计算物理作业

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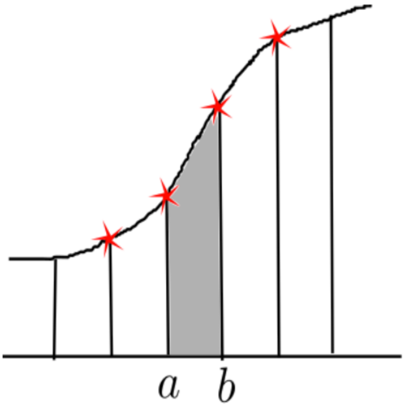
HWI

- 已知曲线过四个点（红色标记），确定中间两点 a,b 之间灰色区域面积。



过 $(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$ N　　N 点多项式插值：

$$y = \sum_i^N l_i(x) y_i, \quad l_i(x) = \frac{(x - x_1)(x - x_2) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_N)}{(x_i - x_1)(x_i - x_2) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_N)}$$

HW1

```
In[3]:= y = FullSimplify[InterpolatingPolynomial[{{x1, y1}, {xa, ya}, {xb, yb}, {x2, y2}}, x]]
```
完全简化 插值多项式

Out[3]=

$$y1 + (x - x1)\left(\frac{y1 - ya}{x1 - xa} + (x - xa)\left(\frac{\frac{-y1+ya}{x1-xa} + \frac{ya-yb}{xa-xb}}{-x1 + xb} + \frac{(x - xb)\left(-\frac{\frac{-y1+ya}{x1-xa} + \frac{ya-yb}{xa-xb}}{-x1+xb} + \frac{\frac{y2-yb}{x2-xb} + \frac{-ya+yb}{xa-xb}}{x2-xa}\right)}{-x1 + x2}\right)\right)$$

```
In[8]:= S = FullSimplify[Integrate[y, {x, xa, xb}], Assumptions → x1 < xa < xb < x2]
```
完全简化 积分 假设

Out[8]=

$$\begin{aligned}&-xa\,y1 + xb\,y1 + \Big((xa - xb)\,\big(xa\,(xa - xb)^2\,xb\,(xa + xb)\,(y1 - y2) +\\
&\quad 3\,x2^2\,(xa + xb)^2\,(xb\,(y1 - ya) + xa\,(y1 - yb)) + 2\,x2^3\,\big(xb^2\,(-y1 + ya) + xa^2\,(-y1 + yb) + 2\,xa\,xb\,(-2\,y1 + ya + yb)\big) +\\
&\quad x2\,\big(2\,xa\,xb^3\,(-y1 + ya) + xb^4\,(-y1 + ya) + xa^4\,(-y1 + yb) + 2\,xa^3\,xb\,(-y1 + yb) + 3\,xa^2\,xb^2\,(-2\,y1 + ya + yb)\big) +\\
&\quad 3\,x1^2\,\big(x2\,\big(xa^2\,(4\,y1 - ya - 3\,yb) + xb^2\,(4\,y1 - 3\,ya - yb) + 2\,xa\,xb\,(2\,y1 - ya - yb)\big) +\\
&\qquad 2\,x2^3\,(-2\,y1 + ya + yb) + (xa + xb)\,\big(xb^2\,(-y2 + ya) + xa^2\,(-y2 + yb) + xa\,xb\,(-4\,y1 + 2\,y2 + ya + yb)\big)\big) +\\
&\quad 2\,x1^3\,\big(xb^2\,(y2 - ya) + xa^2\,(y2 - yb) + 2\,xa\,xb\,(3\,y1 - y2 - ya - yb) + x2^2\,(6\,y1 - 3\,(ya + yb)) +\\
&\qquad 2\,x2\,(xb\,(-3\,y1 + 2\,ya + yb) + xa\,(-3\,y1 + ya + 2\,yb))\big) + x1\,\big(2\,xa\,xb^3\,(y2 - ya) + xb^4\,(y2 - ya) + xa^4\,(y2 - yb) +\\
&\qquad 2\,xa^3\,xb\,(y2 - yb) + 3\,xa^2\,xb^2\,(4\,y1 - 2\,y2 - ya - yb) + 4\,x2^3\,(3\,xa\,y1 + 3\,xb\,y1 - xa\,ya - 2\,xb\,ya - (2\,xa + xb)\,yb) +\\
&\qquad 3\,x2^2\,\big(2\,xa\,xb\,(-2\,y1 + ya + yb) + xb^2\,(-4\,y1 + 3\,ya + yb) + xa^2\,(-4\,y1 + ya + 3\,yb)\big)\big)\big)\Big) \Big/\\
&\quad (12\,(x1 - x2)\,(x1 - xa)\,(x2 - xa)\,(x1 - xb)\,(x2 - xb))\end{aligned}$$

等间距：

```
In[9]:= FullSimplify[S /. {x1 → 2 xa - xb, x2 → 2 xb - xa}]
```
完全简化

Out[9]=

$$\frac{1}{24}\,(xa - xb)\,(y1 + y2 - 13\,(ya + yb))$$

HW2

- 求解方程 $AX^2 + BX + C = 0$ 其中 A,B,C,X 均为矩阵。取 A,B,C 为任意的 3×3 矩阵，找到满足方程的解的 X。
  迭代方程：$X_{n+1} = -B^{-1}(C + AX_n^2)$
- Matlab 程序：

```
clc
clear
A=[-1 2 1; 0 1 0;1 0 3];
B=[2 1 0; 1 -1 -3; 0 3 1];
Binv=inv(B);
C=[3 5 11; -7 -2 13; 35 3 -20];
x0=zeros(3,3);
for i=1:1000
x=-Binv*(A*x0^2+C);
x0=x;
y(:,:,i)=A*x^2+B*x+C;
fnorm1(i) = norm(y(:,:,i), 1);
fnorm2(i) = norm(y(:,:,i), 2);
end
x
yend=A*x^2+B*x+C
hold on
plot(1:1000,fnorm1,'-b ','LineWidth',1.5)
plot(1:1000,fnorm2,'-r ','LineWidth',1.5)
xlabel('i','FontSize', 24,'Interpreter','latex')
ylabel('norm','FontSize', 24,'Interpreter','latex')
legend('norm-1','norm-2')
set(gca, 'FontSize', 24)
box on
```

此参数无解

HW2

```
A=[1 0 0; 0 1 0;0 0 1];
B=[2 0 0; 0 2 0; 0 0 3];
C=[-1 0 0; 1 0 3; 2 0 1];
```

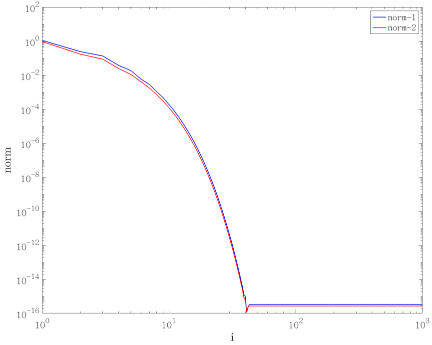
```
x =

   0.414213562373095                   0                   0
  -0.920764671736719                   0  -1.854101966249684
  -0.659576754958315                   0  -0.381966011250105


yend =

   1.0e-15 *

                   0                   0                   0
   0.111022302462516                   0                   0
   0.222044604925031                   0   0.111022302462516
```

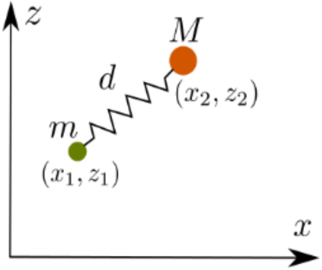


1-范数： $\|x\|_1 = \sum_{i=1}^{N} |x_i|$

2-范数： $\|\mathbf{x}\|_2 = \sqrt{\sum_{i=1}^{N} x_i^2}$

HW3

- 质量分别为 m 和 M 的两球通过劲度系数为 k 的弹簧连接，弹簧自然状态长为 d_0，初始时刻系统位置、弹簧长度任意选取，若沿 x 轴水平抛出，求解之后系统的运动情况，如下图示意。



