

XXZ自旋模型

模型的哈密顿量为：

$$H = -J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z)$$

利用自旋的升降算符可以将x和y方向的自旋化简如下：

$$\begin{cases} S^+ = S^x + i S^y \\ S^- = S^x - i S^y \end{cases} \Rightarrow \begin{cases} S^x = \frac{1}{2} (S^+ + S^-) \\ S^y = -\frac{i}{2} (S^+ - S^-) \end{cases}$$

$$\begin{aligned} S_i^x S_j^x &= \frac{1}{4} (S_i^+ + S_i^-) (S_j^+ + S_j^-) \\ &= \frac{1}{4} (S_i^+ S_j^+ + S_i^+ S_j^- + S_i^- S_j^+ + S_i^- S_j^-) \end{aligned}$$

$$\begin{aligned} S_i^y S_j^y &= -\frac{1}{4} (S_i^+ - S_i^-) (S_j^+ - S_j^-) \\ &= -\frac{1}{4} (S_i^+ S_j^+ - S_i^+ S_j^- - S_i^- S_j^+ + S_i^- S_j^-) \end{aligned}$$

$$\Rightarrow \underline{S_i^x S_j^x + S_i^y S_j^y = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)}$$

如果我们将自旋向上定义为1态，向下定义为0态，那么上式会贡献如下的变换：

$$|01\rangle \rightarrow |10\rangle$$

$$|10\rangle \rightarrow |01\rangle$$

因而据此，我们列出L=5，N=2的OBC下的所有可能情况：

$$\begin{aligned}
① \quad |00011\rangle &\rightarrow |00101\rangle^{②} \\
② \quad |00101\rangle &\rightarrow |01001\rangle^{④} \text{ or } |00011\rangle^{①} \text{ or } |00110\rangle^{③} \\
③ \quad |00110\rangle &\rightarrow |01010\rangle^{⑤} \text{ or } |00101\rangle^{②} \\
④ \quad |01001\rangle &\rightarrow |10001\rangle^{⑦} \text{ or } |00101\rangle^{②} \text{ or } |01010\rangle^{⑤} \\
⑤ \quad |01010\rangle &\rightarrow |10010\rangle^{⑧} \text{ or } |00110\rangle^{③} \text{ or } |01100\rangle^{⑥} \text{ or } |01001\rangle^{④} \\
⑥ \quad |01100\rangle &\rightarrow |10100\rangle^{⑨} \text{ or } |01010\rangle^{⑤} \\
⑦ \quad |10001\rangle &\rightarrow |01001\rangle^{④} \text{ or } |10010\rangle^{⑧} \\
⑧ \quad |10010\rangle &\rightarrow |01010\rangle^{⑤} \text{ or } |10100\rangle^{⑨} \text{ or } |10001\rangle^{⑦} \\
⑨ \quad |10100\rangle &\rightarrow |01100\rangle^{⑥} \text{ or } |11000\rangle^{⑩} \text{ or } |10010\rangle^{⑧} \\
⑩ \quad |11000\rangle &\rightarrow |10100\rangle^{⑨}
\end{aligned}$$

从而，我们可以写出如下的matlab程序进行对角化，求出能谱：

```

clear
dim = 10;
delta = 1;

for J = 0:0.2:10

Hz = diag(ones(1,dim)*(-J)*delta,0);

Hxy = zeros(dim,dim);
Hxy(1,2) = -0.5*J;
Hxy(2,1) = -0.5*J; Hxy(2,3) = -0.5*J; Hxy(2,4) = -0.5*J;
Hxy(3,2) = -0.5*J; Hxy(3,5) = -0.5*J;
Hxy(4,2) = -0.5*J; Hxy(4,5) = -0.5*J; Hxy(4,7) = -0.5*J;
Hxy(5,3) = -0.5*J; Hxy(5,4) = -0.5*J; Hxy(5,6) = -0.5*J; Hxy(5,8) = -0.5*J;
Hxy(6,5) = -0.5*J; Hxy(6,9) = -0.5*J;
Hxy(7,4) = -0.5*J; Hxy(7,8) = -0.5*J;
Hxy(8,5) = -0.5*J; Hxy(8,7) = -0.5*J; Hxy(8,9) = -0.5*J;
Hxy(9,6) = -0.5*J; Hxy(9,8) = -0.5*J; Hxy(9,10) = -0.5*J;
Hxy(10,9) = -0.5*J;

H = Hz + Hxy;

E = eig(H);

plot(J*ones(1,dim),E,'r. ');
xlabel(['$J$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);

