计算物理答案

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1 hw1

该题没有好的迭代方法，

$$X = -B^{-1}AX^2 - B^{-1}C, \tag{1}$$
$$X = \pm\sqrt{-A^{-1}BX - A^{-1}C}, \tag{2}$$
$$X = -X^{-1}A^{-1}(BX + C), \tag{3}$$
$$X = -A^{-1}(BX + C)X^{-1} \tag{4}$$

以上都不很好迭代收敛，与初始值有关。

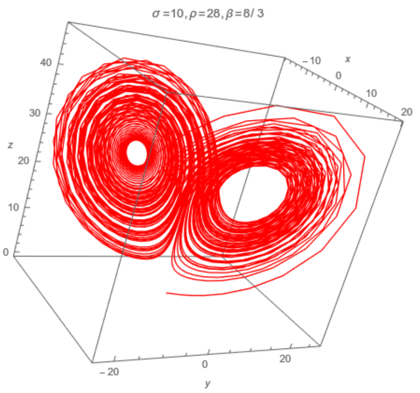
```
clear;
A = rand(3,3);
B = rand(3,3);
C = rand(3,3);
X = zeros(3,3);
N = 1000000;
for n = 1 : N
    Xn = sqrtm(-inv(A)*B*X - inv(A)*C);
    if norm(A*Xn*Xn+B*Xn+C) < 0.001
        X = Xn;
        break;
    else
        X = Xn;
    end
end

%%
clear;
A = rand(3,3);
B = rand(3,3);
C = rand(3,3);
X = rand(3,3);
N = 1000000;
for n = 1 : N
    Xn =  - inv(A)*(B*X+C)*inv(X);
    if norm(A*Xn*Xn+B*Xn+C) < 0.001
```

```
        X = Xn;
        break;
    else
        X = Xn;
    end
end

%%
clear;
A = rand(3,3);
B = rand(3,3);
C = rand(3,3);
X = rand(3,3);
N = 1000000;
for n = 1 : N
    Xn = - inv(X)*inv(A)*(B*X+C);
    if max(max(abs(Xn -X))) < 0.001
        X = Xn;
        break;
    else
        X = Xn;
    end
end
```

2 hw2

NDSolve 求解

```
s = NDSolve[{x'[t] == σ (y[t] - x[t]), y'[t] == ρ x[t] - y[t] - x[t] z[t], z'[t] == x[t] y[t] - β z[t], x[0] == y[0] == z[0] == 1} /. {σ → 10, ρ → 28, β → 8/3}, {x, y, z}, {t, 0, 100}]
    数值求解微分方程组
ParametricPlot3D[Evaluate[{x[t], y[t], z[t]} /. s], {t, 0, 100}, PlotStyle → {{Thickness[0.003], Red}}, AxesLabel → {x, y, z}, PlotLabel → "σ=10,ρ=28,β=8/3"]
绘制三维参数图      计算                                绘图样式      粗细               红色   坐标轴标签              绘图标签

{{x → InterpolatingFunction[ Domain: {{0., 100.}} Output: scalar ], y → InterpolatingFunction[ Domain: {{0., 100.}} Output: scalar ], z → InterpolatingFunction[ Domain: {{0., 100.}} Output: scalar ]}}
```

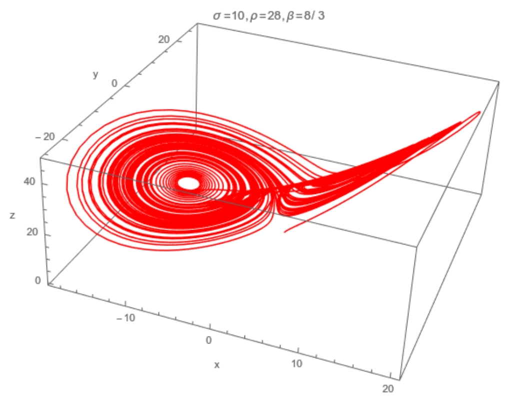


稳定点

```
FullSimplify[Solve[σ (y - x) == 0 && ρ x - y - x z == 0 && x y - β z == 0, {x, y, z}]]
完全简化      解方程

{{x → 0, y → 0, z → 0}, {x → -√β √(-1 + ρ), y → -√β √(-1 + ρ), z → -1 + ρ}, {x → √β √(-1 + ρ), y → √β √(-1 + ρ), z → -1 + ρ}}
```

欧拉迭代

```
x = 1; y = 1; z = 1; σ = 10; ρ = 28; β = 8 / 3; h = 0.01; n = 10000;
xt = Range[1, n]; yt = Range[1, n]; zt = Range[1, n];
     范围              范围              范围
Do[{x = x + h σ (y - x); y = y + h (ρ x - y - x z); z = z + h (x y - β z); xt[[t]] = x; yt[[t]] = y; zt[[t]] = z;}, {t, n}]
Do循环
ListPointPlot3D[Transpose[{xt, yt, zt}], PlotStyle → {{Thickness[0.003], Red}}, AxesLabel → {"x", "y", "z"}, PlotLabel → "σ=10,ρ=28,β=8/3"] /. Point → Line
点集的三维散点图  转置                     绘图样式      粗细               红色   坐标轴标签                    绘图标签                    点       线段
```



稳定性分析

令 $r = (x, y, z)$，$r = \tilde{r} + r^*$

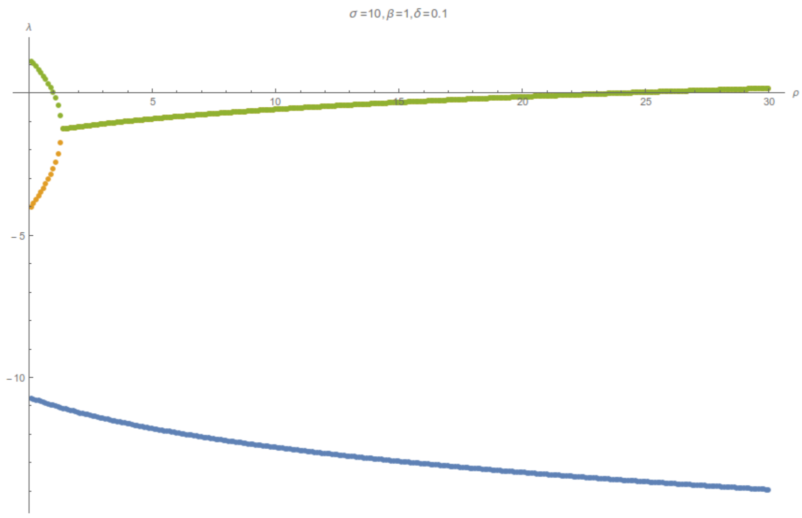
$$\frac{d}{dt}r = f(\tilde{r} + r^*) = f(r^*) + \frac{\partial f}{\partial r}|_{r=r^*} = A\tilde{r} \tag{5}$$

$$A=\begin{pmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} & \frac{\partial f_1}{\partial z} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} & \frac{\partial f_2}{\partial z} \\ \frac{\partial f_3}{\partial x} & \frac{\partial f_3}{\partial y} & \frac{\partial f_3}{\partial z} \end{pmatrix}\Bigg|_{r=r^*}=\begin{pmatrix} -\sigma & \sigma & 0 \\ \rho-z^* & -1 & -x^* \\ y^* & x^* & -\beta \end{pmatrix} \tag{6}$$

$x^*=\pm\sqrt{\beta(\rho-1)},\ y^*=\pm\sqrt{\beta(\rho-1)},\ z^*=\rho-1$

A 的三个本征值的实部都为负数，则系统在 r^* 渐近稳定，只要有一个实部为正，则系统不稳定。但如果有一个本征值实部是负数，从该方向上来看是存在稳定性，系统会绕该方向旋转，如下图

```
Clear["Global`*"]
n = 300; λ1 = Range[1, n]; λ2 = Range[1, n]; λ3 = Range[1, n]; rn = Range[0.1, 0.1 n, 0.1];
Do[
 A = {{-σ, σ, 0}, {ρ - z, -1, -x}, {y, x, -β}} /. {x → √(β (ρ - 1)), y → √(β (ρ - 1)), z → ρ - 1};
 λ = N[Eigenvalues[A /. {σ → 10, ρ → k * 0.1, β → 8 / 3}]]; λ1[[k]] = λ[[1]]; λ2[[k]] = λ[[2]]; λ3[[k]] = λ[[3]], {k, n}]
p1 = ListPlot[{Transpose[{rn, Re[λ1]}], Transpose[{rn, Re[λ2]}], Transpose[{rn, Re[λ3]}]}, PlotStyle → Automatic, AxesLabel → {"ρ", "λ"}, PlotLabel → "σ=10,β=1,δ=0.1"]
```



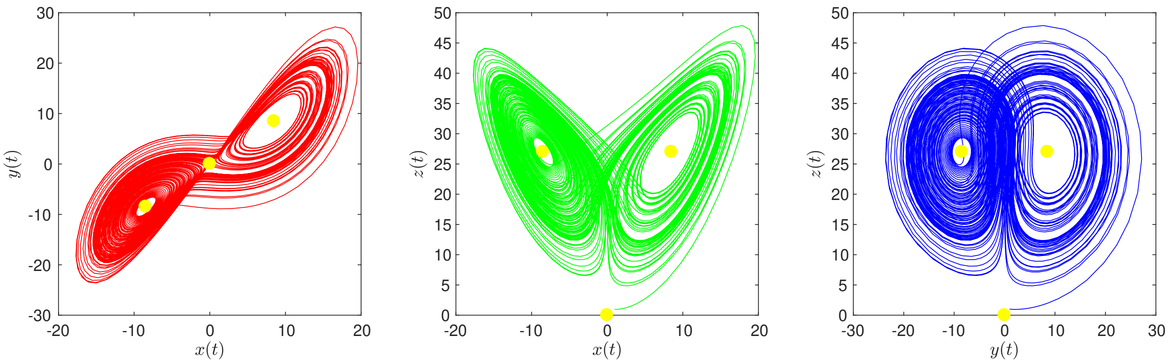


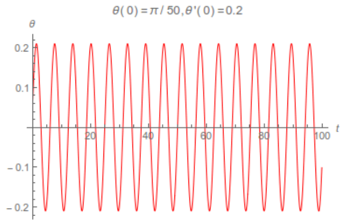
Figure 1: $\sigma=10,\ \beta=8/3,\ \rho=28$

```
sigma = 10;
beta = 8/3;
rho =28;
f = @(t,a) [-sigma*a(1) + sigma*a(2);...
 rho*a(1) - a(2) - a(1)*a(3);...
 -beta*a(3) + a(1)*a(2)];
[t,a] = ode45(f,[0 100],[1 1 1]);
% Runge-Kutta 4th/5th order ODE solver
figure;
% plot3(a(:,1),a(:,2),a(:,3));
%
% hold on;
% plot3(1,1,1,'r.','MarkerSize',15);
% hold on;
% plot3(0,0,0,'r.','MarkerSize',25);
% hold on;
% plot3(-sqrt(beta*(-1+rho)),-sqrt(beta*(-1+rho)),-1+rho,...
'g.','MarkerSize',25);
% hold on;
% plot3(sqrt(beta*(-1+rho)),sqrt(beta*(-1+rho)),-1+rho,...
'r.','MarkerSize',25);
subplot(1,3,1);
plot(a(:,1),a(:,2),'r');
hold on;
plot(0,0,'y.','MarkerSize',25);
hold on;
plot(-sqrt(beta*(-1+rho)),-sqrt(beta*(-1+rho)),'y.','MarkerSize',25);
hold on;
plot(sqrt(beta*(-1+rho)),sqrt(beta*(-1+rho)),'y.','MarkerSize',25);
xlabel(['$x(t)$'],'Interpreter','latex');
ylabel(['$y(t)$'],'Interpreter','latex');



subplot(1,3,2);
plot(a(:,1),a(:,3),'g');
hold on;
plot(0,0,'y.','MarkerSize',25);
hold on;
plot(-sqrt(beta*(-1+rho)),-1+rho,'y.','MarkerSize',25);
hold on;
plot(sqrt(beta*(-1+rho)),-1+rho,'y.','MarkerSize',25);
xlabel(['$x(t)$'],'Interpreter','latex');
ylabel(['$z(t)$'],'Interpreter','latex');

```

```
subplot(1,3,3);
plot(a(:,2),a(:,3),'b');
hold on;
plot(0,0,'y.','MarkerSize',25);
hold on;
plot(-sqrt(beta*(-1+rho)),-1+rho,'y.','MarkerSize',25);
hold on;
plot(sqrt(beta*(-1+rho)),-1+rho,'y.','MarkerSize',25);
xlabel(['$y(t)$'],'Interpreter','latex');
ylabel(['$z(t)$'],'Interpreter','latex');
```

3 hw4

```
θ0 = π / 50; ω = 0.2;
s = NDSolve[{θ''[t] + Sin[θ[t]] == 0, θ[0] == θ0, θ'[0] == ω}, θ, {t, 0, 100}]
    数值求解微分方程组      正弦
Plot[Evaluate[{θ[t]} /. s], {t, 0, 100}, PlotStyle → {Thickness[0.003], Red}, AxesLabel → {t, θ}, PlotLabel → "θ(0)=π/50,θ'(0)=0.2", PlotLegends → LineLegend["Expressions"]]
绘图 计算  绘图样式  粗细  红色  坐标轴标签  绘图标签  绘图的图例  线的图例

{{θ → InterpolatingFunction[ Domain: {{0., 100.}} Output: scalar ]}}
```



对于初始角速度和角度很小，周期近似 $T\approx 2\pi$；对于初始角速度 0，初始角度很大，$T=4\sqrt{l/g}F(\pi/2,\sin^2\dfrac{\theta}{2})$，$F$ 为第一类椭圆积分，这里可以改变数值初始条件，验证这些结果. 讨论初始角度为 0，初始角速度不为 0 的情况等等.

