计算物理作业 2

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June 14, 2019

HW17

- 求解一维单粒子体系 $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_0\sin(qx)\right]\Psi(x)=E\Psi(x)$，参数自取。
- 正交完备基展开：$\Psi=\sum_n c_n\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

  基矢：$\psi_n=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$

  矩阵元：

  $H_{nm}=\langle\psi_n|H|\psi_m\rangle=\frac{\hbar^2}{2m}\left(\frac{\pi n}{L}\right)^2+\int_0^L V_0\sin(qx)\frac{2}{L}\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)dx$

```
Tnn[n_, n_] := h^2/(2 m) (π n/L)^2;

Vnm[n_, m_] := Integrate[V0 (2 Sin[q x])/L Sin[(n π x)/L] Sin[(m π x)/L], {x, 0, L}];
               积分                        正弦            正弦

H = Tnn + Vnm;
```

HW18

- 两粒子系统 $H = H_0 + V$, 单粒子部分 $H_0 = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dy^2}\right)$，相互作用部分 $V = g\delta(x-y)$。任选 Bose/Fermi 子一种情况求解，并且当 $g \to 0$ 和微扰结果比较。
  $\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$
- Fermion
  基矢 $c_{n_1}^\dagger c_{n_2}^\dagger|0\rangle \equiv |n_1 n_2\rangle = \psi_{n_1}(x)\psi_{n_2}(y) - \psi_{n_2}(x)\psi_{n_1}(y)$
  H_0 部分能量：$\frac{\hbar^2\pi^2}{2mL^2}(n_1^2 + n_2^2)$
  相互作用部分：

```
V = FullSimplify[(ψ[n4, x] ψ[n3, y] - ψ[n3, x] ψ[n4, y]) g DiracDelta[x - y] (ψ[n1, x] ψ[n2, y] - ψ[n2, x] ψ[n1, y])]
    |完全简化                                                |狄拉克δ函数
Vnm = Integrate[V, {x, 0, L}, {y, 0, L}]
      |积分
```

$$\frac{4\, g\, \text{DiracDelta}[x-y]\left(\text{Sin}\left[\frac{n2\,\pi\,x}{L}\right]\text{Sin}\left[\frac{n1\,\pi\,y}{L}\right] - \text{Sin}\left[\frac{n1\,\pi\,x}{L}\right]\text{Sin}\left[\frac{n2\,\pi\,y}{L}\right]\right)\left(-\text{Sin}\left[\frac{n4\,\pi\,x}{L}\right]\text{Sin}\left[\frac{n3\,\pi\,y}{L}\right] + \text{Sin}\left[\frac{n3\,\pi\,x}{L}\right]\text{Sin}\left[\frac{n4\,\pi\,y}{L}\right]\right)}{L^2}$$

0

HW18

- Boson

基矢 $a_{n_1}^\dagger a_{n_2}^\dagger|0\rangle \equiv |n_1 n_2\rangle = \psi_{n_1}(x)\psi_{n_2}(y) + \psi_{n_2}(x)\psi_{n_1}(y), \quad n_1 \neq n_2$

$\frac{1}{\sqrt{2}}(a_n^\dagger)^2|0\rangle = \frac{2}{\sqrt{2}}\psi_n(x)\psi_n(y), \quad n_1 = n_2 = n$

H_0 部分能量: $\frac{\hbar^2\pi^2}{2mL^2}(n_1^2 + n_2^2)$

相互作用部分:

```
V = FullSimplify[(2/√2 ψ[n, x] ψ[n, y]) g DiracDelta[x - y] (2/√2 ψ[n, x] ψ[n, y])]
    完全简化                               狄拉克δ函数

Integrate[V, {x, 0, L}, Assumptions → 0 ≤ y ≤ L] /. {n → 1}
积分                     假设

Integrate[%, {y, 0, L}, Assumptions → L > 0]
积分                     假设
```

Out[43]=

$$\frac{8\, g\, \text{DiracDelta}[x-y]\, \text{Sin}\left[\frac{n\pi x}{L}\right]^2 \text{Sin}\left[\frac{n\pi y}{L}\right]^2}{L^2}$$