```

```

hold on;

end

for delta = 0:0.2:10

Hz = diag(ones(1,dim)*(-J)*delta,0);

Hxy = zeros(dim,dim);
Hxy(1,2) = -0.5*J;
Hxy(2,1) = -0.5*J; Hxy(2,3) = -0.5*J; Hxy(2,4) = -0.5*J;
Hxy(3,2) = -0.5*J; Hxy(3,5) = -0.5*J;
Hxy(4,2) = -0.5*J; Hxy(4,5) = -0.5*J; Hxy(4,7) = -0.5*J;
Hxy(5,3) = -0.5*J; Hxy(5,4) = -0.5*J; Hxy(5,6) = -0.5*J; Hxy(5,8) = -0.5*J;
Hxy(6,5) = -0.5*J; Hxy(6,9) = -0.5*J;
Hxy(7,4) = -0.5*J; Hxy(7,8) = -0.5*J;
Hxy(8,5) = -0.5*J; Hxy(8,7) = -0.5*J; Hxy(8,9) = -0.5*J;
Hxy(9,6) = -0.5*J; Hxy(9,8) = -0.5*J; Hxy(9,10) = -0.5*J;
Hxy(10,9) = -0.5*J;

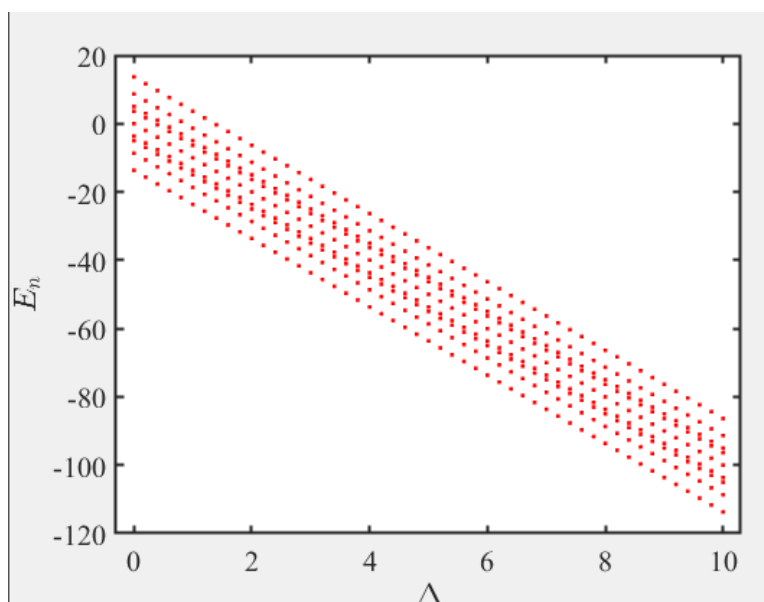
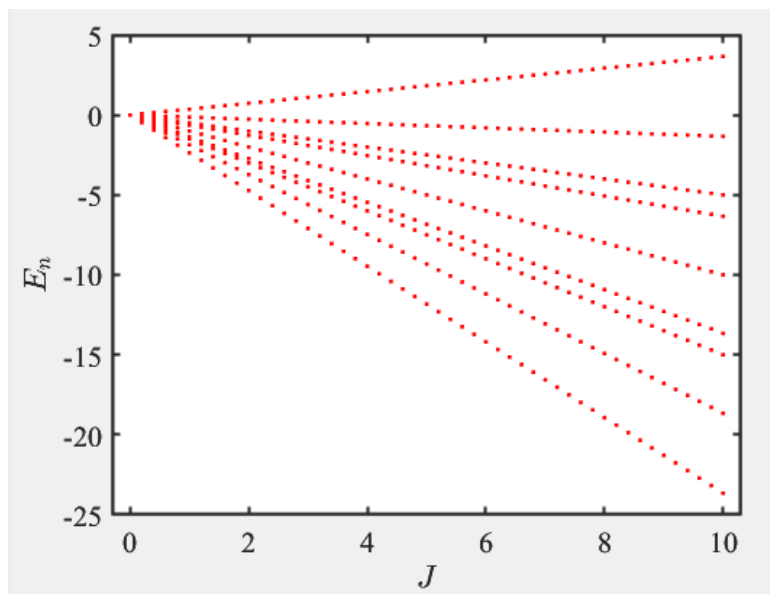
H = Hz + Hxy;

E = eig(H);

figure(2)
plot(delta*ones(1,dim),E,'r. ');
xlabel(['$\Delta$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on;

end