4 hw5

$$L=\frac{1}{2}I_\psi(\dot\psi+\dot\phi\cos\theta)^2+\frac{1}{2}I_0\left(\dot\theta^2+\dot\phi^2\sin\theta^2\right)-mgl\cos\theta \tag{7}$$

$$\frac{\partial L}{\partial\dot\psi}=p_\psi=I_\psi(\dot\psi+\dot\phi\cos\theta)=\text{const}, \tag{8}$$

$$\frac{\partial L}{\partial\dot\phi}=p_\phi=I_\psi(\dot\psi+\dot\phi\cos\theta)\cos\theta+I_0\dot\phi\sin\theta^2=\text{const} \tag{9}$$

用p_ϕ, p_ψ, θ代替$\dot\psi, \dot\phi$，得到$L=\dfrac{1}{2}I_0\dot\theta^2-V_{\text{eff}}(\theta)$，求运动方程$\dfrac{d}{dt}\dfrac{\partial L}{\partial\dot\theta}=\dfrac{\partial L}{\partial\theta}\Rightarrow I_0\ddot\theta=f(\theta)$

对于 L 中的 $\dot\psi, \dot\phi$，用 θ 代替，然后求 $\partial L/\partial\theta$ 会有问题

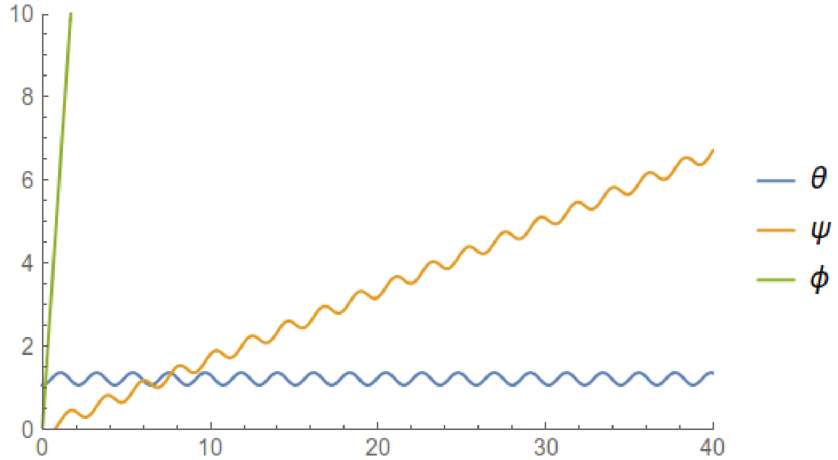
```
L = 1/2 I1 (dψ + dϕ Cos[θ])^2 + 1/2 I0 (dθ^2 + dϕ^2 Sin[θ]^2) - m g l Cos[θ];
                                                                     余弦

s = FullSimplify[Solve[{pψ == D[L, {dψ, 1}], pϕ == D[L, {dϕ, 1}]}, {dϕ, dψ}]]
    完全简化     解方程       偏导                  偏导
FullSimplify[D[L, θ] /. s]
             偏导
FullSimplify[D[L, dθ] /. s]
完全简化     偏导
```

$$\left\{\left\{d\phi\to\frac{(p\phi-p\psi\,\mathrm{Cos}[\theta])\,\mathrm{Csc}[\theta]^2}{I0},\ d\psi\to\frac{p\psi}{I1}+\frac{(-p\phi+p\psi\,\mathrm{Cos}[\theta])\,\mathrm{Cot}[\theta]\,\mathrm{Csc}[\theta]}{I0}\right\}\right\}$$

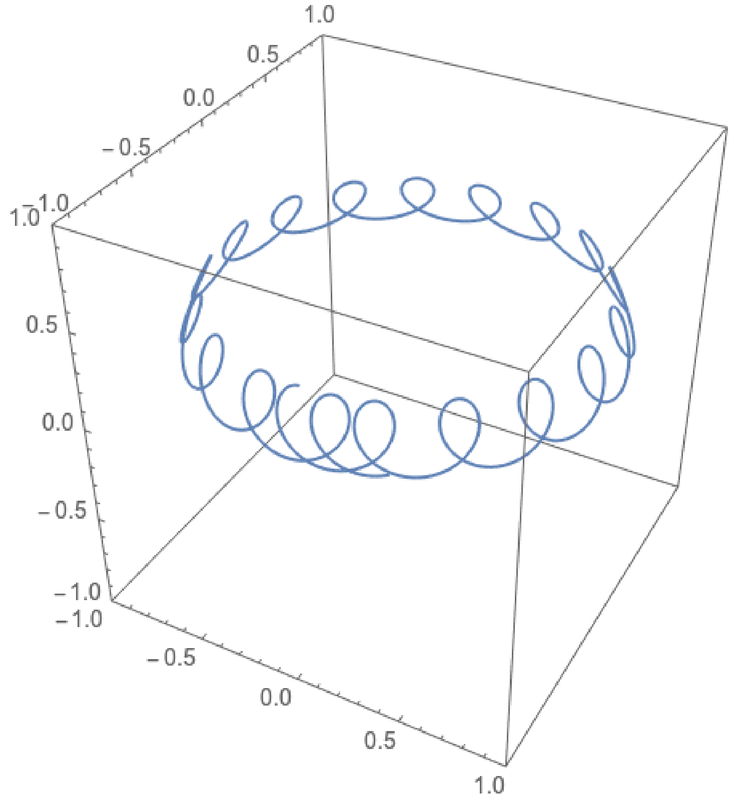
$$\left\{\frac{-p\phi\,p\psi\left(1+2\,\mathrm{Cot}[\theta]^2\right)\mathrm{Csc}[\theta]+\left(p\phi^2+p\psi^2\right)\mathrm{Cot}[\theta]\,\mathrm{Csc}[\theta]^2+g\,I0\,l\,m\,\mathrm{Sin}[\theta]}{I0}\right\}$$

$\{d\theta\ I0\}$

```
Clear["Global`*"];
m = 1; g = 10; l = 1; pψ = 60; pϕ = 25; I0 = 20; I1 = 10;
time = 40;
s =
  NDSolve[
   {I0 θ''[t] ==
     (-pϕ pψ (1 + 2 Cot[θ[t]]^2) Csc[θ[t]] + (pϕ^2 + pψ^2) Cot[θ[t]] Csc[θ[t]]^2 + g I0 l m Sin[θ[t]]) / I0,
    ϕ'[t] == (pϕ - pψ Cos[θ[t]]) Csc[θ[t]]^2 / I0, ψ'[t] == pψ/I1 + (-pϕ + pψ Cos[θ[t]]) Cot[θ[t]] Csc[θ[t]] / I0,
    θ[0] == Pi / 3, θ'[0] == 0, ϕ[0] == 0, ψ[0] == 0},
   {θ[t], ϕ[t], ψ[t]}, {t, 0, time}];
Plot[Evaluate[{θ[t], ϕ[t], ψ[t]} /. s], {t, 0, time}, PlotLegends → {"θ", "ψ", "ϕ"},
 PlotRange → {{0, time}, {0, 10}}]
ParametricPlot3D[{Sin[θ[t]] Sin[ϕ[t]], -Sin[θ[t]] Cos[ϕ[t]], Cos[θ[t]]} /. s,
 {t, 0, time}, PlotRange → {{-1, 1}, {-1, 1}, {-1, 1}}]
```



θ
ψ
ϕ



5 hw6

共振问题

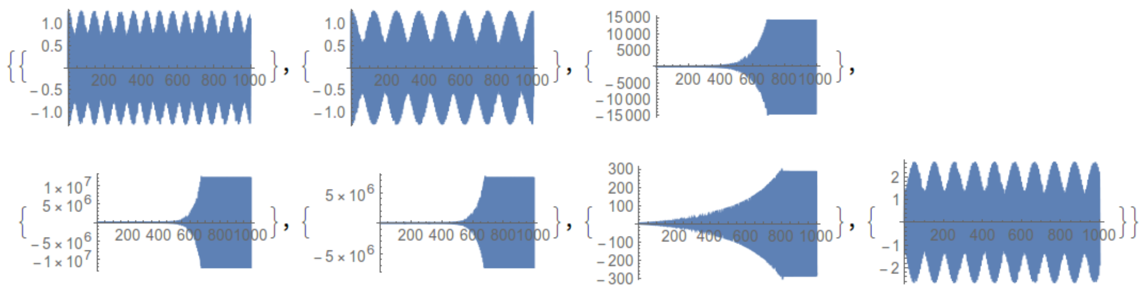
$$
\begin{cases}
\ddot{\theta}+w_0^2(t)\theta=0 \\
w_0(t)=w_0[1+\alpha\cos wt], \alpha\ll 1
\end{cases}
\tag{10}
$$

令 $w=2w_0+\varepsilon$，保留线性项

$$
\ddot{\theta}+w_0^2\left[1+2\alpha\cos\left(2w_0+\varepsilon\right)t\right]\theta=0
\tag{11}
$$

当 $|\varepsilon|<|\alpha w_0|$，系统不稳定；当 $|\varepsilon|>|\alpha w_0|$ ，系统稳定

```
fun[w_, α_, w0_] := {f = NDSolve[{θ''[t] + w0^2 (1 + α Cos[w t])^2 θ[t] == 0, θ[0] == 0, θ'[0] == 1.2}, θ, {t, 0, 1000}];
   Plot[Evaluate[θ[t] /. f], {t, 0, 1000}]};
fun[#, 0.05, 1] & /@ Range[1.9, 2.1, 0.03]
```

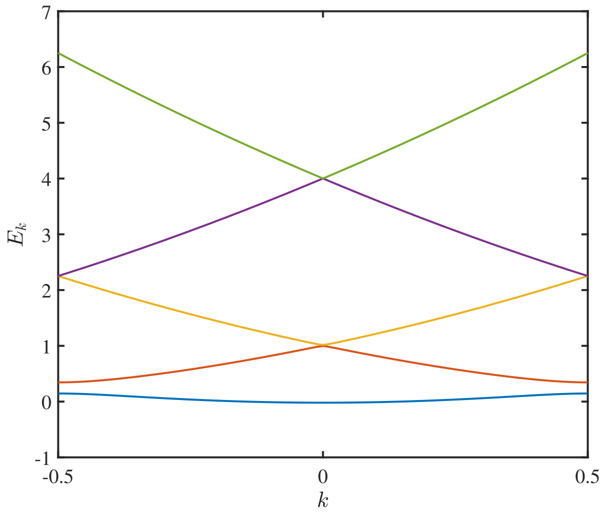


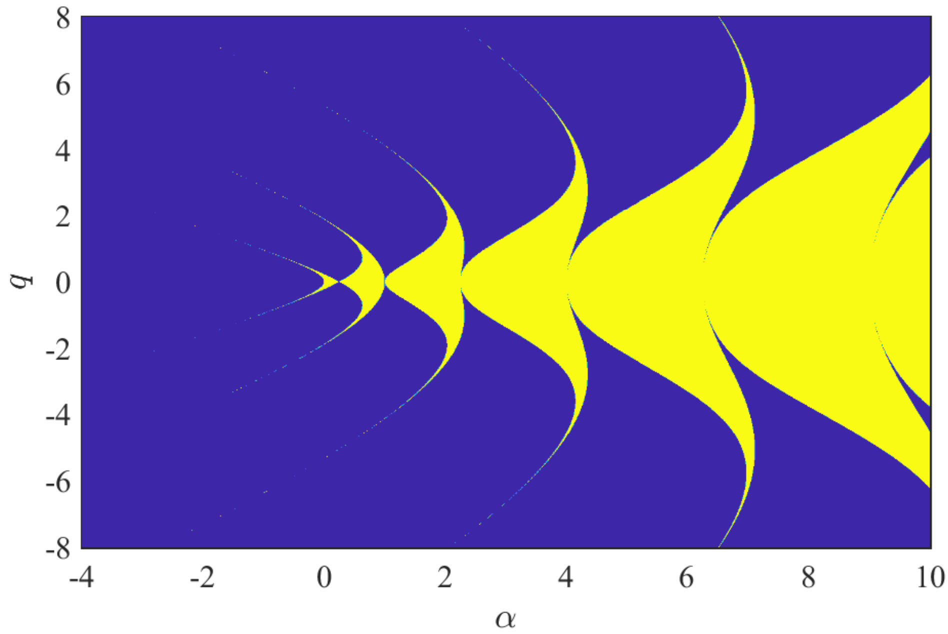
6 hw7

$$
-\frac{d^2}{dx^2}\phi-2q\cos x\phi=\varepsilon\phi
$$

$$
\begin{pmatrix}
\ddots & & & & \\
-q & (1+k)^2 & -q & & \\
 & -q & (0+k)^2 & -q & \\
 & & -q & (-1+k)^2 & -q \\
 & & & & \ddots
\end{pmatrix}
\begin{pmatrix}
\vdots \\ C_1 \\ C_0 \\ C_{-1} \\ \vdots
\end{pmatrix}
=\varepsilon
\begin{pmatrix}
\vdots \\ C_1 \\ C_0 \\ C_{-1} \\ \vdots
\end{pmatrix}
\tag{12}
$$

从矩阵的平移性可以看出 $|k|\leq 1/2$，能带图如下，$q=0.1$。对于给定 a,q，判断稳定区域，稳定对应于波函数是布洛赫波形式或者能量 a 处于能带带宽之中，不稳定对应波函数发散或者能量 a 处于能隙之中。对于判断波函数是否发散，可以给定初始波函数，把上面方程看做含时演化方程，求波函数函数，给定一定幅值限制，超过认为发散，但该方法可能比较耗时，下面是直接从能隙判断






```
clear;

N=10;
G = -N:N;
klist = -0.5:0.01:0.5;
q =0.1;

for ki = 1:length(klist)
    k = klist(ki);
    H = diag((G+k).^2,0)+...
        diag(-q*ones(1,2*N),1)+...
        diag(-q*ones(1,2*N),-1);
    band(:,ki)=eig(H);
end
plot(klist,band(1:5,:),'LineWidth',1.5);
```

```
xlabel(['$k$'],'Interpreter','latex');
ylabel(['$E_k$'],'Interpreter','latex');

fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
%%
% find stable region
clear;

N=21;
G = -N:N;
klist = -0.5:0.01:0;
qlist = -8:0.01:8;
alist = -4:0.01:10;
phase = zeros(length(qlist),length(alist));

for qi = 1:length(qlist)
    q = qlist(qi);
    band = zeros(2*N+1,length(klist));
    for ki = 1:length(klist)
        k = klist(ki);
        H = diag((G+k).^2,0)+...
            diag(-q*ones(1,2*N),1)+...
            diag(-q*ones(1,2*N),-1);
        band(:,ki) = eig(H);
    end

    bandtop = max(band');
    bandbot = min(band');

    for ai = 1:length(alist)
        a = alist(ai);
        if  sum(a < bandtop) + sum(a > bandbot) == 2*N+2
            phase(qi,ai) = 1;
        end
    end
end

[X,Y] = meshgrid(alist,qlist);
pcolor(X,Y,phase);
shading interp;
xlabel(['$\alpha$'],'Interpreter','latex');
ylabel(['$q$'],'Interpreter','latex');