- 系统拉格朗日量

$$L = \frac{1}{2}m\left(\dot{x_1}^2 + \dot{z_1}^2\right) + \frac{1}{2}M\left(\dot{x_2}^2 + \dot{z_2}^2\right) - mgz_1 - Mgz_2 - \frac{1}{2}k\left(\sqrt{(x_1 - x_2)^2 + (z_1 - z_2)^2} - d_0\right)^2$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$$

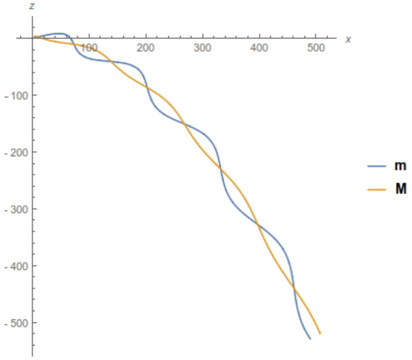
HW3

```
L = 1/2 m ((x1'[t])^2 + (z1'[t])^2) + 1/2 M ((x2'[t])^2 + (z2'[t])^2) - m g z1[t] - M g z2[t] -
    1/2 k (Sqrt[(x1[t] - x2[t])^2 + (z1[t] - z2[t])^2] - d0)^2;

m = 1; M = 3; g = 10; k = 5; d0 = 2;

Eq = {D[D[L, x1'[t]], t] == D[L, x1[t]],  D[D[L, x2'[t]], t] == D[L, x2[t]],
      偏导                  偏导             偏导                   偏导
   D[D[L, z1'[t]], t] == D[L, z1[t]],  D[D[L, z2'[t]], t] == D[L, z2[t]]};
   偏导                  偏导             偏导                  偏导

X0 = {x1[0] == 0, z1[0] == 0, x1'[0] == 80, z1'[0] == 20, x2[0] == 4, z2[0] == 4, x2'[0] == 40, z2'[0] == -10};
result = NDSolve[{Eq, X0}, {x1, z1, x2, z2}, {t, 0, 10}];
         数值求解微分方程组
ParametricPlot[{Evaluate[{x1[t], z1[t]} /. result], Evaluate[{x2[t], z2[t]} /. result]},
绘制参数图        计算                                    计算
 {t, 0, 10}, PlotLegends → {"m", "M"}, AxesLabel → {x, z}]
             绘图的图例                    坐标轴标签
```



HW4

- RK45 算法精度分析

常微分方程: $\begin{cases} y'(x) = f(x, y) \\ y(x_0) = y_0 \end{cases}$ $\quad a \leqslant x \leqslant b$

Taylor 展开至四阶

$$
\begin{cases}
y(x_{n+1}) = y_(x_n) + hy'(x_n) + \dfrac{h^2}{2}y''(x_n) + \dfrac{h^3}{3!}y'''(x_n) + \dfrac{h^4}{4!}y''''(x_n) + \mathrm{O}(h^5) \\
y'(x_n) = f(x_n, y_n) \\
y''(x_n) = f^{(1,0)}(x_n, y_n) + f^{(0,1)}(x_n, y_n) f(x_n, y_n) \\
y'''(x_n) = f(x_n, y_n)^2 f^{(0,2)}(x_n, y_n) + f^{(0,1)}(x_n, y_n) f^{(1,0)}(x_n, y_n) + f(x_n, y_n) \\
\qquad \cdot \left(f^{(0,1)}(x_n, y_n)^2 + 2f^{(1,1)}(x_n, y_n)\right) + f^{(2,0)}(x_n, y_n) \\
y''''(x_n) = f(x_n, y_n)^3 f^{(0,3)}(x_n, y_n) + f^{(1,0)}(x_n, y_n)\left(f^{(0,1)}(x_n, y_n)^2 + 3f^{(1,1)}(x_n, y_n)\right) + f(x_n, y_n)^2 \\
\qquad \cdot \left(4f^{(0,1)}(x_n, y_n) f^{(0,2)}(x_n, y_n) + 3f^{(1,2)}(x_n, y_n)\right) + f^{(0,1)}(x_n, y_n) f^{(2,0)}(x_n, y_n) + f(x_n, y_n) \\
\qquad \cdot \left(f^{(0,1)}(x_n, y_n)^3 + 5f^{(0,1)}(x_n, y_n) f^{(1,1)}(x_n, y_n) + 3\left(f^{(0,2)}(x_n, y_n) f^{(1,0)}(x_n, y_n) + f^{(2,1)}(x_n, y_n)\right)\right) \\
\qquad + f^{(3,0)}(x_n, y_n)
\end{cases}
$$

HW4

- Runge-Kutta45 形式

```
k1 = f[x, y];
k2 = f[x + a h, y + b h k1];
k3 = f[x + c h, y + d1 h k1 + d2 h k2];
k4 = f[x + e h, y + g1 h k1 + g2 h k2 + g3 h k3];
ynadd1 = y + h (c1 k1 + c2 k2 + c3 k3 + c4 k4);

ys = FullSimplify[Series[ynadd1, {h, 0, 4}]]
     |完全简化        |级数
```

$$
\begin{aligned}
& y + (c1 + c2 + c3 + c4)\, f[x, y]\, h + \\
& \left((b\, c2 + c3\, (d1 + d2) + c4\, (g1 + g2 + g3))\, f[x, y]\, f^{(0,1)}[x, y] + (a\, c2 + c\, c3 + c4\, e)\, f^{(1,0)}[x, y]\right) h^2 + \\
& \frac{1}{2} \left(\left(b^2\, c2 + c3\, (d1 + d2)^2 + c4\, (g1 + g2 + g3)^2\right) f[x, y]^2\, f^{(0,2)}[x, y] + \right. \\
& \quad 2\, (a\, c3\, d2 + a\, c4\, g2 + c\, c4\, g3)\, f^{(0,1)}[x, y]\, f^{(1,0)}[x, y] + 2\, f[x, y] \\
& \quad \left((b\, (c3\, d2 + c4\, g2) + c4\, (d1 + d2)\, g3)\, f^{(0,1)}[x, y]^2 + (a\, b\, c2 + c\, c3\, (d1 + d2) + c4\, e\, (g1 + g2 + g3))\, f^{(1,1)}[x, y]\right) + \\
& \quad \left.\left(a^2\, c2 + c^2\, c3 + c4\, e^2\right) f^{(2,0)}[x, y]\right) h^3 + \frac{1}{6} \left(\left(b^3\, c2 + c3\, (d1 + d2)^3 + c4\, (g1 + g2 + g3)^3\right) f[x, y]^3\, f^{(0,3)}[x, y] + \right. \\
& \quad 6\, f^{(1,0)}[x, y] \left(a\, c4\, d2\, g3\, f^{(0,1)}[x, y]^2 + (a\, c\, c3\, d2 + a\, c4\, e\, g2 + c\, c4\, e\, g3)\, f^{(1,1)}[x, y]\right) + 3\, f[x, y]^2 \\
& \quad \left(\left(b^2\, (c3\, d2 + c4\, g2) + c4\, (d1 + d2)\, g3\, (d1 + d2 + 2\, (g1 + g2 + g3)) + 2\, b\, (c3\, d2\, (d1 + d2) + c4\, g2\, (g1 + g2 + g3))\right)\right. \\
& \quad\quad \left. f^{(0,1)}[x, y]\, f^{(0,2)}[x, y] + \left(a\, b^2\, c2 + c\, c3\, (d1 + d2)^2 + c4\, e\, (g1 + g2 + g3)^2\right) f^{(1,2)}[x, y]\right) + \\
& \quad 3 \left(a^2\, (c3\, d2 + c4\, g2) + c^2\, c4\, g3\right) f^{(0,1)}[x, y]\, f^{(2,0)}[x, y] + 3\, f[x, y] \left(2\, b\, c4\, d2\, g3\, f^{(0,1)}[x, y]^3 + \right. \\
& \quad\quad 2\, (c\, c4\, g3\, (g1 + g2 + g3) + a\, (c3\, d2\, (d1 + d2) + c4\, g2\, (g1 + g2 + g3)))\, f^{(0,2)}[x, y]\, f^{(1,0)}[x, y] + \\
& \quad\quad 2\, (b\, (a + c)\, c3\, d2 + b\, c4\, (a + e)\, g2 + c4\, (d1 + d2)\, (c + e)\, g3)\, f^{(0,1)}[x, y]\, f^{(1,1)}[x, y] + \\
& \quad\quad \left.\left.\left(a^2\, b\, c2 + c^2\, c3\, (d1 + d2) + c4\, e^2\, (g1 + g2 + g3)\right) f^{(2,1)}[x, y]\right) + \left(a^3\, c2 + c^3\, c3 + c4\, e^3\right) f^{(3,0)}[x, y]\right) h^4 + O[h]^5
\end{aligned}
$$