```



可以看到，随着 J 的增大，能级的劈裂越来越大；而 z 方向的 δ 仅仅类似于化学势一样，改变绝对能量大小，却不改变相对能差。

Spinless Fermi Hubbard

体系哈密顿量为

$$H = -J \sum_i \left(c_i^\dagger c_{i+1} + \text{h. c.} \right) + U n_i n_{i+1} - \mu n_i$$

利用泡利不相容原理，可以列出 $L=5$ ， $N=2$ 的所有态，并考虑OBC的边条,与之前类似，可以写出如下的matlab代码：

```
clear;
N = 2;
L = 5;
```

```

t = 1;
mu = 1;

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 U = 0:0.2:10
    H = mu*Hmu + (-t)*Ht + U*Hu;
    E = eig(H);
    plot(U*ones(1,length(E)),E,'r. ');
    xlabel(['$U$'],'Interpreter','latex');
    ylabel(['$E_n$'],'Interpreter','latex');
    fonts=15;
    set(gca,'FontSize',fonts);
    set(gca,'FontName','Times');
    set(gca,'LineWidth',1.5)
    xlim([0-0.3,10+0.3]);
    hold on

end

U = 1;

for mu = 0:0.2:10
    H = mu*Hmu + (-t)*Ht + U*Hu;
    E = eig(H);

```

```

figure(2);
plot(mu*ones(1,length(E)),E,'r. ');
xlabel(['$\mu$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on

end

mu = 1;

for t = 0:0.2:10
H = mu*Hmu+(-t)*Ht+U*Hu;
E = eig(H);
figure(3);
plot(t*ones(1,length(E)),E,'r. ');
xlabel(['$t$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on

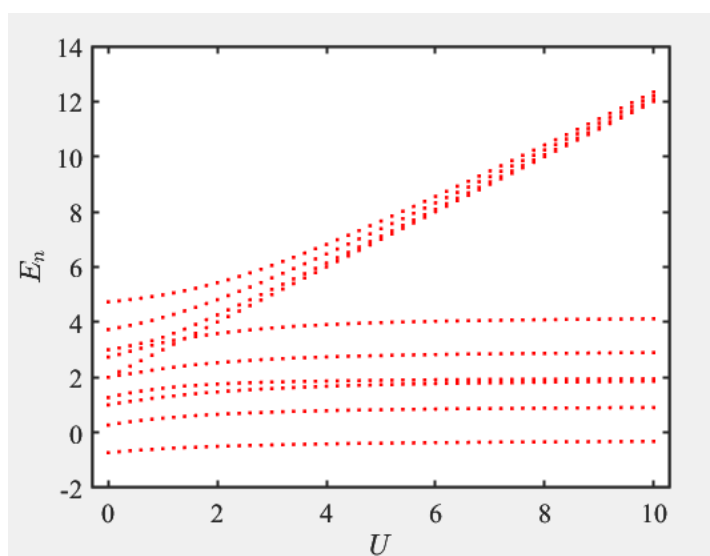
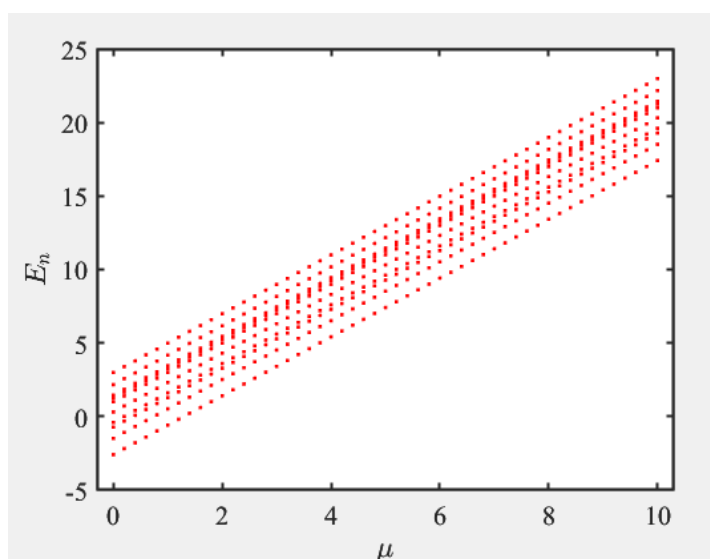
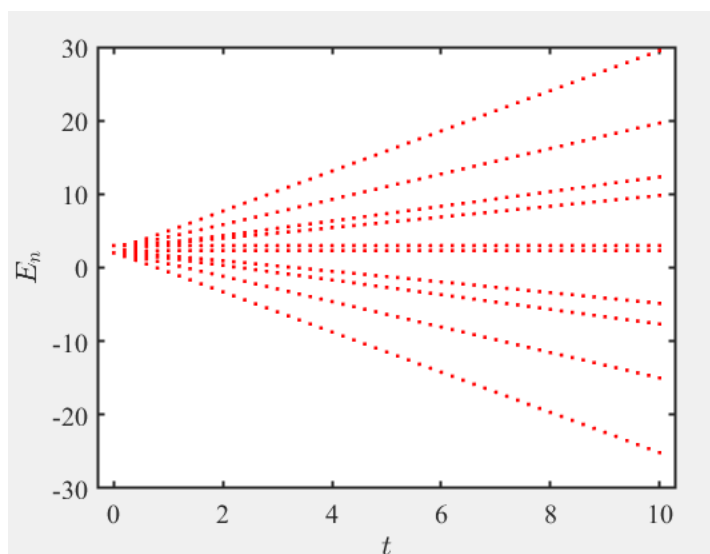
end

tlist = 0:0.1:2*pi;
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

figure(4)
plot(tlist,E,'r. ');
xlabel(['$\theta$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0,2*pi]);

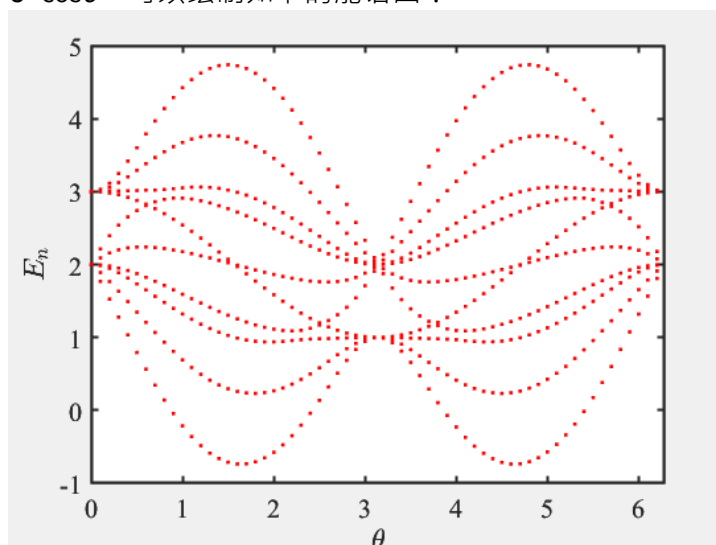
```