```

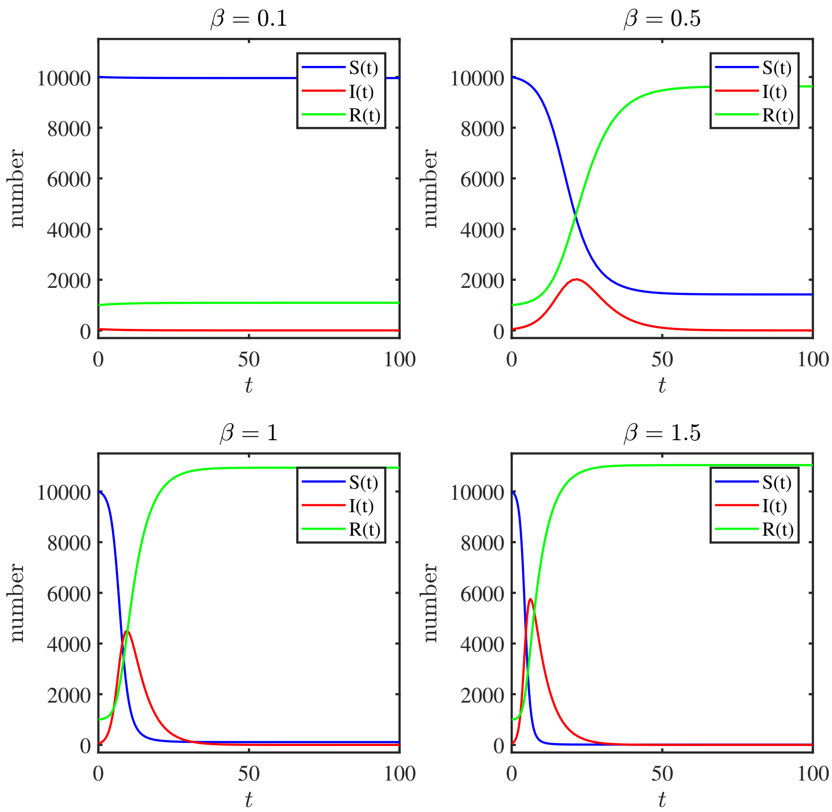
```
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
```

7 hw8

以最简单的模型为例

$$\frac{dS}{dt} = -\frac{\beta IS}{N},\ \frac{dI}{dt} = \frac{\beta IS}{N} - \gamma I,\ \frac{dR}{dt} = \gamma I \tag{13}$$

S 类，缺乏免疫力，容易受到感染；I 类，感染者，容易传播给 S 类的人；R 类，被隔离或者因治愈而具有免疫力。当 $dI/dt < 0$，则 $\beta S(0) < N\gamma$，不会引起感染病爆发




```
clear;
S = 10000;
I = 50;
R = 1000;
N = S+I+R;
gamma = 0.2;
ii = 1;
for beta = [0.1 0.5 1.0 1.5]
    f = @(t,a) [-beta*a(2)*a(1)/N;...
        beta*a(2)*a(1)/N-gamma*a(2);...
        gamma*a(2)];
    [t,a] = ode45(f,[0 100],[S I R]);

    subplot(2,2,ii);
    plot(t,a(:,1),'b','LineWidth',1.5);
    hold on;
```

```
    plot(t,a(:,2),'r','LineWidth',1.5);
    hold on;
    plot(t,a(:,3),'g','LineWidth',1.5);
    xlabel(['$t$'],'Interpreter','latex');
    ylabel('number','Interpreter','latex');
    title(['$\beta␣=' num2str(beta) '$'],'Interpreter','latex');
    legend('S(t)','I(t)','R(t)');
    ii=ii+1;
    fonts=15;
    set(gca,'FontSize',fonts);
    set(gca,'FontName','Times');
    set(gca,'LineWidth',1.5);
    ylim([-300 11500]);
end
```

8 hw9

记 $b=(b_1,b_2,\cdots)$

$$UU^\dagger=1\Rightarrow\sum_k U_{nk}U^\dagger_{km}=\sum_k U_{nk}U^*_{mk}=\delta_{nm} \tag{14}$$

$$\tilde{b}_n=\sum_k U_{nk}b_k,\ \tilde{b}^\dagger_n=\sum_k U^*_{nk}\tilde{b}^\dagger_k \tag{15}$$

利用 $[b_i,b^\dagger_j]=\delta_{ij},\ [b_i,b_j]=[b^\dagger_i,b^\dagger_j]=0$

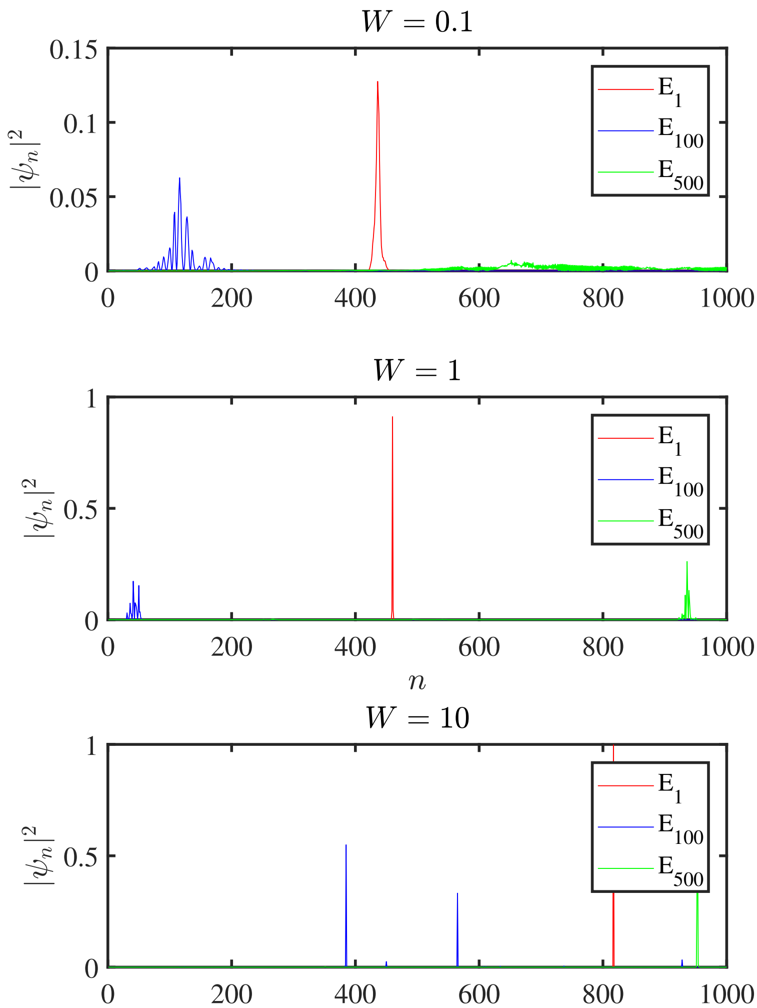
$$[\tilde{b}_n,\tilde{b}^\dagger_m]=[\sum_k U_{nk}b_k,\ \sum_p U^*_{mp}b^\dagger_p]=\sum_{kp}U_{nk}U^*_{mp}[b_k,\ b^\dagger_p]=\sum_k U_{nk}U^\dagger_{mk}=\delta_{nm} \tag{16}$$

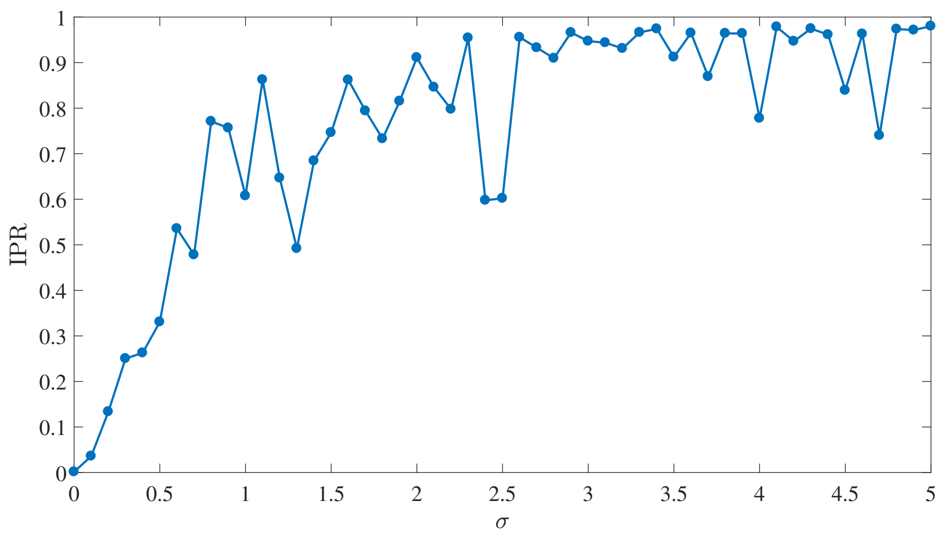
同理可证 $[\tilde{b}_i,\tilde{b}_j]=[\tilde{b}^\dagger_i,\tilde{b}^\dagger_j]=0$，费米子也是同理可证

9 hw10

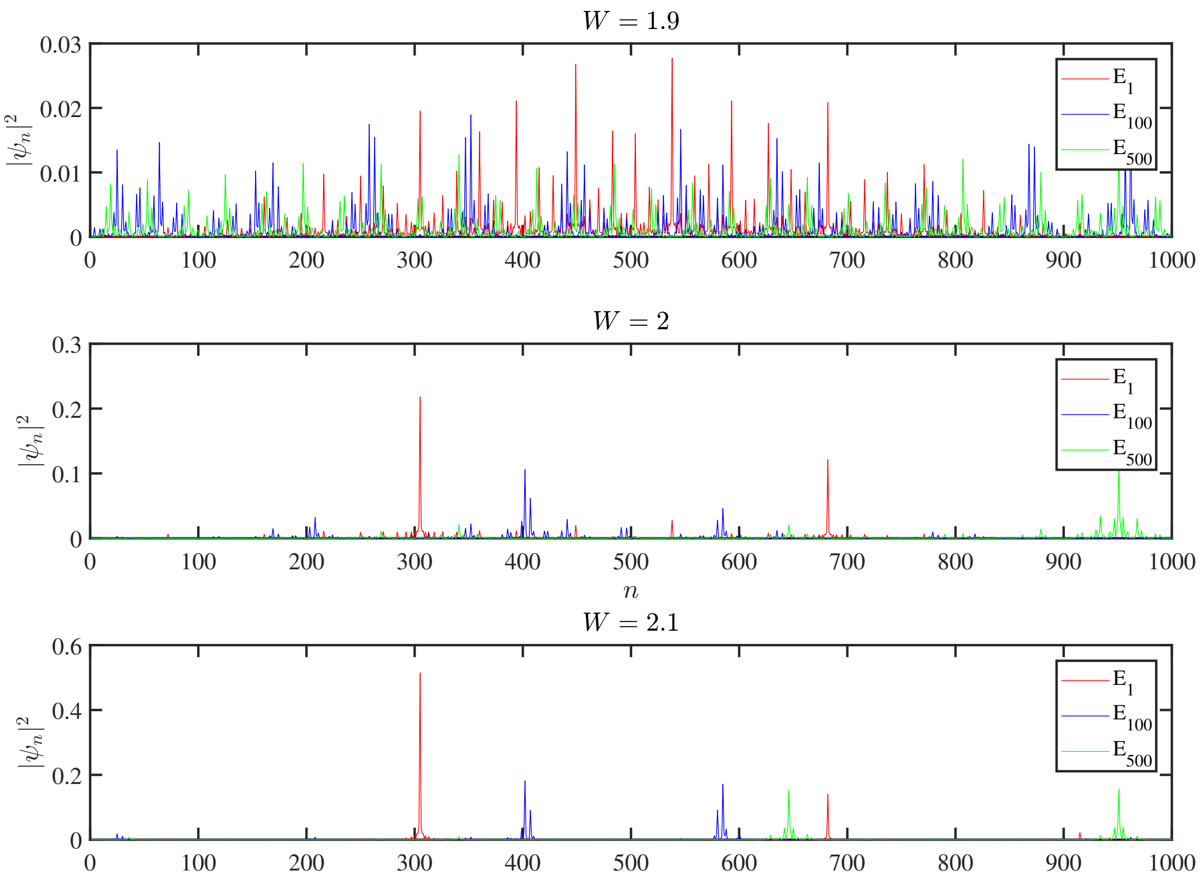
用 IPR $=\sum_n |\psi_n|^4$ 来刻画波函数的局域性，IPR$\sim$1，表示波函数局域，IPR~ 0 表示波函数扩展.