HW4

- 与 Taylor 展开系数对比

$$\begin{cases} y_{n+1} = y_n + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) \\ k_1 = f(x_n, y_n) \\ k_2 = f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1\right) \\ k_3 = f\left(x_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2\right) \\ k_4 = f(x_n + h, y_n + hk_3) \end{cases}$$

- RK45 的精度为 $O(h^4)$, 误差为 $O(h^5)$

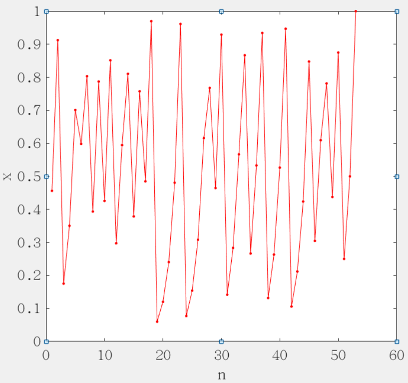
HW5

- Baker's map, 产生随机序列，画出点图。

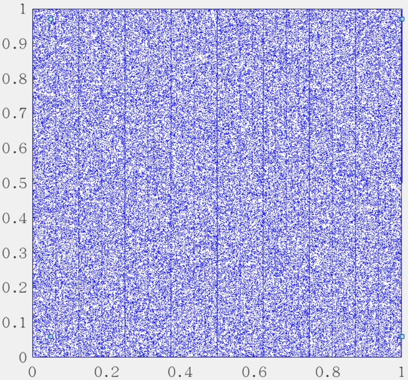
$$S(x,y) = \begin{cases} (2x, y/2), 0 \leq x < 1/2 \\ (2-2x, 1-y/2), 1/2 \leq x < 1 \end{cases}$$

```
clc
clear
for m=1:3000
    x0 = rand(1,1);
    y0 = rand(1,1);
    for n = 1:100
        if x0>=0&&x0<0.5
            x(n) = 2*x0;
            y(n) = y0/2;
            x0 = x(n);y0 = y(n);
        else if x0>=0.5&&x0<1
                x(n) = 2-2*x0;
                y(n) = 1-y0/2;
                x0 = x(n);y0 = y(n);
            end
        end
    end
hold on
scatter(x,y,1,'b','filled')
clear('x','y')
end
```

HW5



x
n
0
10
20
30
40
50
60
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



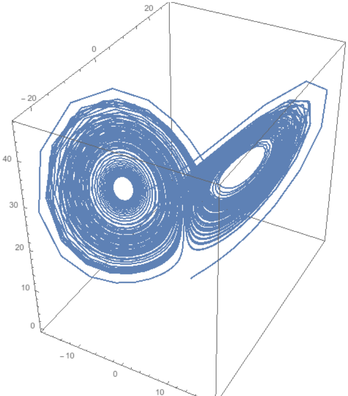
0
0.2
0.4
0.6
0.8
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

HW6

- Lorenz Attractor 自选参数，画出系统运动轨迹。

$$\begin{cases} x' = -\sigma(x-y) \\ y' = x(\rho - z) - y \\ z' = xy - \beta z \end{cases}$$

```
σ = 10; ρ = 28; β = 8 / 3;
s = NDSolve[{x'[t] == -σ (x[t] - y[t]), y'[t] == x[t] (ρ - z[t]) - y[t],
    数值求解微分方程组
     z'[t] == x[t] y[t] - β z[t], x[0] == 1, y[0] == 1, z[0] == 1}, {x, y, z},
    {t, 0, 100}];
ParametricPlot3D[Evaluate[{{x[t], y[t], z[t]}} /. s], {t, 0, 100}]
绘制三维参数图          计算
```



HW7

- 计算 GOE($\beta = 1$),GUE($\beta = 2$),GSE($\beta = 4$)
  (1). 能级间距比分布 $P(r)$，(2). 半圆率，(3). 换不同随机数计算，如均匀、正态分布等。矩阵大小可以选择 100*100, 平均 1000 次。
- 能级间距：$S_n = E_{n+1} - E_n$，能级间距比：

$$r_n = \frac{\min\left(S_n, S_{n+1}\right)}{\max\left(S_n, S_{n+1}\right)}$$

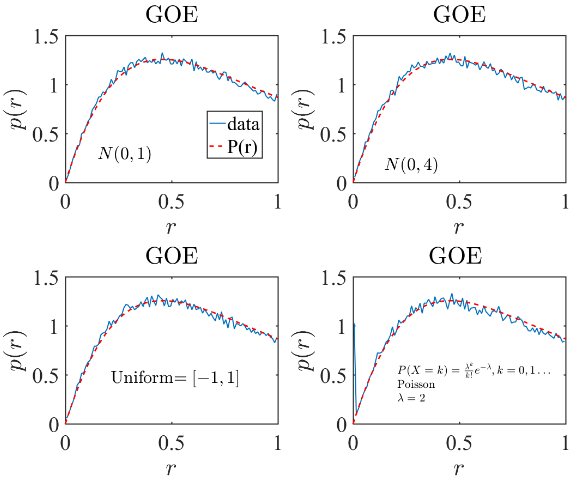
  $P(r)$ 函数：

$$P(r) = \frac{1}{Z_\beta} \frac{\left(r + r^2\right)^\beta}{\left(1 + r + r^2\right)^{1+3\beta/2}}$$

- 半圆率
  $N \to \infty \Rightarrow$ Semicircle Rule: $p(x) = \frac{1}{2\pi}\sqrt{4 - x^2}$

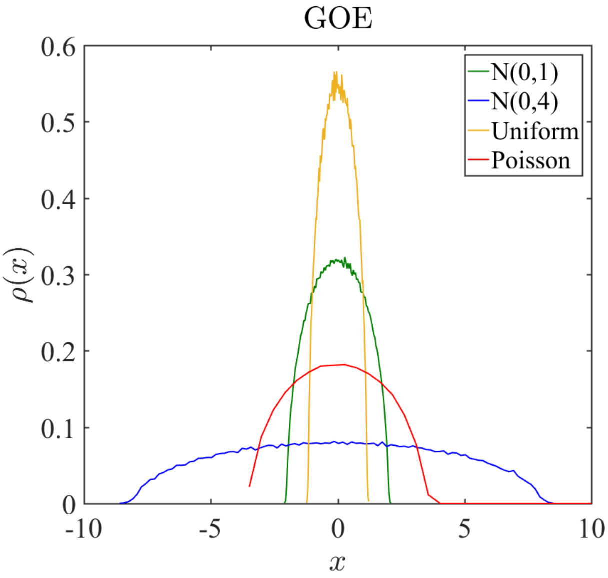
HW7

- 能级间距比分布 $P(r)$



HW7

- 半圆率



HW7

- GSE:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \frac{1}{2}(a+d)I - \frac{i}{2}(a-d)e_1 - \frac{1}{2}(b-c)e_2 + \frac{i}{2}(b+c)e_3$$

