$.

It's a bit strange that the probability of $|0\rangle \to |3\rangle$ is so small, since it's also on-resonance with ω_2. I think it's because in this coupling driving field, one-photon absorption effect is much weaker, and the one-photon transition probabilities from ground state to 2nd and higher excited states are already very small.

This is the end of my computational project. Important codes are in appendix.

THANKS for reading!

Appendix

```
function [P1] = transition_probability(A, omega, T)
    a = -20;
    b = +20;
    L = b-a;
    N = 10^3;
    X1 = a+L*(0:N-1)/N;         %N grid points for FFT
    X2 = a+L*(1:N-1)/N;         %N-1 for DVR
    P = (2*pi/L)*[0:N/2-1,-N/2:-1];
    M = 10^3;
    dt = T/M;
    dx = L/N;

    UV_base = exp(-1i*(X1.^2/2)*dt/2);    % One-step propagator in position space
    UT = exp(-1i*(P.^2/2)*dt);       % One-step propagator in momentum space

    % ground & first state

    % theory
    % n=0;
    % Hn = hermiteH(n, X1);
    % psi00 = (1 / sqrt(2^n * factorial(n) * sqrt(pi))) * exp(-X1.^2 / 2) .* Hn;
    %plot (X1(1:N),abs(psi00(1:N)).^2,'LineWidth',3,'LineStyle',':')
    %hold on

    %DVR method
    Tmatrix = zeros(N-1);       % Kinetic energy in DVR, (N-1)*(N-1) dimensional
    Vmatrix = (1/2)*diag(X2(1:N-1).^2);   % Potential energy in DVR
    nsum = 1:N-1;
    nsquare = (1:N-1).^2;
    c = (1/2)*(pi/L)^2*(2/N);
    for i1 = 1:N-1
        for i2 = i1:N-1
            Tmatrix(i1,i2) = c*sum(nsquare.*sin(nsum*pi*i1/N).*sin(nsum*pi*i2/N));
            Tmatrix(i2,i1) = Tmatrix(i1,i2);    % T is Hermitian
        end
    end
    Hamiltonian = Tmatrix+Vmatrix;           % Total Hamiltonian
    [vec,~] = eig(Hamiltonian);  % Eigenstates and eigenvalues
    vec0 = vec(1:N-1,1)./sqrt(sum(abs(vec(1:N-1,1)).^2*dx));  %ground state
    vec1 = vec(1:N-1,2)./sqrt(sum(abs(vec(1:N-1,2)).^2*dx));  %first excited state
    psi0 = [0;vec0]; %extend to N dimension
    psi1 = [0;vec1];
```

```
    %time evolution
    psi_tem=psi0'; %transpose if DVR
    %psi_tem=psi00
    P1_p=0;
    for m = 1:M
        t = m*dt;
        V_t = A * sin(X1).* cos(omega * t);

        %transition probability (1st perturbation)
        p_1=sum(psi1(1:N)'*diag(V_t(1:N))*psi0(1:N).*(L/N));
        pt=p_1*exp(1i*t)*dt;
        P1_p= P1_p+pt;

        %with RWA
        %V_rwa=A*sin(X1)
        %p_1rwa=sum(phi1(1:N)'*diag(V_rwa(1:N))*phi0(1:N).*L/N);
        %P1_rwa=p_1rwa*(exp(1i*(omega-1))-1)/(omega-1)

        UV_t = UV_base .* exp(-1i * V_t * dt / 2);
        psi_1 = UV_t.*psi_tem;
        phi_2 = fft(psi_1);
        phi_3 = UT.*phi_2;
        psi_3 = ifft(phi_3);
        psi_4 = UV_t.*psi_3;
        psi_tem = psi_4;
    end

    psi=psi_tem(1:N)';      %final state
    P1 = [abs(psi1(1:N)'*psi(1:N)*L/N)^2,abs(P1_p)^2];    %transition probability

    %P1_perturbation_rwa=abs(P1_rwa)^2

    % plot (X1(1:N),abs(psi(1:N)).^2,'LineWidth',2)
    % hold on
end
```

```
a = -20;
b = +20;
L = b-a;
N = 10^3;
X1 = a+L*(0:N-1)/N;        %N grid points for FFT
P = (2*pi/L)*[0:N/2-1,-N/2:-1];
M = 10^3;
T = 6*pi;
dt = T/M;

UV_base = exp(-1i*(X1.^2/2)*dt/2);    % One-step propagator in position space
UT = exp(-1i*(P.^2/2)*dt);       % One-step propagator in momentum space


% theory
psi0 = (1 / sqrt(2^0 * factorial(0) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(0, X1);
psi1 = (1 / sqrt(2^1 * factorial(1) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(1, X1);
psi2 = (1 / sqrt(2^2 * factorial(2) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(2, X1);
psi3 = (1 / sqrt(2^3 * factorial(3) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(3, X1);
psi4 = (1 / sqrt(2^4 * factorial(4) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(4, X1);
psi5 = (1 / sqrt(2^5 * factorial(5) * sqrt(pi))) * exp(-X1.^2 / 2) .* hermiteH(5, X1);


%time evolution
psi_tem=psi0;

for m = 1:M
    t = m*dt;
    A = 1;
    o1 = 1;
    o2 = 3;
    V_t = A * sin(X1).* cos(o1 * t).* cos(o2 * t);
    UV_t = UV_base .* exp(-1i * V_t * dt / 2);
    psi_1 = UV_t.*psi_tem;
    phi_2 = fft(psi_1);
    phi_3 = UT.*phi_2;
    psi_3 = ifft(phi_3);
    psi_4 = UV_t.*psi_3;
    psi_tem = psi_4;
end

psi=psi_tem(1:N)';      %final state
P1 = abs(psi1(1:N)*psi(1:N)*L/N)^2;    %transition probability
P2 = abs(psi2(1:N)*psi(1:N)*L/N)^2;
P3 = abs(psi3(1:N)*psi(1:N)*L/N)^2;
```