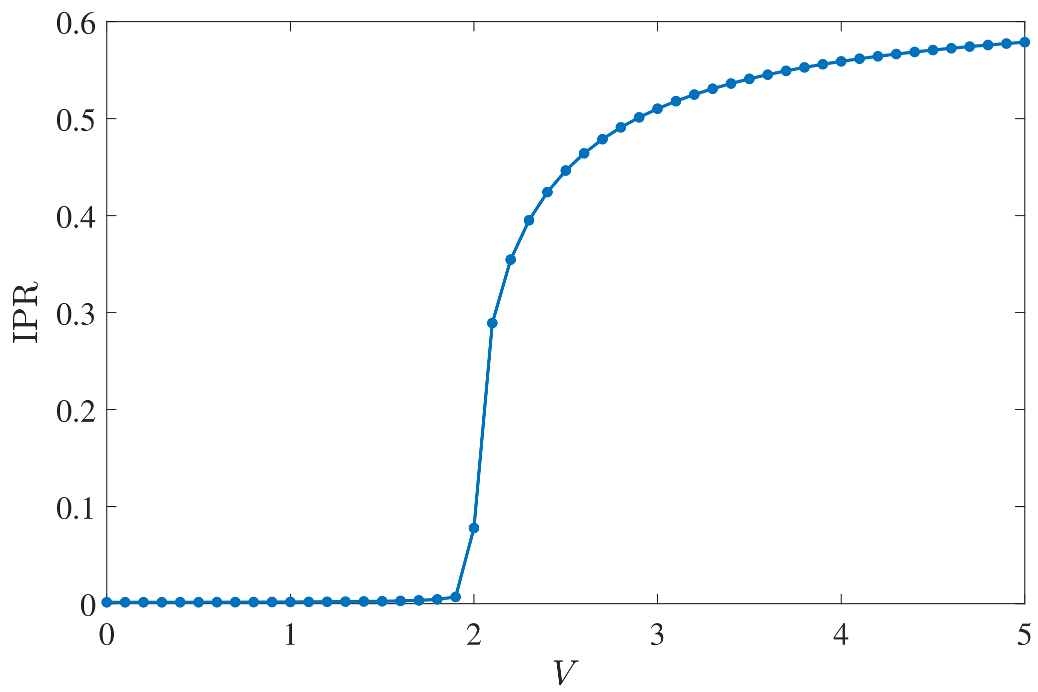
考虑高斯形无序





考虑 $V\cos 2\pi q i$ 无序，$q=(\sqrt{5}-1)/2$





扩展态到局域态的相变点在 $V=2$ $(t=1)$

```
clear;
mu = 1;
t = 1;
N = 1000;
ii=1;
si=1;
for sigma = [0.1 1 10]
    H =zeros(N,N);
    Ht = diag([t*ones(1,N-1)],-1)+...
        diag([t*ones(1,N-1)], 1);
    Hmu = diag(normrnd(0,sigma,[1,N]),0) + mu;
    H = Ht + Hmu;
    [U,E]=eig(H);

    subplot(3,1,ii);
    plot(1:N,abs(U(:,1)).^2,'r');
    hold on;
    plot(1:N,abs(U(:,100)).^2,'b');
    hold on;
    plot(1:N,abs(U(:,500)).^2,'g');
    legend('E_1','E_{100}','E_{500}');
    ii=ii+1;
    ylabel(['$|\psi_n|^2$'],'Interpreter','latex');
    title(['$W=' num2str(sigma) '$'],'Interpreter','latex');
    if ii==3
        xlabel(['$n$'],'Interpreter','latex');
    end
    fonts=15;
    set(gca,'FontSize',fonts);
    set(gca,'FontName','Times');
    set(gca,'LineWidth',1.5)
end

%%


clear;
mu = 1;
t = -1;
N = 1000;
ii=1;
si=1;
for sigma = 0:0.1:10
    H =zeros(N,N);
    Ht = diag([t*ones(1,N-1)],-1)+...
```

```
        diag([t*ones(1,N-1)], 1);
    Hmu = diag(normrnd(0,sigma,[1,N]),0) + mu;
    H = Ht + Hmu;
    [U,E]=eig(H);
    IPR(si)=sum(abs(U(:,1)).^4);
    si=si+1;
end
plot(0:0.1:10, IPR,'-');





%%%  cos(2*pi*q*i)
%%
clear;
mu = 1;
t = 1;
N = 1000;
ii=1;
si=1;
q = (sqrt(5)-1)/2;
for V = [1.9 2 2.1]
    H =zeros(N,N);
    Ht = diag([t*ones(1,N-1)],-1)+...
        diag([t*ones(1,N-1)], 1);
    Hmu = diag(V*cos(2*pi*q*[1:N]),0) + mu;
    H = Ht + Hmu;
    [U,E]=eig(H);

    subplot(3,1,ii);
    plot(1:N,abs(U(:,1)).^2,'r');
    hold on;
    plot(1:N,abs(U(:,100)).^2,'b');
    hold on;
    plot(1:N,abs(U(:,500)).^2,'g');
    legend('E_1','E_{100}','E_{500}');
    ii=ii+1;
    ylabel(['$|\psi_n|^2$'],'Interpreter','latex');
    title(['$W=' num2str(V) '$'],'Interpreter','latex');
    if ii==3
        xlabel(['$n$'],'Interpreter','latex');
    end
    fonts=15;
    set(gca,'FontSize',fonts);
    set(gca,'FontName','Times');
```

```
    set(gca,'LineWidth',1.5)
end



%%
clear;
mu = 1;
t = -1;
N = 1000;
ii=1;
si=1;
q = (sqrt(5)-1)/2;
for V = 0:0.1:10
    H =zeros(N,N);
    Ht = diag([t*ones(1,N-1)],-1)+...
        diag([t*ones(1,N-1)], 1);
    Hmu = diag(V*cos(2*pi*q*[1:N]),0) + mu;
    H = Ht + Hmu;
    [U,E]=eig(H);
    IPR(si)=sum(abs(U(:,1)).^4);
    si=si+1;
end
plot(0:0.1:10, IPR,'-');
```

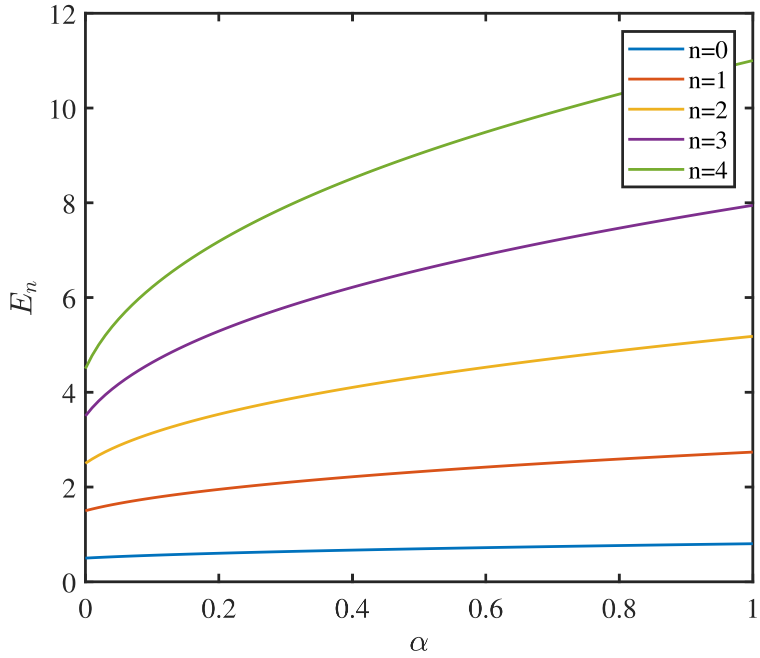
10 hw11

$$
\begin{aligned}
\left(a+a^{\dagger}\right)^{4}=&\, a^{\dagger 4}+a^{4}+2a^{\dagger 3}a+2a^{\dagger}aa^{\dagger 2}+2a^{\dagger 2}\\
&+2a^{2}a^{\dagger}a+2a^{\dagger}a^{3}+2a^{2}+a^{\dagger 2}a^{2}+a^{2}a^{\dagger 2}+2a^{\dagger}aa^{\dagger}a+4a^{\dagger}a+1
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
\left(a+a^{\dagger}\right)^{4}|n\rangle =&\sqrt{(n+4)(n+3)(n+2)(n+1)}|n+4\rangle+\sqrt{n(n-1)(n-2)(n-3)}|n-4\rangle\\
&+2(2n+3)\sqrt{(n+1)(n+2)}|n+2\rangle+2(2n-1)\sqrt{n(n-1)}|n-2\rangle\\
&+\left(6n^{2}+6n+3\right)|n\rangle
\end{aligned}
\tag{18}
$$

$$
\langle m|H|n\rangle=\langle m\left|H_{0}\right|n\rangle+\langle m|V|n\rangle \tag{19}
$$

取 $w=1,\ m=1,\ \hbar=1$




```
clear;
alist = 0:0.01:1;

N = 20;
H = zeros(N,N);
for ai = 1:length(alist)
    a = alist(ai);
    for mi = 1:N
        for ni =1:N
            m = mi−1;
            n = ni−1;
            if m == n
                H(ni,ni) = 0.5+n+(6*n^2+6*n+3)*a/4;
            end
```

```
            if m == n+4
                H(mi,ni) = a/4*sqrt((n+4)*(n+3)*(n+2)*(n+1));
                H(ni,mi) = H(mi,ni);
            end
            if m == n+2
                H(mi,ni) = a/4*(4*n+6)*sqrt((n+1)*(n+2));
                H(ni,mi) = H(mi,ni);
            end
        end
    end
    E(:,ai)=eig(H);
end
plot(alist,E(1:5,:),'LineWidth',1.5);
xlabel(['$\alpha$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
legend('n=0','n=1','n=2','n=3','n=4');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5);
```

11 hw12

Fermi-Hubbard model(spinless)

$$\begin{aligned} V &= g\int \phi^{\dagger}\left(\boldsymbol{x}_1\right)\phi^{\dagger}\left(\boldsymbol{x}_2\right)v\left(\boldsymbol{x}_1-\boldsymbol{x}_2\right)\phi\left(\boldsymbol{x}_2\right)\phi\left(\boldsymbol{x}_1\right)d\boldsymbol{x}_1 d\boldsymbol{x}_2 \\ &= g\sum_{nmkl} C_n^{\dagger}C_m^{\dagger}C_l C_k \int \varphi_n^*\left(\boldsymbol{x}_1\right)\varphi_m^*\left(\boldsymbol{x}_2\right)v\left(\boldsymbol{x}_1-\boldsymbol{x}_2\right)\varphi_k\left(\boldsymbol{x}_1\right)\varphi_l\left(\boldsymbol{x}_2\right)d\boldsymbol{x}_1 d\boldsymbol{x}_2 \end{aligned} \tag{20}$$

由于泡利不相容原理，考虑紧邻

$$\begin{cases} n\neq m & |n-m|=1 & n=k \\ k\neq l & |k-l|=1 & m=l \end{cases} \tag{21}$$

则

$$\begin{aligned} V &= U\sum_n C_n^{\dagger}C_{n+1}^{\dagger}C_{n+1}C_n \\ &= U\sum_n C_n^{\dagger}C_n C_{n+1}^{\dagger}C_{n+1} \\ &= U\sum_n N_n N_{n+1} \end{aligned} \tag{22}$$

Fermi-Hubbard model(spinful)

$$V = U\sum_{nmkl}\sum_{\sigma,\sigma'} C_{n,\sigma}^{\dagger}C_{m,\sigma'}^{\dagger}C_{l,\sigma'}C_{k,\sigma} \tag{23}$$

取 $n=m=k=l,\ \sigma'=\bar{\sigma}$

$$\begin{aligned} V &= U\sum_{n\sigma} C_{n\sigma}^{\dagger}C_{n\bar{\sigma}}^{\dagger}C_{n\bar{\sigma}}C_{n\sigma} \\ &= U\sum_{n\sigma} C_{n\sigma}^{\dagger}C_{n\sigma}C_{n\bar{\sigma}}^{\dagger}C_{n\bar{\sigma}} \\ &= U\sum_n N_{n\uparrow}N_{n\downarrow} \end{aligned} \tag{24}$$

12 hw13

2. **Fermi-Hubbard model**

(1) $H=\sum_i(-tC_i^\dagger C_{i+1}+\mathrm{h.c.})+\mu C_i^\dagger C_i+Un_{i\uparrow}n_{i\downarrow}$

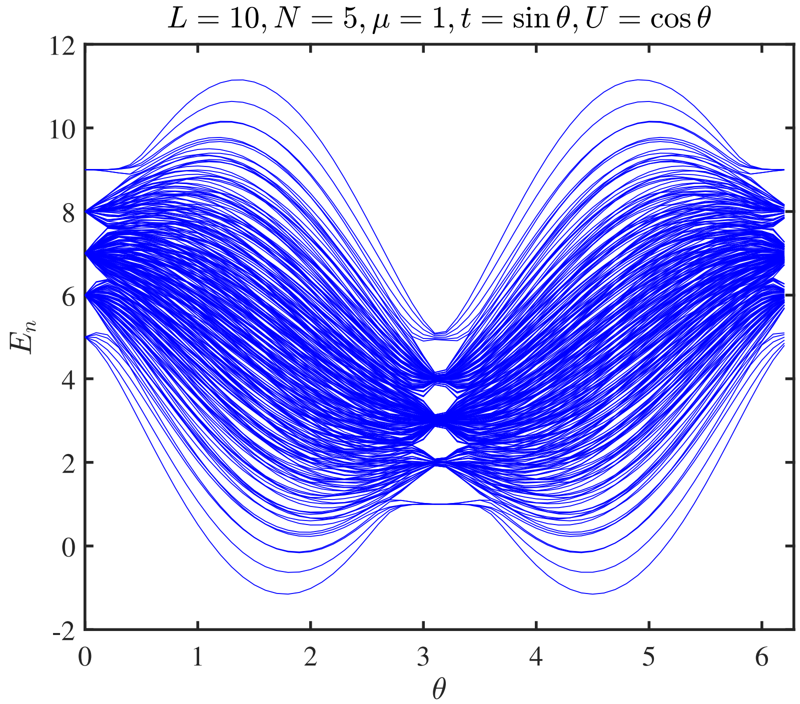
(2) Spinless F-H model (L个格子，N 个粒子)处理:

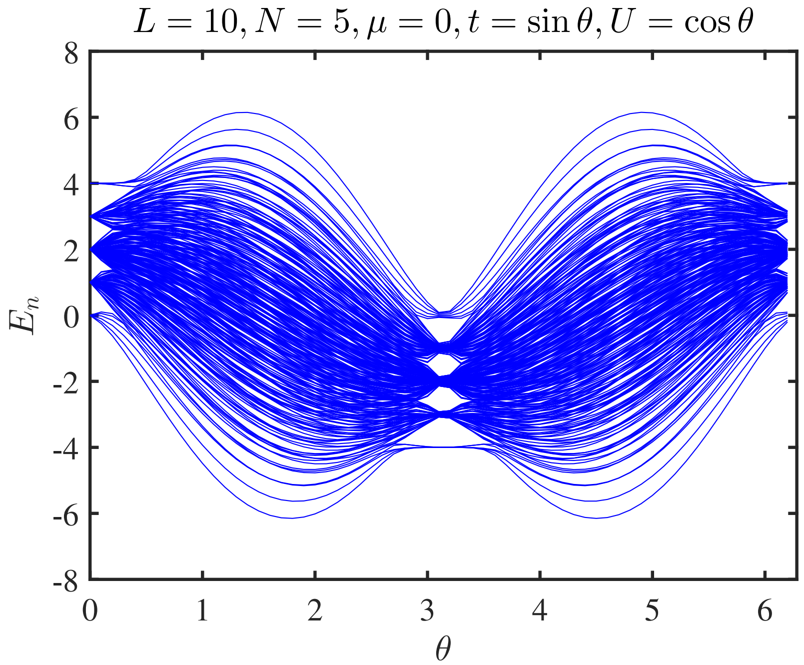
a. Hillbert-Space 的构建：二进制表$(1,2,3\cdots 2^L)$，判断1的个数是否为N，是则为基矢$|\psi_i\rangle$

b. $|\psi_i\rangle=x_1+x_2\cdot 2+\cdots+x_L\cdot 2^{L-1}$，$|\psi_j\rangle=y_1+y_1\cdot 2+\cdots+y_L\cdot 2^{L-1}$，满足$||\psi_i\rangle-|\psi_j\rangle|=2^{\alpha-1}$的$\langle\psi_i|C_\alpha^\dagger C_{\alpha+1}|\psi_j\rangle$不为0

c. $\langle\psi_i|n_\alpha n_{\alpha+1}|\psi_j\rangle=x_\alpha x_{\alpha+1}\delta_{ij}$

$$H=-t\sum_i\left(c_i^\dagger c_{i+1}+\mathrm{h.c.}\right)+\sum_i Un_in_{i+1}-\mu n_i \tag{25}$$





```
clear;
N = 5;
L = 10;
mu = 1;

tlist = 0:0.1:2*pi;

ii = 1;
for n = 0:2^L-1
    base = dec2bin(n,L);
    if sum(base-'0') == N
        basis(ii,:) = base;
        basiss(ii) = n;
        ii = ii+1;
    end
end
dim = length(basis);

Hmu =  N*diag(ones(1,dim),0);

Hu = zeros(dim,dim);
for di =1:dim
    Hu(di,di) = sum(diff(find(basis(di,:)-'0'==1))==1);
end

Ht = zeros(dim,dim);
for di = 1:dim
    for dj = di:dim
        for li = 1:L-1
            bij = abs(basiss(dj) - basiss(di));
            if abs(bij - 2^(li-1)) < 0.00001
                Ht(di,dj) = Ht(di,dj) + 1;
            end
        end
        Ht(dj,di) = Ht(di,dj);
    end
end

for ti = 1:length(tlist)
    theta = tlist(ti);
    t = sin(theta);
    U = cos(theta);
    H = mu*Hmu+(-t)*Ht+U*Hu;
    E(:,ti) = eig(H);
end
```

```
plot(tlist,E,'b');
 xlabel(['$\theta$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
title(['$L=' num2str(L) ',N=' num2str(N) ...
        ',\mu=' num2str(mu) ',t=\sin{\theta},' ...
        'U=\cos{\theta}' '$'],'Interpreter','latex');

fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0,2*pi]);
```

13 hw14

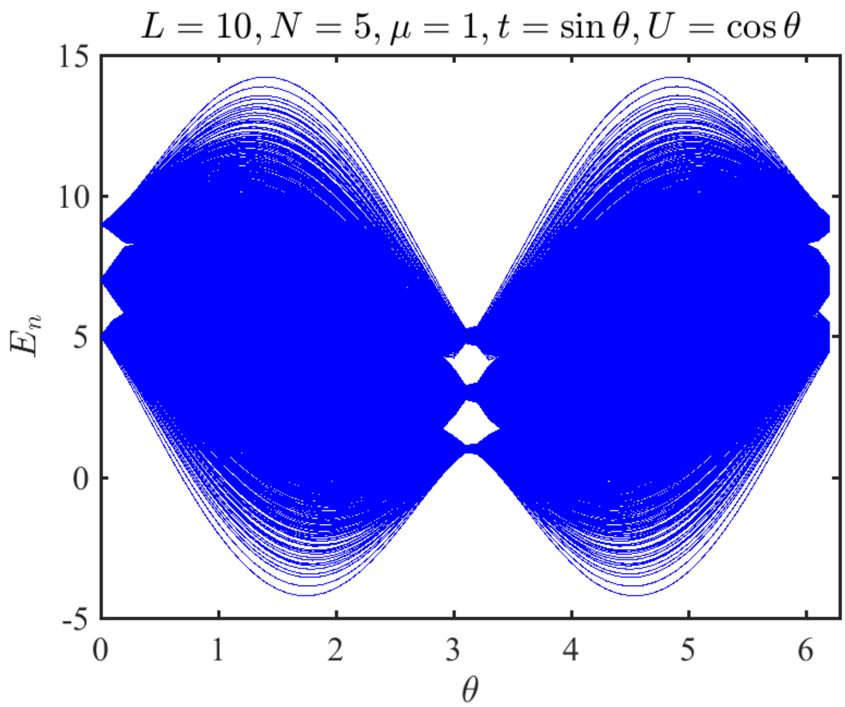
Bose-Hubbard model

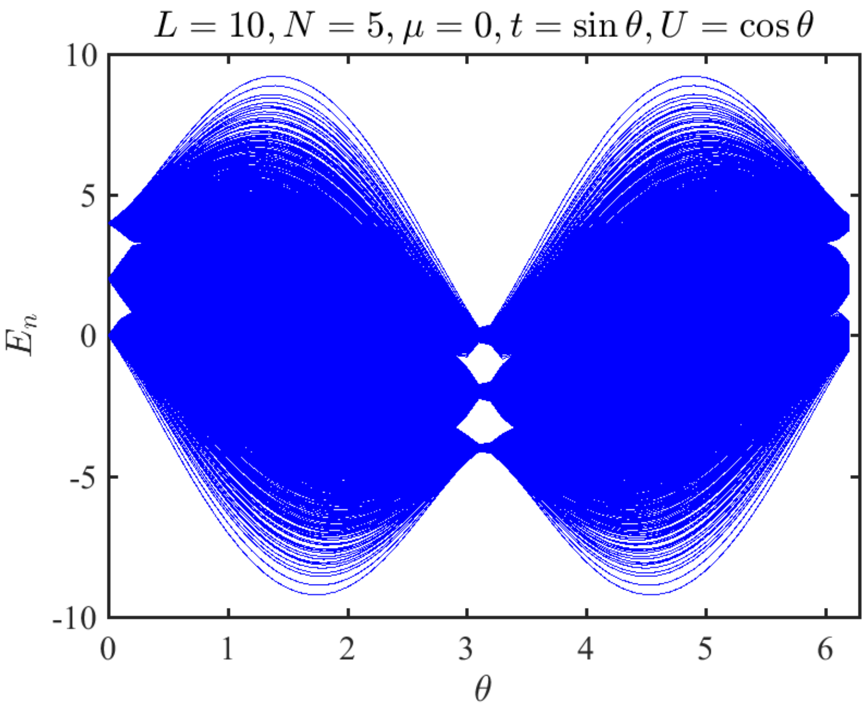
$$H=\sum_i\left(-tC_i^\dagger C_{i+1}+\text{h.c.}\right)+\mu C_i^\dagger C_i+Un_i\left(n_i-1\right) \tag{26}$$

对于 $\langle\psi_i|C_\alpha^\dagger C_{\alpha+1}|\psi_j\rangle$，不为 0 的项需满足

$$|\psi_i-\psi_j|=3^\alpha-3^{\alpha-1} \tag{27}$$

$$|\psi_i\rangle=x_1+x_2\cdot 3+\cdots+x_L\cdot 3^{L-1},|\psi_j\rangle=y_1+y_1\cdot 3+\cdots+y_L\cdot 3^{L-1} \tag{28}$$






```
clear;
N = 5;
L = 10;
mu = 1;
Q = 3;


tlist =0:0.1:2*pi;

ii = 1;
for n = 0:Q^L-1
    base = dec3bin(n,L);
    if sum(base-'0') == N
        basis(ii,:) = base;
        basiss(ii) = n;
        ii = ii+1;
    end
end
dim = length(basis);

Hmu = N*diag(ones(1,dim),0);

Hu = zeros(dim,dim);
for di =1:dim
    base = [];
    for li =1:L
        base = [base str2num(basis(di,li))];
    end
```

```
    Hu(di,di) = sum(base.*(base-1));
end

Ht = zeros(dim,dim);
for di = 1:dim
    for dj = di:dim
        for li = 1:L-1
            bij =  basiss(dj) - basiss(di);
            if abs(bij - 2*3^(li-1)) < 0.00001
                state = basis(dj,:);
                aa = sqrt(str2num(state(L-li+1))+1)*...
                     sqrt(str2num(state(L-li)));
                Ht(di,dj) = Ht(di,dj) + aa;
            end
        end
        Ht(dj,di) = Ht(di,dj);
    end
end

for ti = 1:length(tlist)
    theta = tlist(ti);
     t = sin(theta);
     U = cos(theta);
    H = mu*Hmu+(-t)*Ht+U*Hu;
    E(:,ti) = eig(H);
end
plot(tlist,E,'b');
xlabel(['$\theta$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
title(['$L=' num2str(L) ',N=' num2str(N) ...
    ',\mu=' num2str(mu) ',t=\sin{\theta},' ...
    'U=\cos{\theta}' '$'],'Interpreter','latex');

fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0,2*pi]);


function out = bin3dec( a )

out = 0;
for ii = 1:length(a)
    out = out+ str2num(a(ii))*3^(length(a)-ii);
end
```

```
end


function out = dec3bin(b,L)
out=[];
while (b>0)
    c=mod(b,3);
    out=[num2str(c) out];
    b=(b-c)/3;
end

for ii = 1:L-length(out)
    out = ['0' out];
end
end
```

14 hw15

给定 A,B, 随机产生 a, b, c, d, 作缩放 $a \to xa$, $b \to xb$, $c \to xc$, $d \to xd$, 使得满足方程 $x^2\left(a^2+b^2+c^2+d^2\right)+x^4Aabcd=B$, 解出 x，得到缩放后的 a,b,c,d 和 $f=a+b+c+d$

(A,B)	$f_{\max}$	a	b	c	d	$f_{\min}$	a	b	c	d
（1,2）	2.6818	0.6698	0.6710	0.6693	0.6717	1.4246	0.0009	0.0008	1.4142	0.0087
（1,5）	4.0000	0.9997	0.9980	1.0027	0.9996	2.2529	0.0033	0.0001	2.2360	0.0134
（3,2）	2.4897	0.6230	0.6222	0.6233	0.6213	1.4184	0.0011	0.0021	0.0009	1.4142
（3.5）	3.8726	1.2978	1.2766	0.0002	1.2980	2.2537	0.0034	2.2360	0.0043	0.0100
（8.2）	2.4492	0.0001	0.8155	0.8167	0.8169	1.4266	0.0086	0.0022	1.4142	0.0015
（8,5）	3.8724	0.0000	1.3147	1.2714	1.2862	2.2620	2.2360	0.0019	0.0030	0.0211
(20,40)	10.9469	3.8050	3.4759	3.865e-07	3.6659	4.5917	1.1468	1.1488	1.1459	1.1501

从表可以看到，最大值有两种情况，$a=b=c=d$ 或者 $a=b=c$, $d=0$; 最小值 $a=b=c=0, d\neq 0$

代入方程 $(a^2+b^2+c^2+d^2)+Aabcd=B$

$$\begin{cases} \text{当 } 0<AB<\dfrac{64}{9} \quad f_{\max}=4\sqrt{\dfrac{-2+\sqrt{4+AB}}{A}} \quad a=b=c=d=\sqrt{\dfrac{-2+\sqrt{4+AB}}{A}} \\ \text{当 } AB>\dfrac{64}{9} \quad f_{\max}=\sqrt{3B} \quad a=b=c=\sqrt{\dfrac{B}{3}} \quad d=0 \end{cases} \tag{29}$$

$$AB<192,\ f_{\min}=\sqrt{B} \quad a=\sqrt{B} \quad b=c=d=0 \tag{30}$$

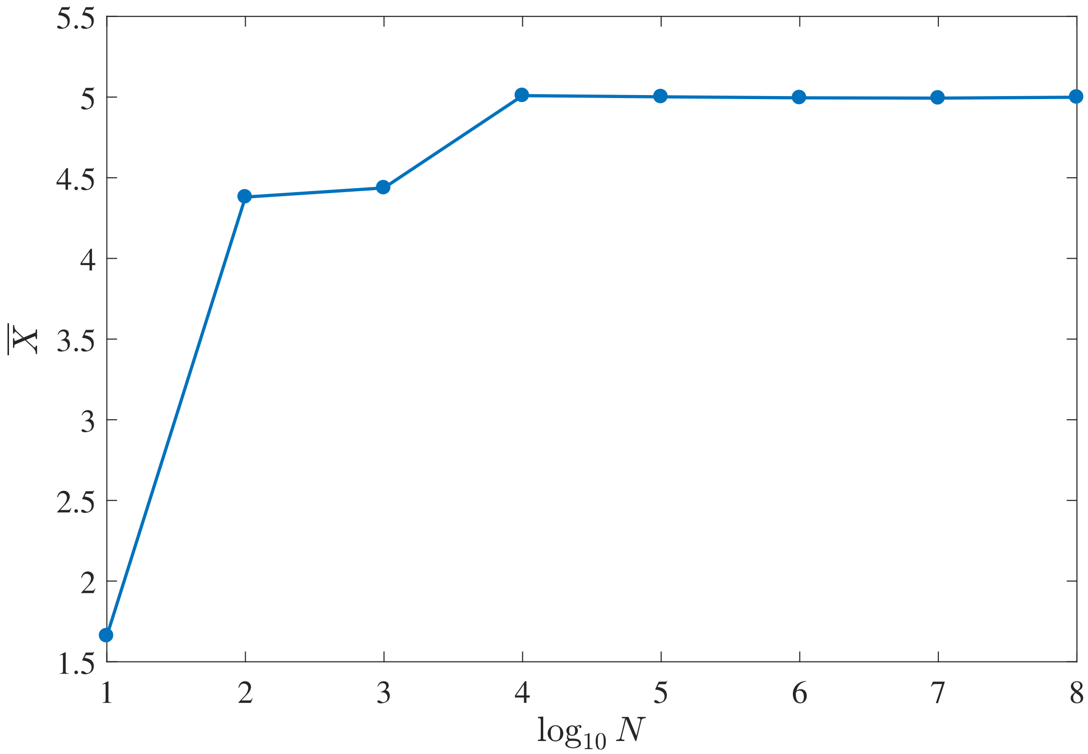
$$AB>192,\ f_{\min}=4\sqrt{\frac{-2+\sqrt{4+AB}}{AB}},\ a=b=c=d \tag{31}$$