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad e_1 = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad e_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad e_3 = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}$$

能级两两简并，所以在计算时要注意，只需取能级的一半：
E = E(1:2:end) or E = E(2:2:end)

HW8

- 计算四个粒子 $\langle x_1x_2x_3x_4 \,|\partial x_1|\, x_1x_2x_3x_4\rangle$
- $|x_1x_2x_3x_4\rangle = a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger|0\rangle$

$$\begin{aligned}
\langle x_1x_2x_3x_4 \,|\partial x_1|\, x_1x_2x_4x_4\rangle &= \left\langle 0 \left| a_1 a_2 a_3 a_4 \partial x_1 a_1^\dagger a_2^\dagger a_3^\dagger a_4^\dagger \right| 0 \right\rangle \\
&= \left\langle 0 \left| a_1 a_2 a_3 \partial x_1 a_1^\dagger a_2^\dagger a_3^\dagger a_4 a_4^\dagger \right| 0 \right\rangle \\
&= \left\langle 0 \left| a_1 a_2 a_3 \partial x_1 a_1^\dagger a_2^\dagger a_3^\dagger \left(1 + a_4^\dagger a_4\right) \right| 0 \right\rangle \\
&= \left\langle 0 \left| a_1 a_2 a_3 \partial x_1 a_1^\dagger a_2^\dagger a_3^\dagger \right| 0 \right\rangle \\
&= \left\langle 0 \left| a_1 \partial x_1 a_1^\dagger \right| 0 \right\rangle \\
&= \langle x_1 \,|\partial x_1|\, x_1\rangle
\end{aligned}$$

HW9

- 相互作用项 $\int dxdy\Psi^\dagger(x)\Psi^\dagger(y)g\delta(x-y)\Psi(y)\Psi(x) = g\sum_{n_1 n_2 n_3 n_4} C^\dagger_{n_1} C^\dagger_{n_2} C_{n_3} C_{n_4} \int W^*_{n_1} W^*_{n_2} W_{n_3} W_{n_4} dx$, 若 C_n 为费米子，做最低阶近似。

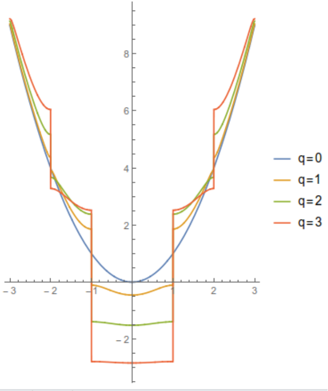
$$\sum_{n_1 n_2 n_3 n_4} C^\dagger_{n_1} C^\dagger_{n_2} C_{n_3} C_{n_4} \int W^*_{n_1} W^*_{n_2} W_{n_3} W_{n_4} dx$$
$$= \sum_i C^\dagger_i C^\dagger_{i+1} C_i C_{i+1} \int W^*_i W^*_{i+1} W_i W_{i+1} dx$$
$$\Rightarrow U n_i n_{i+1}$$

$n_i = C^\dagger_i C_i$

HW10

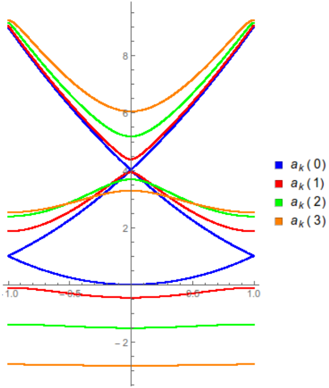
- Mathematica 里 Mathieu 函数．(1) 画能带 (变化 q 的大小)，(2) 画出 Bloch 波函数，(3) 计算 Wannier 函数 (Mathematica 编程计算)
- (1).

```
Plot[Table[MathieuCharacteristicA[k, q], {q, 0, 3}] // Evaluate, {k, -3, 3},
|绘图   |表格    |马提厄偶函数特征值                                   |计算
 PlotLegends → LineLegend[{"q=0", "q=1", "q=2", "q=3"}], AspectRatio → 1.5]
 |绘图的图例    |线的图例                                    |宽高比
```



HW10

```
Block[{range = {-1., 1} 2.999, n = 5000, translate = Mod[# + 1, 2] - 1 &, grid, data, datareduced},
|块                                                  |模余
  grid = Subdivide[Sequence @@ range, n];
         |等分划分    |序列
  data = Table[{#, MathieuCharacteristicA[#, q]} & ~ ParallelMap ~ grid, {q, 0, 3}];
         |表格       |马提厄偶函数特征值              |并行映射
  datareduced = MapAt[translate, data, {All, All, 1}];
                |作用于                   |全部 |全部
  ListPlot[datareduced, AspectRatio → 1.5, PlotLegends → SwatchLegend[Array[StringTemplate["a_k(``)"], 5, 0]],
  |绘制点集              |宽高比            |绘图的图例      |样本图例      |数组   |字符串模板
   PlotStyle → Thread[{{Blue, Red, Green, Orange}, PointSize[.005]}]]]
   |绘图样式    |逐项作用  |蓝色  |红色 |绿色   |橙色     |点的大小
```

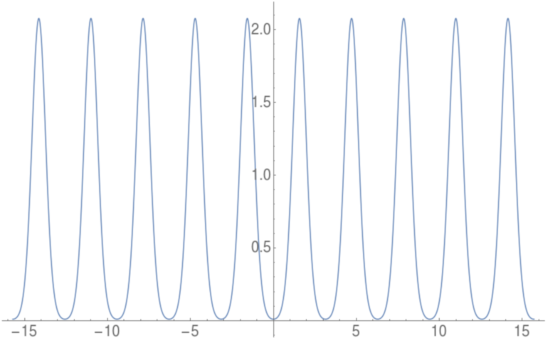


From 曾俊杰

HWIO

▸ (2)

```
ψ[k_, q_] := MathieuC[MathieuCharacteristicA[k, q], q, z] +
             马提厄偶函数 马提厄偶函数特征值
   I MathieuS[MathieuCharacteristicB[k, q], q, z];
   ·· 马提厄奇函数 马提厄奇函数特征值
Plot[Abs[ψ[0.2, 10]], {z, -5 π, 5 π}]
绘图  绝对值
```



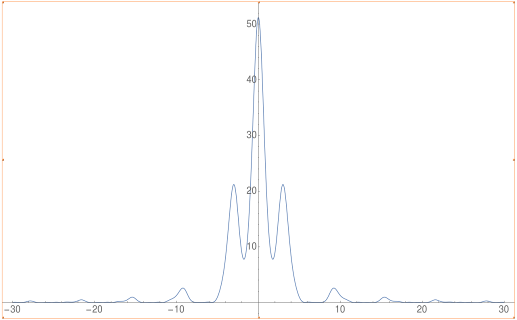
HW10

- (3)