Out[44]=

$$\frac{8\, g\, (-1+2\,\text{HeavisideTheta}[L])\, \text{HeavisideTheta}[y - L\,\text{HeavisideTheta}[-L]]\, \text{Sin}\left[\frac{\pi y}{L}\right]^4}{L^2}$$

Out[45]=

$$\frac{3\, g}{L}$$

HW18

相互作用部分矩阵元：

40]:=

```
V = FullSimplify[(ψ[n4, x] ψ[n3, y] + ψ[n3, x] ψ[n4, y]) g DiracDelta[x - y] (ψ[n1, x] ψ[n2, y] + ψ[n2, x] ψ[n1, y])]
    完全简化                                                狄拉克δ函数
Integrate[V, {x, 0, L}, Assumptions → 0 ≤ y ≤ L] /. {n1 → 1, n2 → 2, n3 → 3, n4 → 4}
积分                     假设
Integrate[%, {y, 0, L}, Assumptions → L > 0]
积分                     假设
```

ıt[40]=

$$\frac{4\, g\, \mathrm{DiracDelta}[x-y]\left(\mathrm{Sin}\left[\frac{n2\,\pi\,x}{L}\right]\mathrm{Sin}\left[\frac{n1\,\pi\,y}{L}\right]+\mathrm{Sin}\left[\frac{n1\,\pi\,x}{L}\right]\mathrm{Sin}\left[\frac{n2\,\pi\,y}{L}\right]\right)\left(\mathrm{Sin}\left[\frac{n4\,\pi\,x}{L}\right]\mathrm{Sin}\left[\frac{n3\,\pi\,y}{L}\right]+\mathrm{Sin}\left[\frac{n3\,\pi\,x}{L}\right]\mathrm{Sin}\left[\frac{n4\,\pi\,y}{L}\right]\right)}{L^2}$$

ıt[41]=

$$\frac{16\, g\,(-1+2\,\mathrm{HeavisideTheta}[L])\,\mathrm{HeavisideTheta}[y-L\,\mathrm{HeavisideTheta}[-L]]\,\mathrm{Sin}\left[\frac{\pi\,y}{L}\right]\mathrm{Sin}\left[\frac{2\,\pi\,y}{L}\right]\mathrm{Sin}\left[\frac{3\,\pi\,y}{L}\right]\mathrm{Sin}\left[\frac{4\,\pi\,y}{L}\right]}{L^2}$$

ıt[42]=

$$\frac{2\,g}{L}$$

HW19

Holstein–Primakoff(HP)变换，Spin系统和Bose系统之间的变换，设变换形式：

$$\begin{cases} S^{\dagger} = f(n)a^{\dagger} \\ S^{-} = af(n) \\ S^{z} = g(n) \end{cases}$$

得到关系式：

$$\begin{cases} f^2(n) = B_1 + B_2 n \\ g(n) = A + n \end{cases}$$

确定A, B_1, B_2可以得到：
$$\begin{cases} S_i^{\dagger} = (\sqrt{2S-n})a_i \\ S_i^{-} = a_i^{\dagger}\sqrt{2S-n} \\ S_i^{z} = S-n \end{cases} \text{ or } \begin{cases} S_i^{\dagger} = a_i^{\dagger}(\sqrt{2S-n}) \\ S_i^{-} = \sqrt{2S-n}a_i \\ S_i^{z} = n-S \end{cases}$$
其中$n = a_i^{\dagger}a_i$