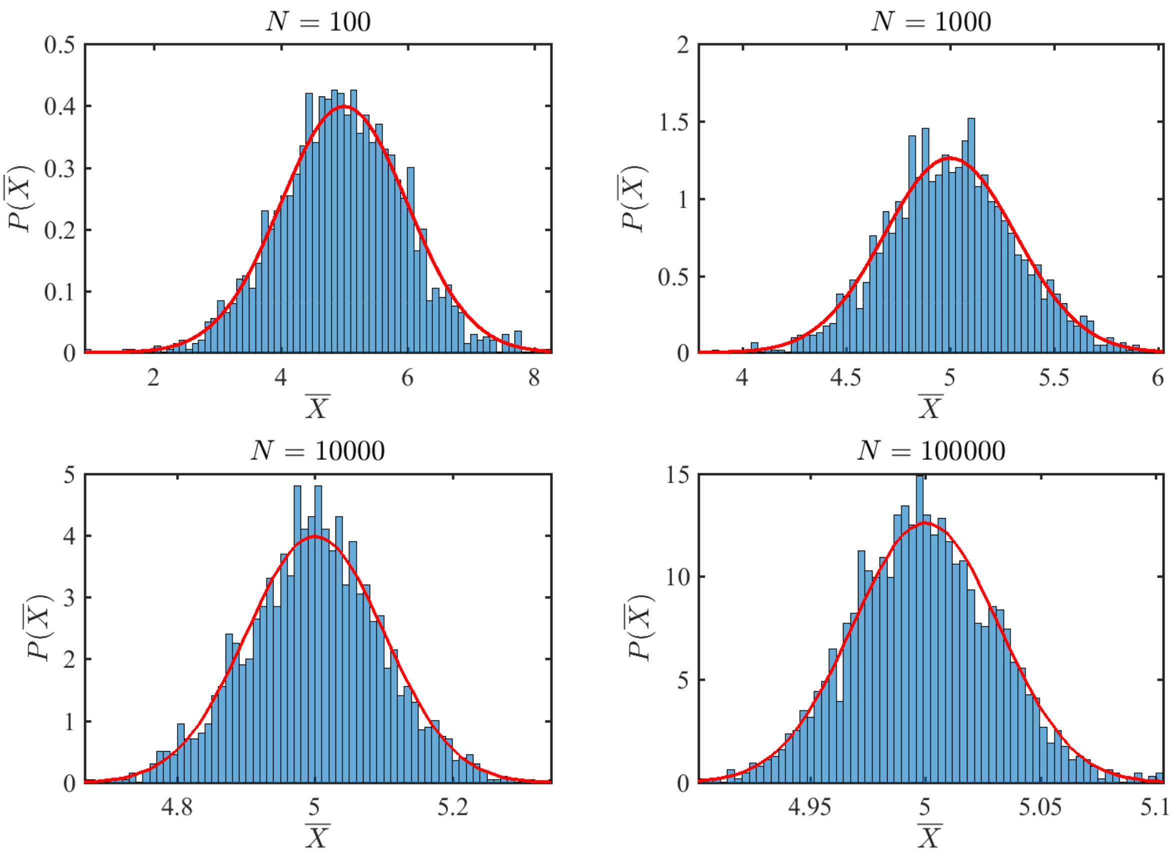
```

clear;
N = 10000000;
ii = 1;
for A = [1 3 8]
    for B = [2 5]
        a = rand(1,N);
        b = rand(1,N);
        c = rand(1,N);
        d = rand(1,N);
        p = a.^2 + b.^2 + c.^2 +d.^2;
        q = a.*b.*c.*d;
        xx = (-p + sqrt(p.^2 + 4.*A.*B.*q))./(2.*A.*q);
        x = sqrt(xx);
        f  = x.*(a + b + c + d);
        [fmax(ii),numax] = max(f);
        abdcmax(ii,:) = x(numax).*[a(numax), b(numax), c(numax), d(numax)];
        [fmin(ii),numin] = min(f);
        abcdmin(ii,:) = x(numin).*[a(numin), b(numin), c(numin), d(numin)];
        ii=ii+1;
```

```
        end
end
```

15 hw16

简单来说，记 $Y=(X_1+X_2+\cdots+X_N)$，当实验次数 N 足够多，N 次实验的平均值 Y 趋于期望值 μ (即大数定理)；N 次实验的平均值 Y 会服从正态分布，$P(Y)\sim e^{-(Y-\mu)^2/(2\sigma^2/N)}$ (中心极限定理)，σ 是分布 $P(X)$ 的标准差。





```
clear;
a = [];
for n = 10.^[1:8]
    a =[a mean(normrnd(5,10,[1,n]))];
end

% plot(1:8,a,'o');

ii = 1;
m = 2000;
for n = 10.^[2:5]
    dn = 1/sqrt(n);
    b(ii,:) = mean(normrnd(5,10,[n,m]));
    subplot(2,2,ii);
    histogram(b(ii,:),[-5:dn:10],'Normalization','pdf');
    hold on;
    x = -5:dn:15;
    A = 1/sqrt(2*10^2*pi/n);
    plot(x,A*exp(-(x-5).^2/(2*10^2/n)),'r');
    xlim([min(b(ii,:)) max(b(ii,:))]);
    ii = ii+1;

    xlabel(['$\overline{X}$'],'Interpreter','latex');
    ylabel(['$P(\overline{X})$'],'Interpreter','latex');
    title(['$N = ' num2str(n) '$'],'Interpreter','latex');

    fonts=15;
    set(gca,'FontSize',fonts);
    set(gca,'FontName','Times');
    set(gca,'LineWidth',1.5)
end
```

16 hw17

差分法

$$\frac{d^2 f}{dx^2} = \frac{f(x+h) + f(x-h) - 2f(h)}{h^2} + O\left(h^2\right) \tag{32}$$

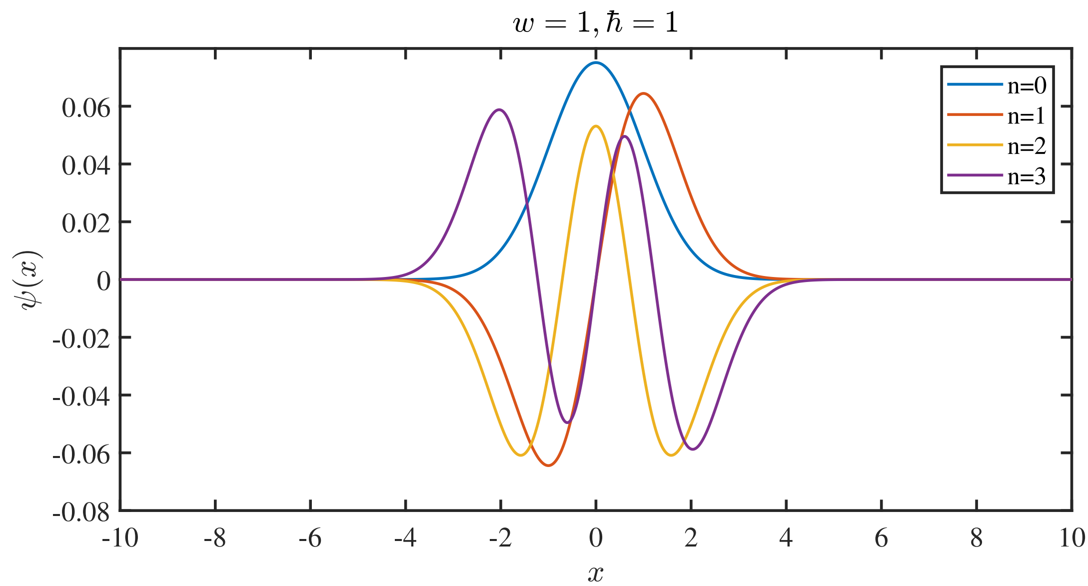
对于

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\omega^2 x^2,\ m = 1,\ \hbar = 1 \tag{33}$$

离散化

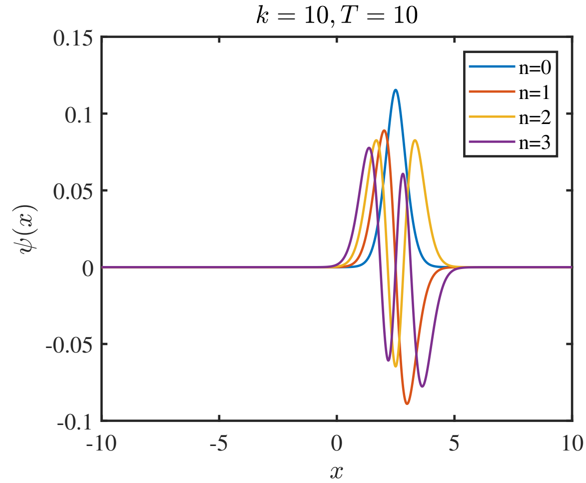
$$\begin{aligned} H\psi_n &= -\frac{1}{2}\frac{d^2\psi_n}{dx_n^2} + \frac{1}{2}\omega^2 x_n^2 \psi_n \\ &= -\frac{1}{2h^2}\left(\psi_{n+1} + \psi_{n-1} - 2\psi_n\right) + \frac{1}{2}\omega^2 (nh)^2 \psi_n \\ &= E\psi_n \end{aligned} \tag{34}$$

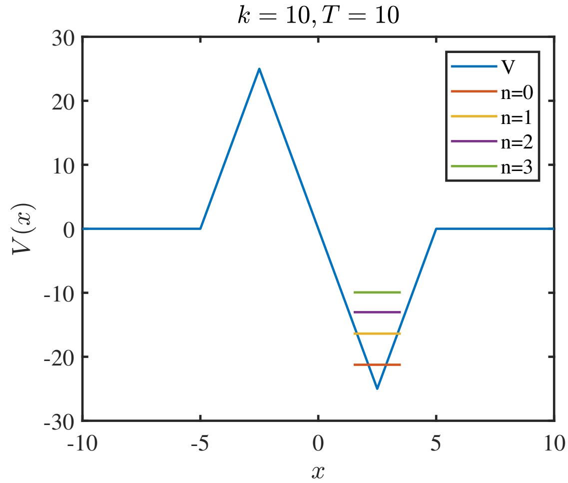
$$\begin{aligned} &H = T + V \\ &= -\frac{1}{2h^2}\begin{pmatrix} \ddots & \ddots & \ddots & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \end{pmatrix} + \begin{pmatrix} \ddots & & \\ & \frac{1}{2}w^2(nh)^2 & \\ & & \ddots \end{pmatrix} \end{aligned} \tag{35}$$

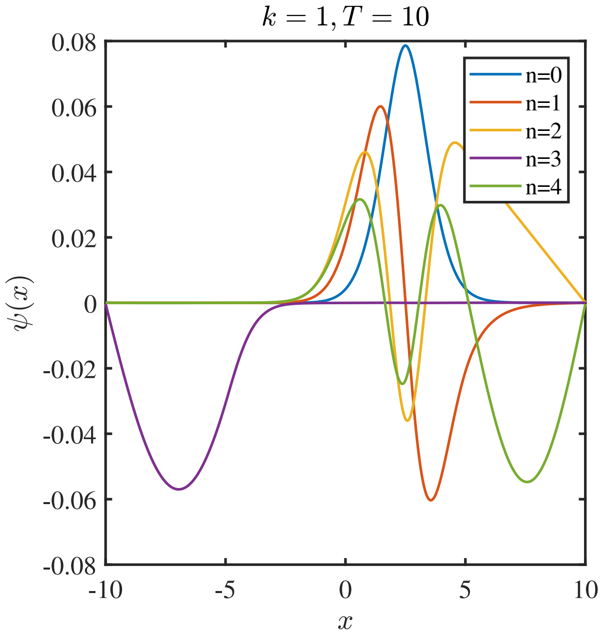


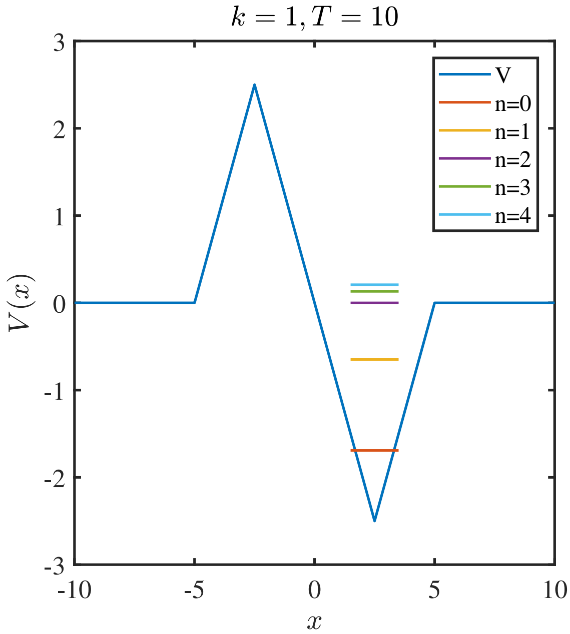
可验证波函数奇偶宇称和能级能量，$E_n = \hbar w(n + 1/2)$
三角势

$$V(x) = \begin{cases} 0, & x < -T/2 \\ kx + kT/2, & -T/2 \le x \le -T/4 \\ -kx, & -T/4 \le x \le T/4 \\ kx - kT/2, & T/4 \le x \le T/2 \\ 0, & X > T/2 \end{cases} \tag{36}$$