分别变化 t, μ, U ，并保持其他参数为1，可以绘制如下能谱：



可以看到，随着 t 的增大，能级的劈裂越来越大；而化学势改变绝对能量大小，却不改变相对能差。对于相互作用能 U ，其能谱难以简单概况，有一部分能级相互靠近且不断升高，而剩下

的几乎保持不变，这也许就是Hubbard model的困难和微妙的体现。如果我们设 $t=\sin\theta$ 而 $U=\cos\theta$ ，可以绘制如下的能谱图：



Spinless Bose Hubbard

体系的哈密顿量为

$$H = -J \sum_i \left(c_i^\dagger c_{i+1} + \text{h.c.} \right) + \frac{U}{2} n_i (n_i - 1) - \mu n_i$$

由于boson不受泡利不相容原理的限制，因此同一个态上允许存在多个粒子，从而matlab程序改写如下：

```
clear;
N = 2;
L = 5;
t = 1;
mu = 1;
Q = 3;

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
end
```



```

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 U = 0:0.2:10
H = mu*Hmu+(-t)*Ht+U*Hu;
E = eig(H);
plot(U*ones(1,length(E)),E,'r. ');
xlabel(['$U$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on

end

U = 1;

for mu = 0:0.2:10
H = mu*Hmu+(-t)*Ht+U*Hu;
E = eig(H);
figure(2);
plot(mu*ones(1,length(E)),E,'r. ');
xlabel(['$\mu$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on

end

```

```

mu = 1;

for t = 0:0.2:10
H = mu*Hmu+(-t)*Ht+U*Hu;
E = eig(H);
figure(3);
plot(t*ones(1,length(E)),E,'r. ');
xlabel(['$t$'],'Interpreter','latex');
ylabel(['$E_n$'],'Interpreter','latex');
fonts=15;
set(gca,'FontSize',fonts);
set(gca,'FontName','Times');
set(gca,'LineWidth',1.5)
xlim([0-0.3,10+0.3]);
hold on

end

tlist = 0:0.1:2*pi;
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
figure(4)
plot(tlist,E,'r. ');
xlabel(['$\theta$'],'Interpreter','latex');
ylabel(['$E_n$'],'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];