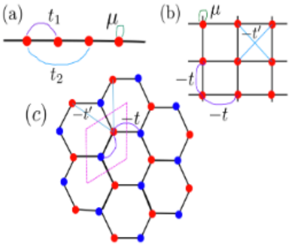
$$\psi_{nk(r)} = N^{-1/2} \sum_{l} e^{ik\cdot R} w_n(r-R)$$

$$w_n(r-R) = N^{-1/2} \sum_{k\in BZ} e^{-ik\cdot R} \psi_{nk}(r)$$

```
Wannier = 0.0; n = 30; q = -0.5;
For[i = 0, i < n, i++,
For循环
  Wannier = Wannier + 1 / Sqrt[n] (Exp[-I k R] (MathieuC[MathieuCharacteristicA[k, q], q, x] +
                          平方根    指…    虚数单位 马提厄偶函数 马提厄偶函数特征值
        I MathieuS[MathieuCharacteristicA[k, q], q, x]) /. {k → -1 + 2 i / n , R → 0})];
        ·· 马提厄奇函数 马提厄偶函数特征值
Plot[Abs[Wannier] ^2, {x, -30, 30}, PlotRange → All]
绘图  绝对值                        绘制范围      全部
```



HW11



(1) 图a的k空间H_k表达式；变化参数问什么时候能带从$m^* > 0$变为$m^* < 0$

(2) 图b的k空间H_k表达式；画出能带图．其中$-t$近邻跃迁，$-t'$次近邻跃迁

(3) 图c的Graphene model的k空间H_k表达式；画出能带图；什么时候出现Dirac点．其中$-t$近邻跃迁，$-t'$次近邻跃迁

(4) 将以下两个动量空间的哈密顿量变到实空间，并在正方形格子中画出Tight-Binding model

$$H_1 = \frac{k_x^2+k_y^2}{2m} + \lambda(k_x\sigma_x - k_y\sigma_y) - \mu$$

$$H_2 = \frac{k_x^2+k_y^2}{2m} + \lambda(k_x\sigma_y - k_y\sigma_x) - \mu$$

(5) 写出下面哈密顿量的Tight-Binding model

$$H = \begin{pmatrix} k^2 - \mu & \alpha\left(k_x + \mathrm{i}k_y\right) \\ \alpha\left(k_x - \mathrm{i}k_y\right) & \mu - k^2 \end{pmatrix}$$

HW11

- (1)

$$H=\Sigma_i\left[-t_1\left(c_i^\dagger c_{i+1}+\mathrm{hc.}\right)-t_2\left(c_i^\dagger c_{i+2}+\mathrm{hc.}\right)-\mu c_i^\dagger c_i\right]$$

FT $:c_n=\frac{1}{\sqrt{N}}\sum_k c_k e^{ikn}$

$\Rightarrow \qquad H_k=-\sum_k[2t_1\cos k+2t_2\cos 2k+\mu]c_k^\dagger c_k$

有效质量

$$\frac{1}{m^*}=\frac{\partial^2 E_k}{\partial k^2}$$

```
Ek = -(2 t1 Cos[k] + 2 t2 Cos[2 k] + u);
       余弦            余弦
m = FullSimplify[1 / D[D[Ek, k], k]]
    完全简化            偏导
FullSimplify[Series[m, {k, 0, 1}]]
完全简化      级数
```

$$\frac{1}{2\,t1\,\mathrm{Cos}[k]+8\,t2\,\mathrm{Cos}[2\,k]}$$

$$\frac{1}{2\,t1+8\,t2}+O[k]^2$$

$k\to 0$, If $t_1+4t_2>0$, then $m^*>0$; If $t_1+4t_2<0$, then $m^*<0$

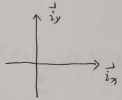
HWII

- (2)

$$H = -t \sum_{\langle \vec{n},\vec{m}\rangle} \left(C_{\vec{n}}^{+} C_{\vec{m}} + h.c \right) - t' \sum_{\langle\langle \vec{n},\vec{m}\rangle\rangle} \left(C_{\vec{n}}^{+} C_{\vec{m}} + h.c \right) - \mu \sum_{\vec{n}} C_{\vec{n}}^{+} C_{\vec{n}}$$

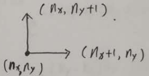
$\langle \vec{n},\vec{m}\rangle$ 近临　　　$\vec{n} = n_x \vec{i}_x + n_y \vec{i}_y$

$\langle\langle n,\vec{m}\rangle\rangle$ 次近临



FT: $C_{\vec{n}} = \frac{1}{\sqrt{N_x N_y}} \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{n}}$

① $\langle \vec{n},\vec{m}\rangle$: $\begin{cases} (n_x, n_y) \to (n_x, n_y+1) \\ (n_x, n_y) \to (n_x+1, n_y). \end{cases}$



$$\sum_{\langle \vec{n},\vec{m}\rangle} C_{\vec{n}}^{+} C_{\vec{m}} + h.c$$

$$= \frac{1}{N_x N_y} \sum_{\langle \vec{n},\vec{m}\rangle} \sum_{\vec{k}\vec{k}'} C_{\vec{k}}^{+} e^{-i\vec{k}\cdot\vec{n}} \quad C_{\vec{k}'} e^{i\vec{k}'\cdot\vec{m}} + h.c$$

$$= \frac{1}{N_x N_y} \sum_{\langle \vec{n},\vec{m}\rangle} \sum_{\vec{k}\vec{k}'} C_{\vec{k}}^{+} C_{\vec{k}'} \; e^{-i(k_x n_x + k_y n_y)} \; e^{i(k'_x m_x + k'_y m_y)} + h.c$$

$$= \frac{1}{N_x N_y} \sum_{\langle \vec{n},\vec{m}\rangle} \sum_{\vec{k}\vec{k}'} C_{\vec{k}}^{+} C_{\vec{k}'} \; e^{-i(k_x n_x - k'_x m_x)} \; e^{-i(k_y n_y - k'_y m_y)} + h.c$$

$$= \sum_{\vec{k}} \left(2\cos k_x + 2\cos k_y \right) C_{\vec{k}}^{+} C_{\vec{k}}$$

HW11

- (2)

② $\langle\langle \vec{n}, \vec{m} \rangle\rangle$: $\begin{cases} (n_x, n_y) \to (n_x+1, n_y+1) \\ (n_x, n_y) \to (n_x+1, n_y-1) \end{cases}$

$$\sum_{\langle\langle \vec{n}, \vec{m}\rangle\rangle} C^\dagger_{\vec{n}} C_{\vec{m}} + h.c.$$

$$= \frac{1}{N_x N_y} \sum_{\langle\langle \vec{n}, \vec{m}\rangle\rangle} \sum_{\vec{k}\vec{k}'} C^\dagger_{\vec{k}} C_{\vec{k}'} e^{-i(k_x n_x - k'_x m_x)} e^{-i(k_y n_y - k'_y m_y)} + h.c.$$

$$= \frac{1}{N_x N_y} \sum_{\langle\langle \vec{n}, \vec{n}\rangle\rangle} \sum_{\vec{k}\vec{k}'} C^\dagger_{\vec{k}} C_{\vec{k}'} \Big[e^{-i(k_x - k'_x)n_x + i k'_x} e^{-i(k_y - k'_y)n_y + i k'_y} + e^{-i(k_x - k'_x)n_x + i k'_x} e^{-i(k_y - k'_y)n_y - i k'_y} \Big] + h.c.$$

$$= \sum_{\vec{k}} \left(\left[e^{i(k_x + k_y)} + e^{i(k_x - k_y)} \right] + h.c. \right) C^\dagger_{\vec{k}} C_{\vec{k}}$$

$$= \sum_{\vec{k}} \left(2\cos(k_x + k_y) + 2\cos(k_x - k_y) \right) C^\dagger_{\vec{k}} C_{\vec{k}}$$