对于 $k=1$, 能级 $n=3,4$，已经高于势阱，波函数会隧穿该三角势，不是衰减函数，差分法对于这些态应该是失效的；对于 $k=10$，势阱较深，束缚态与谐振子波函数相似。

```
%% V = 1/2 * W^2 * x^2
clear;
h = 0.01;
N = 1000;
w=1;

Ht = (diag(ones(1,2*N+1)*(-2),0) +...
      diag(ones(1,2*N),-1) +...
      diag(ones(1,2*N), 1))*(-1/(2*h^2));

Hv = diag( ((-N:N).*h).^2*w^2/2, 0);

H = Ht + Hv;
[U,E]=eig(H);

plot((-N:N)*h,U(:,1:4),'LineWidth',1.5);
```

```
xlabel(['$x$'],'Interpreter','latex');
ylabel(['$\psi(x)$'],'Interpreter','latex');
title(['$w=1,\hbar=1$'],'Interpreter','latex')
legend('n=0','n=1','n=2','n=3');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5);

%% V = kx, -kx...

clear;
k = 1;
T = 10;
h = 0.01;
N = 1000;

V = zeros(1,2*N+1);
Ht = (diag(ones(1,2*N+1)*(-2),0) +...
      diag(ones(1,2*N),-1) +...
      diag(ones(1,2*N), 1))*(-1/(2*h^2));

for ni = 1:2*N+1
    x = (ni-1-N)*h;
    if x < -T/2 | x > T/2
        V(ni) = 0;
    elseif x >= -T/2 & x <= -T/4
        V(ni) = k*x +k*T/2;
    elseif x >= -T/4 & x <= T/4
        V(ni) = -k*x;
    elseif x >= T/4 & x <= T/2
        V(ni) = k*x - k*T/2;
    end
end
Hv = diag(V,0);
H = Ht + Hv;
[U,E]=eig(H);

subplot(1,2,1);
plot((-N:N)*h,U(:,1:5),'LineWidth',1.5);
xlabel(['$x$'],'Interpreter','latex');
ylabel(['$\psi(x)$'],'Interpreter','latex');
legend('n=0','n=1','n=2','n=3','n=4');
title(['$k=' num2str(k) ',T=' num2str(T) '$'],'Interpreter','latex')
fonts=15;
set(gca,'FontSize',fonts);
```

```
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5);

subplot(1,2,2);
plot((-N:N)*h,V,'-','LineWidth',1.5);
hold on;
plot([0.15*T 0.35*T],[diag(E(1:5,1:5)),...
    diag(E(1:5,1:5))],'-','LineWidth',1.5);
xlabel(['$x$'],'Interpreter','latex');
ylabel(['$V(x)$'],'Interpreter','latex');
title(['$k=' num2str(k) ',T=' num2str(T) '$'],'Interpreter','latex')
legend('V','n=0','n=1','n=2','n=3','n=4');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5);
```

17 hw18

	加法	减法	乘法	除法	sin	cos	sqrt	exp	赋值	空循环
时间 (s)	1.1776	1.1227	1.1213	1.1207	10.2701	10.0805	8.1305	2.5951	1.0797	1.0799

循环 20000*20000 次 (MATLAB)

18 hw19

用 rand() 函数产生随机点 (x, y)，区间在 [-1,1] 之间。判断满足 $\sqrt{(x^2+y^2)} < 1$ 的点数 N_p，总点数 N，$\pi = 4 * N_p/N$

N	10^2	10^3	10^4	10^5	10^6	10^7	10^8
π	3.08000	3.20800	3.13120	3.14240	3.14187	3.14137	3.14156

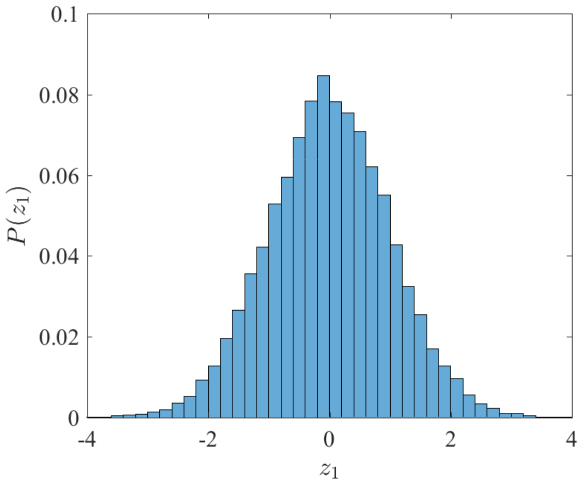
满足大数定理，误差 $\sim 1/\sqrt{N}$

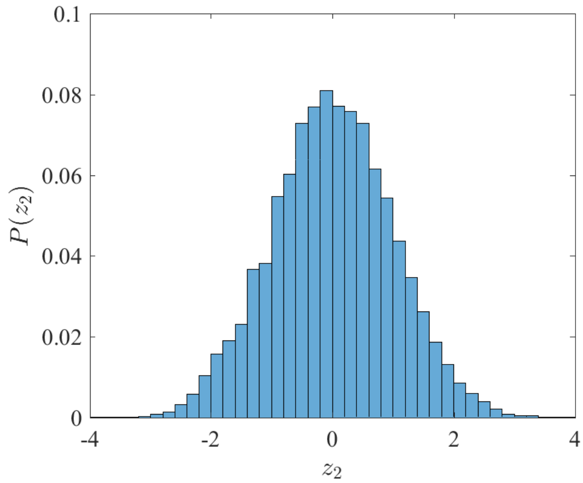
```
clear;
Pi = [];
for N = 1e2*10.^[0:1:6]
    x = 2*rand(1,N)-1;
    y = 2*rand(1,N)-1;
    Pi = [Pi 4*sum(x.^2+y.^2 < 1)/N];
end
```

19 hw20

Box-Muller 算法

$$z_1 = \sqrt{-2\ln\xi_1}\cos 2\pi\xi_2, z_2 = \sqrt{-2\ln\xi_1}\sin 2\pi\xi_2 \tag{37}$$





关联函数

$$\langle (z_1 - \langle z_1\rangle)(z_2 - \langle z_2\rangle)\rangle = \langle z_1 z_2\rangle - \langle z_1\rangle\langle z_2\rangle \approx 0 \tag{38}$$

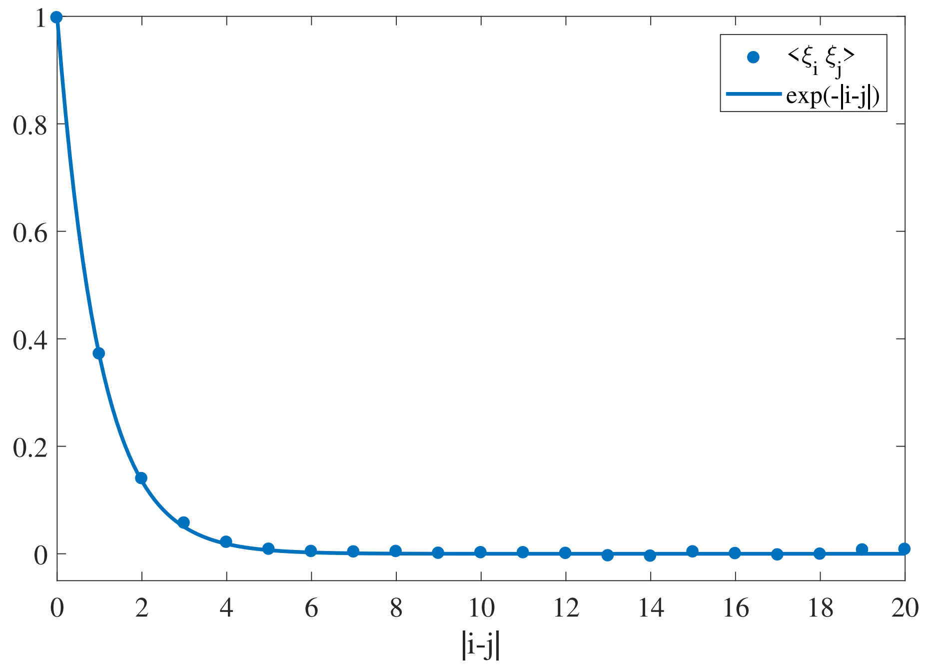
```
clear;
N=100;
xi1 = rand(1,N);
xi2 = rand(1,N);
z1 = sqrt(-2*log(xi1)).*cos(2*pi*xi2);
z2 = sqrt(-2*log(xi1)).*sin(2*pi*xi2);

subplot(1,2,1);
h1=histogram(z1,[-4:0.2:4],'Normalization','pdf');

subplot(1,2,2);
h2=histogram(z2,[-4:0.2:4],'Normalization','pdf');

mean(mean(z1'*z2)) -  mean(z1)*mean(z2);
```

20 hw21

$$\xi_i = \sum_j w_{ij}\eta_j,\ \overline{\xi_i} = 0 \Rightarrow \overline{\eta_j} = 0,\ \langle \xi_i \xi_j \rangle = \sum_{i'j'} w_{ii'} w_{jj'} \langle \eta_{i'} \eta_{j'} \rangle = \sum_k w_{ik} w_{jk} \xrightarrow{w=w^T} (w^2)_{ij} \tag{39}$$

$$\Rightarrow (w^2)_{ij} = f(i-j),\ w^2 = U^\dagger \lambda U \xrightarrow{\lambda>0} w = U^\dagger \sqrt{\lambda} U \tag{40}$$

关联函数取 $\langle \xi_i \xi_j \rangle = e^{-\alpha|i-j|}$



```
clear;
N = 100;
xij = zeros(N,N);
for n = 1:5000
    eta = randn(N,1);
    WW = zeros(N,N);
    alpha = 1;
    for nij = -N+1:N-1
        WW = WW + diag(exp(-alpha*abs(nij)*ones(1,N-abs(nij))),nij);
    end
    [U,E] = eig(WW);
    W = U*sqrt(abs(E))*U';
    xi = W*eta;
    xij = xij + xi*xi';
end

xij = xij / n;
for ij = 0:10
    f(ij+1) = mean(diag(xij,ij));
end
plot(0:10,f,'o');
hold on;
plot(0:10,exp(-alpha*(0:10)));
```

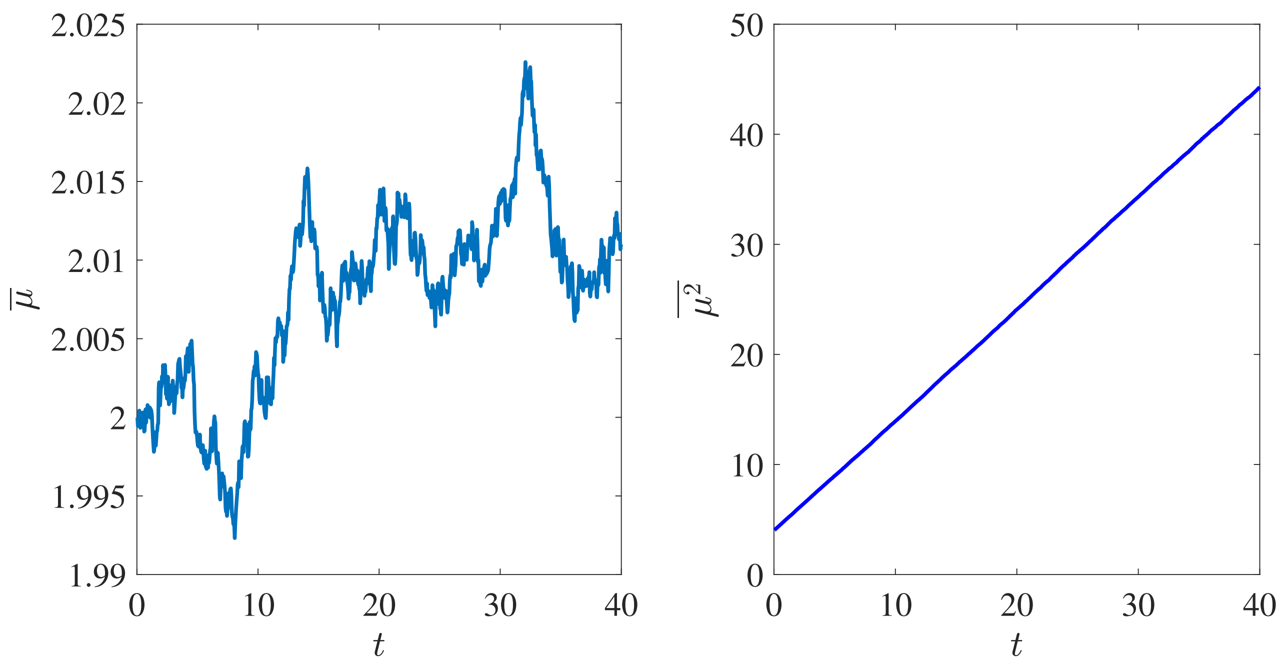
21 hw22

离散化关键 $\delta w_t \sim N(0, \sqrt{\delta t})$，0 是随机分布均值，$\sqrt{\delta t}$ 是标准差，N 是正态分布

对于 $\dot{u} = \xi$，速度的平均值和方差有解析解，平均值等于初始速度，方差与时间成正比，数值结果与解析结果一致

$$\overline{u} = \overline{u(0)} + \int_0^t \overline{(\xi(t')}dt' = u(0), \tag{41}$$

$$\overline{u^2} = u^2(0) + \int_0^t \langle \xi(t_1)\xi(t_2) \rangle dt_1 dt_2 = u^2(0) + Dk_{\mathrm{B}}T \int_0^t \delta(t_1 - t_2) dt_1 dt_2 = u^2(0) + Dk_{\mathrm{B}}Tt \tag{42}$$




```
clear;
dt = 0.04;
A = 1;
n = 1000;
m = 100000;
xi = sqrt(A)*normrnd(0,sqrt(dt),[n,m]);
vt = zeros(1,m)+2;
for ti = 1:n

    vt= vt + xi(ti,:);
    mu(ti) = mean(vt);
    mu2(ti)= mean(vt.^2);
end
t = dt*(1:n);
subplot(1,2,1);
plot(t,mu);
subplot(1,2,2);
plot(t,mu2,'b');
```