```

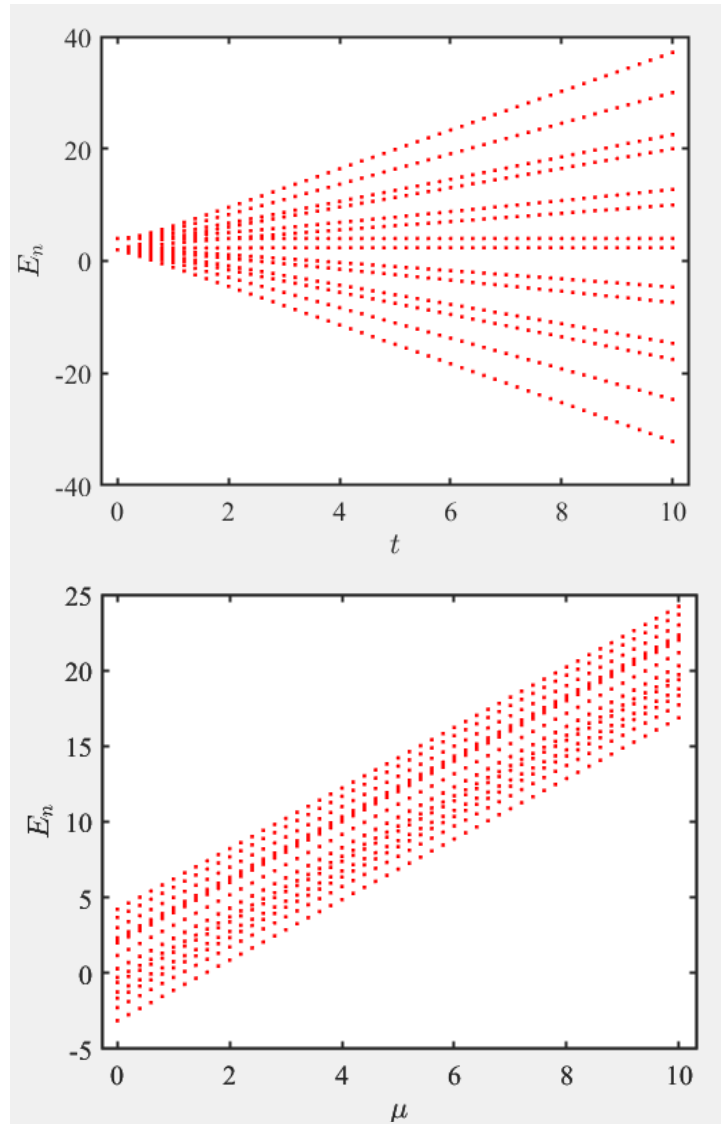
```

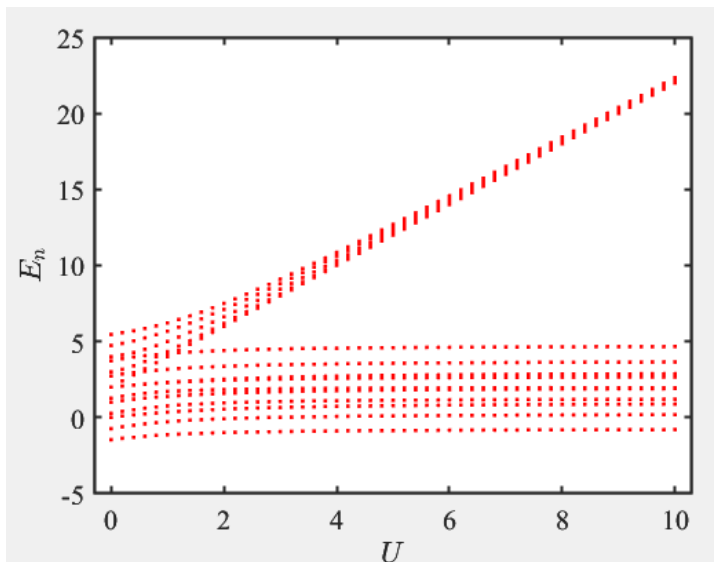
b=(b-c)/3;
end

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

```

分别变化 t, μ, U ，并保持其他参数为1，可以绘制如下能谱：





可以看到，随着 t 的增大，能级的劈裂越来越大；而化学势改变绝对能量大小，却不改变相对能差。对于相互作用能 U ，其能谱难以简单概况，有一部分能级相互靠近且不断升高，而剩下的几乎保持不变，这也许就是Hubbard model的困难和微妙的体现。如果我们设 $t=\sin\theta$ 而 $U=\cos\theta$ ，可以绘制如下的能谱图：