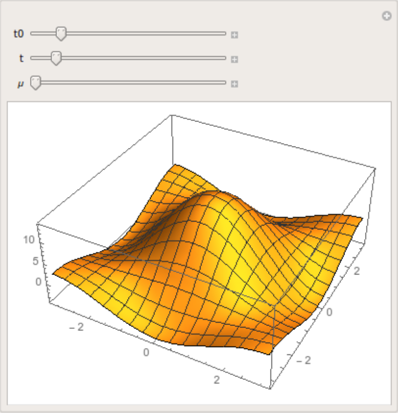
$$= \sum_{\vec{k}} 4 \cos k_x \cos k_y \, C^\dagger_{\vec{k}} C_{\vec{k}}.$$

HW11

- (2)

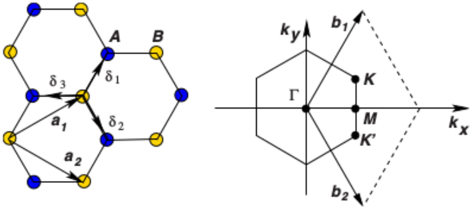
$$H_k = \sum_{\vec{k}} \underbrace{\left[-2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu\right]}_{E_k} C^{\dagger}_{\vec{k}} C_{\vec{k}}$$

```
Manipulate[Plot3D[-2 t0 (Cos[kx] + Cos[ky]) - 4 t Cos[kx] Cos[ky] - μ,
交互式操作    绘制三维图形    余弦    余弦    余弦    余弦
  {kx, -π, π}, {ky, -π, π}], {t0, -2, 2}, {t, -2, 2}, {μ, -2, 2}]
```



HW11

- (3) Graphene model



$$a_1 = \frac{a}{2}(3, \sqrt{3}), \quad a_2 = \frac{a}{2}(3, -\sqrt{3})$$

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}) \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3}) \quad \delta_3 = -a(1, 0)$$

Tight-binding Hamiltonian

$$H = -t \sum \sum_{\langle i,j \rangle} \left(a_i^\dagger b_j + \text{h.c.} \right)$$
$$- t' \sum_{\langle\langle i,j \rangle\rangle} \left(a_i^\dagger a_j + b_i^\dagger b_j + \text{h.c.} \right)$$

HW11

- (3) FT

$$a_{\vec{n}} = \frac{1}{\sqrt{N}} \sum a_{\vec{k}} e^{i\vec{k}\cdot\vec{n}}$$

$$b_{\vec{n}} = \frac{1}{\sqrt{N}} \sum b_{\vec{k}} e^{i\vec{k}\cdot\vec{n}}$$

- 对角化

$$E_{\pm}(\mathbf{k}) = \pm t\sqrt{3 + f(\mathbf{k})} - t' f(\mathbf{k})$$

$$f(\mathbf{k}) = 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\cos\left(\frac{3}{2}k_x a\right)$$

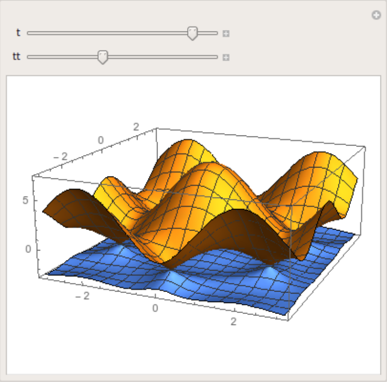
- Dirac points:

$$\boldsymbol{K} = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right), \quad \boldsymbol{K}' = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$$

Ref: Neto, AH Castro, et al. "The electronic properties of graphene." Reviews of modern physics 81.1 (2009): 109.

HW11

```
Manipulate[
交互式操作
 Plot3D[{t Sqrt[3 + 2 Cos[Sqrt[3] ky ] + 4 Cos[Sqrt[3] / 2 ky ] Cos[3 / 2 kx]] -
 绘制三维图形 平方根 余弦 平方根 余弦 平方根 余弦
    tt (2 Cos[Sqrt[3] ky ] + 4 Cos[Sqrt[3] / 2 ky ] Cos[3 / 2 kx]),
       余弦 平方根 余弦 平方根 余弦
   - t Sqrt[3 + 2 Cos[Sqrt[3] ky ] + 4 Cos[Sqrt[3] / 2 ky ] Cos[3 / 2 kx]] -
     平方根 余弦 平方根 余弦 平方根 余弦
    tt (2 Cos[Sqrt[3] ky ] + 4 Cos[Sqrt[3] / 2 ky ] Cos[3 / 2 kx])}, {kx, -π, π},
       余弦 平方根 余弦 平方根 余弦
  {ky, -π, π}], {t, -2, 2}, {tt, -2, 2}]
```



HW11

- (4) 利用变换: $\sum_n \left(\lambda c^\dagger_{n\uparrow} c_{n+1\downarrow} + \lambda c^\dagger_{n\downarrow} c_{n+1\uparrow} + \text{ h.c. }\right)$

  If $\lambda = 1 \Rightarrow \sum_k \left(2\cos k c^\dagger_{k\uparrow} c_{k\downarrow} + h.c.\right)$

  If $\lambda = i \Rightarrow \sum_k \left(-2\sin k c^\dagger_{k\uparrow} c_{k\downarrow} + h.c.\right)$

$$H_1 = \frac{k_x^2 + k_y^2}{2m} + \lambda (k_x \sigma_x - k_y \sigma_y) - \mu .$$

$$\frac{k_x^2 + k_y^2}{2m} \longrightarrow -2t(\cos k_x + \cos k_y)$$

$$k_x \to \sin k_x \qquad k_y \longrightarrow \sin k_y$$

$$H_1 = -2t(\cos k_x + \cos k_y) + \lambda(\sin k_x \sigma_x - \sin k_y \sigma_y) - \mu$$

$$= -2t(\cos k_x + \cos k_y) + \lambda \begin{pmatrix} 0 & \sin k_x + i \sin k_y \\ \sin k_x - i \sin k_y & 0 \end{pmatrix} - \mu$$

$$= \begin{pmatrix} -2t(\cos k_x + \cos k_y) - \mu & \lambda(\sin k_x + i \sin k_y) \\ \lambda(\sin k_x - i\sin k_y) & -2t(\cos k_x + \cos k_y) - \mu \end{pmatrix}.$$

$$\Rightarrow \sum_k (c^\dagger_{k\uparrow} \quad c^\dagger_{k\downarrow}) \, H_1(k) \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}. \qquad \sigma = \{\uparrow, \downarrow\}$$

HW11

- (4)

$$\Rightarrow H_1(k) = \sum_{k\sigma} [-2t(\cos k_x + \cos k_y) - \mu] c^\dagger_{k\sigma} c_{k\sigma}$$

$$+ \lambda \sum_k [(\sin k_x + i \sin k_y) c^\dagger_{k\uparrow} c_{k\downarrow} + (\sin k_x - i \sin k_y) c^\dagger_{k\downarrow} c_{k\uparrow}]$$

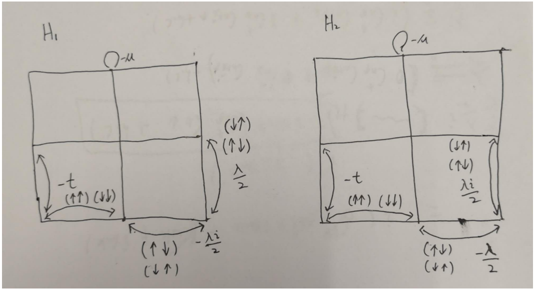
$$= \sum_{k\sigma} [-2t(\cos k_x + \cos k_y) - \mu] c^\dagger_{k\sigma} c_{k\sigma}$$

$$+ \lambda \sum_k (\sin k_x \, c^\dagger_{k\uparrow} c_{k\downarrow} + h.c) + \lambda \sum_k (i \sin k_y \, c^\dagger_{k\uparrow} c_{k\downarrow} + h.c)$$

$$= \sum_{\langle n,m \rangle} (-t c^\dagger_{n\sigma} c_{m\sigma} + h.c) + \sum_n -\mu c^\dagger_{n\sigma} c_{n\sigma}$$

$$+ \sum_n \left[-\frac{\lambda i}{2} (c^\dagger_{n\uparrow} c_{n+\hat{x}\downarrow} + c^\dagger_{n\downarrow} c_{n+\hat{x}\uparrow}) + h.c \right]$$

$$+ \sum_n \left[\frac{\lambda}{2} (c^\dagger_{n\uparrow} c_{n+\hat{y}\downarrow} + c^\dagger_{n\downarrow} c_{n+\hat{y}\uparrow}) + h.c \right]$$