22 hw23

对于 $m\dot{v} = -\eta v + \xi$，存在解析结果

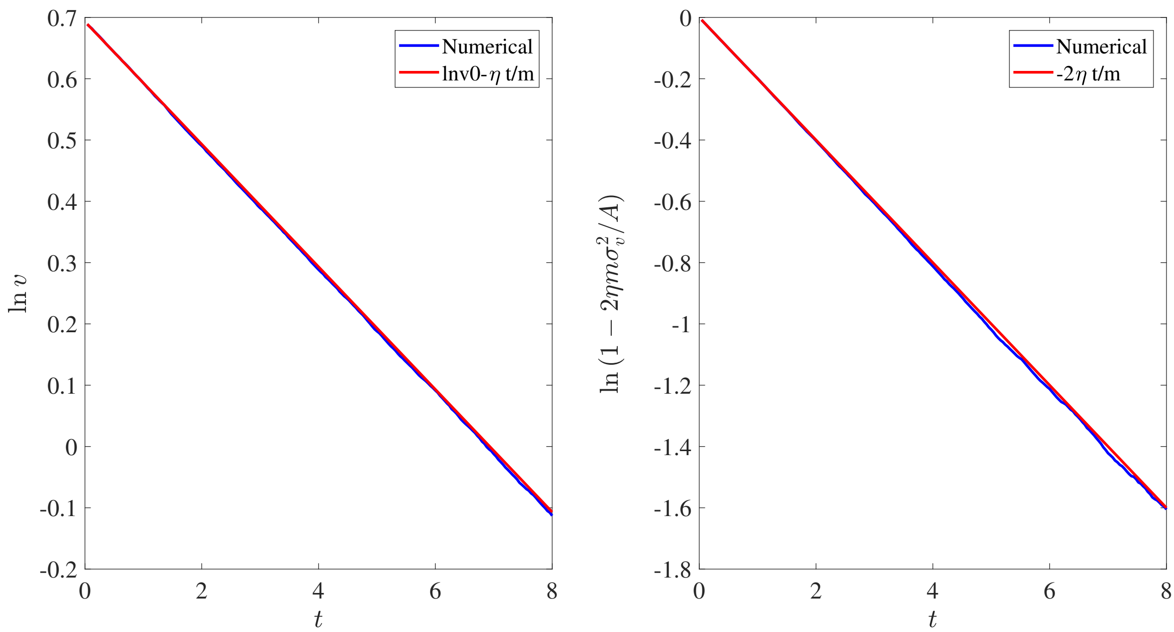
$$\overline{v} = e^{-\eta/mt}v_0 + \sqrt{A}/m\int_0^t e^{-\eta/m(t-t')}\overline{dw_{t'}} = e^{-\eta/mt}v_0, \tag{43}$$

$$\overline{v^2} = \overline{v}^2 + A/m^2\int_0^t e^{-\eta/m(t-t')}e^{-\eta/m(t-t'')}\overline{dw_{t'}dw_{t''}} = \overline{v}^2 + A/m^2\int_0^t e^{-2\eta/m(t-t')}dt' = \overline{v}^2 + \frac{A(1-e^{-\frac{2\eta t}{m}})}{2\eta m} \tag{44}$$

程序采用方法一，$m = 1, A = 1, \eta = 0.1, v(0) = 2$，

数值处理 $dv = adt + bdw_t$，$a(v,t)$，$b = b(v,t)$，Ref：Numerical Solution Of SDE(第一章)

方法一 $v_{n+1} = v_n + a(v_n,t_n)\Delta_n + b(v_n,t_n)\Delta w_n$；方法二 $v_{n+1} = v_n + a\Delta_n + b\Delta w_n + \frac{1}{2}bb'(\Delta w_n^2 - \Delta_n)$



数值结果与解析结果一致

```
clear;
dt = 0.04;
A = 1;
eta = 0.1;
n = 200;
m = 100000;
xi = sqrt(A)*normrnd(0,sqrt(dt),[n,m]);
vt = zeros(1,m)+2;
for ti = 1:n

    vt= vt + (-eta*vt)*dt + xi(ti,:);
    mu(ti) = mean(vt);
    mu2(ti)= mean(vt.^2);
end
t = dt*(1:n);
subplot(1,2,1);
plot(t,log(abs(mu)),'b');
hold on;
plot(t,log(2)+(-eta*t),'r');
subplot(1,2,2);
plot(t,log(1-2*eta*(mu2-abs(mu).^2)/A),'b');
hold on;
plot(t,-2*eta*t,'r');
```

23 hw24

数值求 Black-Scholes Eq，

$$dS = \mu S dt + \sigma S dw \tag{45}$$

可以用

数值处理 $dv = adt + bdw_t$，$a(v,t)$，$b = b(v,t)$，Ref：Numerical Solution Of SDE(第一章)

方法一 $v_{n+1} = v_n + a(v_n, t_n)\Delta_n + b(v_n, t_n)\Delta w_n$；方法二 $v_{n+1} = v_n + a\Delta_n + b\Delta w_n + \frac{1}{2}bb'(\Delta w_n^2 - \Delta_n)$

Black-Scholes Eq 是有解析结果，

$$\begin{aligned} dS = \mu S dt + \sigma S dw, dY = \frac{\partial Y}{\partial S}dS + \frac{1}{2}\frac{\partial^2 Y}{\partial S^2}dS^2 = \frac{\partial Y}{\partial S}\mu S dt + \frac{\partial Y}{\partial S}\sigma S dw + \frac{1}{2}\frac{\partial^2 Y}{\partial S^2}\sigma^2 S^2 dt \\ \text{令} Y = \ln S, \Rightarrow dY = d\ln S = \left(\mu - \frac{1}{2}\sigma^2\right)dt + \sigma dw \end{aligned} \tag{46}$$

然后类比布朗运动，求出解析解

24 hw25

转移矩阵的步骤网站上写的很清楚了，下面直接给出程序

可以得到，取 $E=0$，$V=V\cos(2\pi qn)$，$V=1.9,2,2.1$，关联长度 $\xi=27589,6610.9,10.2415$，从扩展到局域，与作业 10 一致

```

clear;
E=0;
V=1.9;
T=[-E,-1;1,0];
N=100000;
n=10;

RR=eye(2);
gamma=zeros(2,1);
q=(sqrt(5)-1)/2;
Vlist=V*cos(2*pi*q*(1:N));
vi=1;
for ni=1:N/n
    if ni==1
        Tn=eye(2);
        for ii=1:n
            Ti=T+[Vlist(vi),0;0,0];
            Tn=Ti*Tn;
            vi=vi+1;
        end
        [Q,R]=qr(Tn);
    else
        Tn=Q;
        for ii=1:n
            Ti=T+[Vlist(vi),0;0,0];
            Tn=Ti*Tn;
            vi=vi+1;
        end
        [Q,R]=qr(Tn);
    end

    gamma=gamma+(-log(diag(abs(R)).^2)/N);

end

xi=max(abs(1./gamma));
```

25 hw26

选了一个比较简单的积分函数

```
Integrate[x^2 + y^2 + z^2, {x, -a, b}, {y, -a, b}, {z, -a, b}]
积分
```

$$(a+b)^3\left(a^2-a\,b+b^2\right)$$

$$\int_a^b f(x)dx=\int_a^b \frac{f(x)}{P(x)}P(x)dx=\frac{1}{N}\sum_i\int_a^b\frac{f(x)}{P(x)}\delta\left(x-x_i\right)dx=\frac{1}{N}\sum_i\frac{f\left(x_i\right)}{P\left(x_i\right)} \tag{47}$$

程序中 $a=-2,b=2$，选择一个随机分布函数，范围在 $[-2,2]$，随机抽取 N 个 x_i，

```

clear;
for N = 10.^[2 4 6 8]

    x = 4*rand(N,1)−2;
    y = 4*rand(N,1)−2;
    z = 4*rand(N,1)−2;

    f = x.^2 + y.^2 + z.^2;
    P = (1/4)^3;
    intf = sum(f./P)/N

end
```

26 hw27

一维经典 Ising model

考虑周期性边界条件，对于一个格子上的自旋 σ_i 作翻转，前后的构型能量变化为 $\Delta E=2J(\sigma_i\sigma_{i-1}+\sigma_i\sigma_{i+1})$，$\sigma_i$ 翻转前的自旋，只需把文章程序中

```
rand(N)

neighbors = circshift(grid, [ 0  1]) + ...
            circshift(grid, [ 0 −1]) + ...
            circshift(grid, [ 1  0]) + ...
            circshift(grid, [−1  0]);
```

改为

```
rand(1,N)

neighbors = circshift(grid, [ 0  1]) + circshift(grid, [ 0 −1]);
```

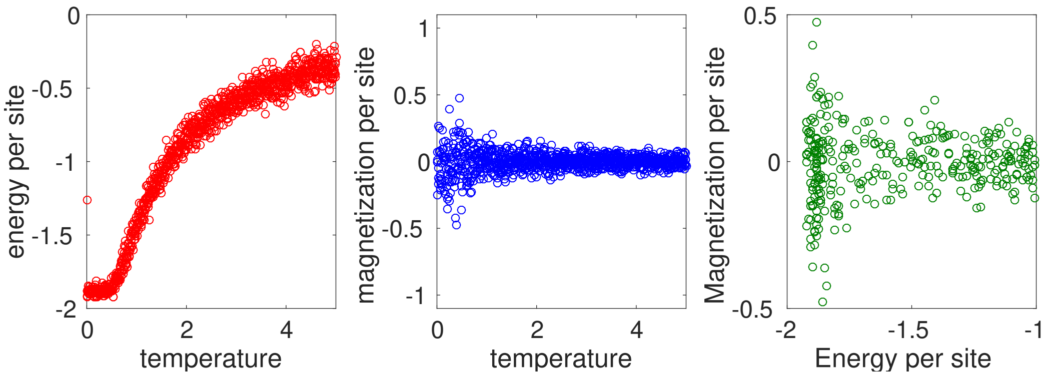


Figure 2: 链长 1000，迭代 1000

从图磁距与温度的变化图，可以看到一维经典 Ising model 没有发生相变

27 HW28

二维经典 Ising model

同样考虑周期性边界条件，对于一个格子上的自旋 $\sigma_{i,j}$ 作翻转，前后的构型能量变化为 $\Delta E = 2J\sigma_{i,j}(\sigma_{i,j-1} + \sigma_{i,j+1} + \sigma_{i,j-1} + \sigma_{i,j+1})$，$\sigma_{i,j} + 2h\sigma_{i,j}$，$\sigma_{i,j}$ 翻转前的自旋，只需把文章程序中

```
% Calculate the change in energy of flipping a spin
DeltaE = 2 * J * (grid .* neighbors);
```

改为

```
% Calculate the change in energy of flipping a spin
DeltaE = 2 * J * (grid .* neighbors) + 2*h*grid;
```

磁场 $h = 0$，相变区间在 $T = 2 \sim 3$（$k_{\mathrm{B}} = 1$）

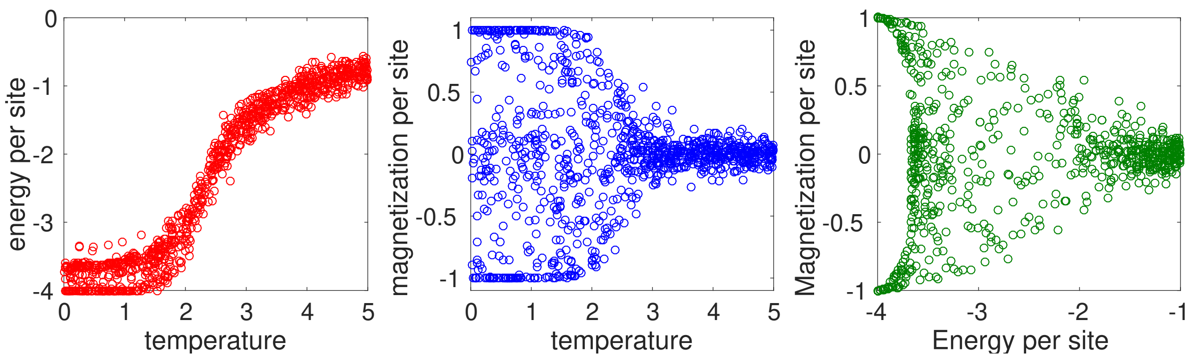


Figure 3: 格子 25*25，迭代 800

磁场不为 0 时，

28 hw32

势场为 Kronig-Penney 势，周期为 a，

$$V(x) = \begin{cases} V_0, & na < x < b + na \\ 0, & b + na < x < a + na \end{cases} \tag{48}$$

$$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x) \tag{49}$$

$$V(x)=\sum_n C_n e^{iG_n x} \tag{50}$$

$$C_n=\frac{1}{a}\int_0^a V(x)e^{-iG_n x}dx=\frac{iV_0(e^{-\frac{2i\pi bn}{a}}-1)}{2\pi n},\ n\neq 0 \tag{51}$$

$$C_n=V_0\frac{b}{a},\ n=0 \tag{52}$$

所以在基矢 $e^{iG_n x}$ 下

$$H\psi_k=E_k\psi_k,\ \psi_k=e^{ikx}u_k(x)=\sum_n C_n e^{ikx}e^{iG_n x} \tag{53}$$

$$H_{nm}(k)=\frac{\hbar^2}{2m}(k+G_n)^2\delta_{nm}+V_0 b/a\delta_{nm},\ n=m \tag{54}$$

$$H_{nm}(k)=\frac{iV_0(e^{-\frac{2i\pi(n-m)b}{a}}-1)}{2\pi(n-m)},\ n\neq m \tag{55}$$

```
clear;
V0 = 4;
a = 2;
b = 1;
N = 50;
dk = 0.01;
G = (-N:N)*2*pi/a;
H = zeros(2*N+1,2*N+1);
Hv = zeros(2*N+1,2*N+1);
H0 = zeros(2*N+1,2*N+1);

for n = -N:N
    for m = -N:N
        if  n == m
            Hv(n+N+1,m+N+1) = b/a;
        else
            ee = exp(-i*2*(n-m)*pi*b/a);
            Hv(n+N+1,m+N+1) = i*(ee-1)/(2*(n-m)*pi);
        end
    end
end

klist = -pi/a:dk:pi/a;
for ki = 1:length(klist)
    k = klist(ki);
    H0 = diag((k+G).^2,0);
    H = V0*Hv + H0;
    band(:,ki) = eig(H);
end
```

```
figure;
plot(klist,band(1:5,:),'LineWidth',1.5);
xlabel(['$k$'],'Interpreter','latex');
ylabel(['$E_k$'],'Interpreter','latex');
title(['$' 'V_0=' num2str(V0) ',a=' num2str(a)...
        '$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
```

29 hw35

s-wave 程序

```
clear;
N = 1000;
mu = 1;
t = 3;
delta = 0.1;
V = 1;

mulist = mu+V*(rand(1,N)-0.5);
H0 = zeros(N,N);
Hd = diag(ones(1,N)*delta,0);
Ht = diag(ones(1,N-1)*(-t),-1)+diag(ones(1,N-1)*(-t),1);
Hmu = diag(mulist,0);
Hmt = Hmu + Ht;
H = [Hmt,H0,H0,Hd;...
    H0,Hmt,-Hd,H0;...
    H0,-Hd,-Hmt,H0;...
    Hd,H0,H0,-Hmt]/2;
E=eig(H);


plot(E(2*N-50:2*N+50),'b.');
```