HW11

- (5)

$$H = \begin{pmatrix} k^2 - \mu & \alpha(k_x + i k_y) \\ \alpha(k_x - i k_y) & \mu - k^2 \end{pmatrix}$$

$$= \begin{pmatrix} c_{k\uparrow}^{+} & c_{k\downarrow}^{+} \end{pmatrix} \begin{pmatrix} -2t(\cos k_x + \cos k_y) - \mu & \alpha(\sin k_x + i \sin k_y) \\ \alpha(\sin k_x - i \sin k_y) & \mu + 2t(\cos k_x + \cos k_y) \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix}$$

$$\Rightarrow H = -t \sum_{\langle n,m \rangle} \left(c_{n\uparrow}^{+} c_{m\uparrow} - c_{n\downarrow}^{+} c_{m\downarrow} + h.c. \right)$$

$$- \mu \sum_{n} \left(c_{n\uparrow}^{+} c_{n\uparrow} - c_{n\downarrow}^{+} c_{n\downarrow} \right)$$

$$+ \sum_{n} \left[-\frac{\alpha i}{2} \left(c_{n\uparrow}^{+} c_{n+\hat{x}\downarrow} + c_{n\downarrow}^{+} c_{n+\hat{x}\uparrow} \right) + h.c. \right]$$

$$+ \sum_{n} \left[\frac{\alpha}{2} \left(c_{n\uparrow}^{+} c_{n+\hat{y}\downarrow} + c_{n\downarrow}^{+} c_{n+\hat{y}\uparrow} \right) + h.c. \right]$$

HW12

- 利用差分方法求解下列哈密顿量

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$
$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \alpha x^4$$

差分：

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} = -\frac{\hbar^2}{2m}\frac{1}{(\delta x)^2}\begin{pmatrix} -2 & 1 & 0 & \ddots \\ 1 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & 1 \\ \ddots & 0 & 1 & -2 \end{pmatrix}$$

HW12

- $$\frac{1}{2}m\omega^2 x^2 = \frac{1}{2}m\omega^2 \begin{pmatrix} x_1^2 & \cdots & \ddots \\ \vdots & \ddots & \vdots \\ \ddots & \cdots & x_N^2 \end{pmatrix}$$

$$\alpha x^4 = \alpha \begin{pmatrix} x_1^4 & \cdots & \ddots \\ \vdots & \ddots & \vdots \\ \ddots & \cdots & x_N^4 \end{pmatrix}$$

例如：$x \in [-1, 1]$, $\delta x = 0.002$, $N = 1001$

HW13

- 三体系统在平衡位置附近的震动问题：

$H = p_1^2 + p_2^2 + p_3^2 + \omega^2(x_1^2 + x_2^2 + x_3^2) + \alpha(x_1x_2 + x_1x_3 + x_2x_3)$ (1). 求系统的震动过程以及频率；(2). 转化为Bose子模型再求解；(3). 证明(1)与(2)等价（相同的一套代数）。

- (2)

$$\begin{cases} \dot{q}_i = \frac{\partial H}{\partial P_i} \\ \dot{p}_i = -\frac{\partial H}{\partial q_i} \end{cases}$$

$$\Rightarrow X = \begin{pmatrix} q \\ p \end{pmatrix} \Rightarrow \dot{X} = DX \Rightarrow$$

解为：

$$\Rightarrow X \sim \sum_i X_i e^{i\omega_i t} \Rightarrow i\omega X = DX$$

- (2)

$$\begin{cases} p_i = -i\left(a_i - a_i^+\right)\sqrt{\frac{\omega}{2}} \\ x_i = \left(a_i + a_i^+\right)/\sqrt{2\omega} \end{cases}$$

HW13

$$D1 = \begin{pmatrix} 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \\ -2\omega^2 & -\alpha & -\alpha & 0 & 0 & 0 \\ -\alpha & -2\omega^2 & -\alpha & 0 & 0 & 0 \\ -\alpha & -\alpha & -2\omega^2 & 0 & 0 & 0 \end{pmatrix}; \quad D2 = \begin{pmatrix} 2\omega & \frac{\alpha}{2\omega} & \frac{\alpha}{2\omega} & 0 & \frac{\alpha}{2\omega} & \frac{\alpha}{2\omega} \\ \frac{\alpha}{2\omega} & 2\omega & \frac{\alpha}{2\omega} & \frac{\alpha}{2\omega} & 0 & \frac{\alpha}{2\omega} \\ \frac{\alpha}{2\omega} & \frac{\alpha}{2\omega} & 2\omega & \frac{\alpha}{2\omega} & \frac{\alpha}{2\omega} & 0 \\ 0 & -\frac{\alpha}{2\omega} & -\frac{\alpha}{2\omega} & -2\omega & -\frac{\alpha}{2\omega} & -\frac{\alpha}{2\omega} \\ -\frac{\alpha}{2\omega} & 0 & -\frac{\alpha}{2\omega} & -\frac{\alpha}{2\omega} & -2\omega & -\frac{\alpha}{2\omega} \\ -\frac{\alpha}{2\omega} & -\frac{\alpha}{2\omega} & 0 & -\frac{\alpha}{2\omega} & -\frac{\alpha}{2\omega} & -2\omega \end{pmatrix};$$

```
E1 = Eigenvalues[-I D1]
```
特征值 虚数单位

```
E2 = Eigenvalues[D2]
```
特征值

$$\left\{-i\sqrt{2}\sqrt{\alpha-2\omega^2},\ -i\sqrt{2}\sqrt{\alpha-2\omega^2},\ i\sqrt{2}\sqrt{\alpha-2\omega^2},\ i\sqrt{2}\sqrt{\alpha-2\omega^2},\ -2i\sqrt{-\alpha-\omega^2},\ 2i\sqrt{-\alpha-\omega^2}\right\}$$

$$\left\{-\frac{2\sqrt{\alpha\omega^2+\omega^4}}{\omega},\ \frac{2\sqrt{\alpha\omega^2+\omega^4}}{\omega},\ -\frac{\sqrt{2}\sqrt{-\alpha\omega^2+2\omega^4}}{\omega},\ -\frac{\sqrt{2}\sqrt{-\alpha\omega^2+2\omega^4}}{\omega},\ \frac{\sqrt{2}\sqrt{-\alpha\omega^2+2\omega^4}}{\omega},\ \frac{\sqrt{2}\sqrt{-\alpha\omega^2+2\omega^4}}{\omega}\right\}$$

```
E1 /. {α → 0.3, ω → 1.} // Sort
```
排序

```
E2 /. {α → 0.3, ω → 1.} // Sort
```
排序

{-2.28035 + 0. i, -1.84391 + 0. i, -1.84391 + 0. i, 1.84391 + 0. i, 1.84391 + 0. i, 2.28035 + 0. i}

{-2.28035, -1.84391, -1.84391, 1.84391, 1.84391, 2.28035}

HW14

- 多体系统求解：(1). 3 个格点，2 个粒子的 Bose-Hubbard model 计算能谱

$$H = -t\sum_{ij}(b_i^\dagger b_j + h.c.) + \frac{U}{2}\sum_i n_i(n_i - 1)$$

(2). 4 个格点，2 个粒子的 Fermi-Hubbard model 计算能谱

$$H = -t\sum_{ij}(c_i^\dagger c_j + h.c.) + U\sum_i n_i n_{i+1}$$

HW14

$|1\rangle \equiv |200\rangle$

$|2\rangle \equiv |110\rangle$

$|3\rangle \equiv |101\rangle$

$|4\rangle \equiv |020\rangle$

$|5\rangle \equiv |011\rangle$

$|6\rangle \equiv |002\rangle$

$$\begin{cases} b^+ |n\rangle = \sqrt{n+1}\, |n+1\rangle \\ b\, |n\rangle = \sqrt{n}\, |n-1\rangle \end{cases}$$

~~例:~~

$T = -t\,(b_1^+ b_2 + b_2^+ b_3 + b_2^+ b_1 + b_3^+ b_2)$ 开边界

$T = -t\,(b_1^+ b_2 + b_2^+ b_3 + b_3^+ b_1 + b_2^+ b_1 + b_3^+ b_2 + b_1^+ b_3)$ 闭边界.

例① $-t\,(b_1^+ b_2 + b_2^+ b_3 + b_2^+ b_1 + b_3^+ b_2)\,|200\rangle$

$= -t\,(0 + 0 + \sqrt{2}\,|110\rangle + 0) = -t\sqrt{2}\,|110\rangle$

$\Rightarrow \quad H_{12} = -\sqrt{2}\,t$

②: $-t\,(b_1^+ b_2 + b_2^+ b_3 + b_2^+ b_1 + b_3^+ b_2)\,\underset{2}{|110\rangle}$

$= -t\,(\sqrt{2}\,\underset{1}{|200\rangle} + 0 + \sqrt{2}\,\underset{4}{|020\rangle} + \underset{3}{|101\rangle})$

$\Rightarrow \quad H_{21} = -\sqrt{2}\,t, \quad H_{23} = -t, \quad H_{24} = -\sqrt{2}\,t$

HW14

$$H1 = \begin{pmatrix} U & -\sqrt{2}\,t & 0 & 0 & 0 & 0 \\ -\sqrt{2}\,t & 0 & -t & -\sqrt{2}\,t & 0 & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & -\sqrt{2}\,t & 0 & U & -\sqrt{2}\,t & 0 \\ 0 & 0 & -t & -\sqrt{2}\,t & 0 & -\sqrt{2}\,t \\ 0 & 0 & 0 & 0 & -\sqrt{2}\,t & U \end{pmatrix};$$

```
Eigenvalues[H1] /. {U → 0.3, t → 0.8} // Sort
特征值                                    排序
```

{-2.15663, -0.991271, 0.0747542, 0.3, 1.29127, 2.38188}

$$H2 = \begin{pmatrix} U & -t & 0 & 0 & 0 & 0 \\ -t & 0 & -t & -t & 0 & 0 \\ 0 & -t & 0 & 0 & -t & 0 \\ 0 & -t & 0 & U & -t & 0 \\ 0 & 0 & -t & -t & 0 & -t \\ 0 & 0 & 0 & 0 & -t & U \end{pmatrix};$$

```
Eigenvalues[H2] /. {U → 0.3, t → 0.8} // Sort
特征值                                    排序
```

{-1.74588, -0.728508, 0.059899, 0.15, 0.878508, 1.83598}

HW15

- 根据以前步骤 (1) 计算 $[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + A\cos(x)]\psi(x) = \lambda\psi(x)$ 本征值，(2). 检查 N_c 多少时结果收敛，(3). 画出能带和 Mathieus 和 Mathieuc 比较。

$$\begin{bmatrix} \ddots & \ddots & & \ddots & & & \\ & \frac{A}{2} & \frac{\hbar^2}{2m}(k+1)^2 & & \frac{A}{2} & & \\ & & & \frac{A}{2} & \frac{\hbar^2}{2m}k^2 & \frac{A}{2} & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix}$$

HW15

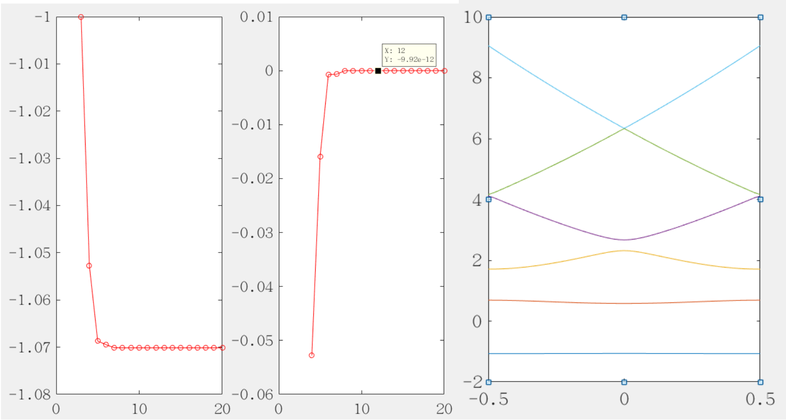
- MATLAB 程序

```
function [ E ] = HW15func( N,kk )
A = 2;
H = zeros(N,N);
for i=1:N-1
   H(i,i+1) = A/2;
end
H = H + H';
for n=1:length(kk)
     k = kk(n);
     for j = 1:N
         H(j,j) = ((N+1)/2+k-j)^2;
         E(:,n) = eig(H);
     end
end
end
```

```
clear
clc
n = 0;
for N = 3:20
     n = n + 1;
     kk = [-0.5:0.02:0.5];
     [ E ] = HW15func( N,kk );
     Emin(n) = min(E(1,:));
end
figure(1)
subplot(1,2,1)
plot(3:20,Emin,'-ro')
subplot(1,2,2)
plot(4:20,diff(Emin),'-ro')
figure(2)
plot(kk,E(1:6,:))
```

HW15

- MATLAB 程序



$$[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (a - 2q\cos(2x))]y = 0$$

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + A\cos(x) - \lambda]\psi(x) = 0$$

HW16

- 找几个任意 2 维图形（矩形，圆，椭圆，操场，心形等），计算本征值以及波函数的空间分布。参考之前 PPT
- MATLAB 程序

```
clc
clear
h=ezplot('-x^2*y^3+(x^2+y^2-1)^3=0',[-1.3,1.3,-1.2,1.4]);
A = h.ZData;
A = A(1:3:end,1:3:end);
a = length(A);
for i=1:a
    for j=1:a
        if A(i,j)>=0
            A(i,j) = 0;
        else
            A(i,j) = 1;
        end
    end
end
```

HW16

```
[h,l] = find(A);
C = find(A);
for i = 1:length(C)
    for j = 1:length(C)
        if i==j
           H(i,j) = -4;
        else if (abs(h(i)-h(j))==0 && abs(l(i)-l(j))==1)...
                 || (abs(l(i)-l(j))==0 && abs(h(i)-h(j))==1)
                H(i,j) = 1;
            else
                H(i,j) = 0;
            end
        end
    end
end
[V,D] = eig(-H);
E=diag(D);
sp = 0;
for k=1:9
    sp = 1+sp;
    subplot(3,3,sp)
for i = 1:length(C)
    M(h(i),l(i)) = abs(V(i,k)).^2;
end
surf(M,'FaceColor','interp','LineStyle','none')
colorbar
colormap(hot)
view(2)
xla=xlabel('$x$');
yla=ylabel('$y$');
zla=zlabel('$|\psi|^2$');
tit =title(strcat('$\psi_{',num2str(k),'}$'));
set([xla,yla,zla,tit],'Interpreter','latex');
set(gca,'linewidth',1.5,'fontsize',20,'fontname','Times');
end
```