作业19 找到上面参数A, B_1, B_2之间的关系

- 利用对易关系

$$\left[S^+, S^-\right] = 2S^z$$

$$\left[S^Z, S^+\right] = S^+$$

$$S^2 = (S^z)^2 + \frac{1}{2}\left(S^+S^- + S^-S^+\right) = S(S+1)$$

- 得到

$$f^2(n)n - f^2(n+1)(n+1) = 2g(n)$$

$$g(n) - g(n-1) = 1$$

$$g^2(n) + \frac{1}{2}\left[f^2(n)n + f^2(n+1)(n+1)\right] = S(S+1)$$

$\Rightarrow$

$$-2\mathrm{B}_2 n - B_1 - B_2 = 2A + 2n$$

$$A^2 + \frac{1}{2}(B_1 - 1) + (2A + B_1 - 1)\,n = S(S+1)$$

$\Rightarrow$

$$A = -S, B1 = 1 + 2S, B2 = -1$$

$$A = 1 + S, B1 = -1 - 2S, B2 = -1$$

HW20

(1). Schwinger Boson $\begin{cases} S^{\dagger} = a^{\dagger}b \\ S^{-} = b^{\dagger}a \\ S^{z} = (a^{\dagger}a - b^{\dagger}b)/2 \end{cases}$

(a).证明$[S^{\dagger}, S^{-}] = 2S_z$; (b). 计算$S^2$; (c). 证明基矢$|S,m\rangle = \frac{(a^{\dagger})^{S+m}(b^{\dagger})^{S-m}}{\sqrt{(S+m)!(S-m)!}}|0\rangle$是算符$S^2, S^z$的本征态，对应本征值$S(S+1), m$，这里$a^{\dagger}a + b^{\dagger}b = 2S$

(2). Schwinger Fermion同样计算(1)中的问题

(3). Dyson–Maleev变化

$$\begin{cases} J^{\dagger} = a \\ J^{-} = a^{\dagger}(2S - n) \\ J^{z} = S - a^{\dagger}a \end{cases}$$

计算$[J^{\dagger}, J^{\dagger}], J^2$

(4). $\vec{J} = \frac{1}{2}a^{\dagger}\vec{\sigma}a$，证明$\vec{J}$和$\vec{\sigma}$有相同对易关系，计算$J^2$

- (1a)

$$\begin{aligned}
\left[S^{+}, S^{-}\right] &= S^{+}S^{-} - S^{-}S^{+} = a^{+}bb^{+}a - b^{+}aa^{+}b \\
&= a^{+}abb^{+} - aa^{+}b^{+}b \\
&= a^{+}a\left(b^{+}b + 1\right) - \left(a^{+}a + 1\right)b^{+}b = a^{+}a - b^{+}b \\
&= 2S^{z}
\end{aligned}$$

HW20

- (1b)

$$S^2 = (S^z)^2 + \frac{1}{2}\left(S^+S^- + S^-S^+\right)$$
$$= \left[\frac{a^+a - b^+b}{2}\right]^2 + \frac{1}{2}\left(a^+bb^+a + b^+aa^+b\right)$$
$$= \frac{a^+a + b^+b}{2}\left(\frac{a^+a + b^+b}{2} + 1\right)$$
$$= \frac{n_a + n_b}{2}(\frac{n_a + n_b}{2} + 1) = S(S+1)$$

- (1c)

$$|S, m\rangle = \frac{\left(a^+\right)^{S+m}\left(b^+\right)^{S-m}}{\sqrt{(S+m)!(S-m)!}}|0\rangle = |S+m\rangle_a|S-m\rangle_b$$

$$S^2|S+m\rangle_a|S-m\rangle_b = \frac{n_a + n_b}{2}(\frac{n_a + n_b}{2} + 1)|S+m\rangle_a|S-m\rangle_b$$
$$= \frac{n_a + n_b}{2}\left[\frac{1}{2}(S+m+S-m) + 1\right]|S+m, S-m\rangle$$
$$= S(S+1)|S+m\rangle_a|S-m\rangle_b$$
$$S^z|S+m\rangle_a|S-m\rangle_b = m|S+m\rangle_a|S-m\rangle_b$$

HW20

- (3)

$$[J^+, J^-] = J^+J^- - J^-J^+ = aa^+(2S-n) - a^+(2S-n)a = 2J^z$$

$$\begin{aligned} J^2 &= (J^z)^2 + \frac{1}{2}\left(J^+J^- + J^-J^+\right) \\ &= (S-n)^2 + \frac{1}{2}((n+1)(2S-n) + n(2S-n+1)) \\ &= S(S+1) \end{aligned}$$

- (4) 二分量：$a^\dagger = \left(a_1^\dagger, a_2^\dagger\right)$

$$J_0 = \frac{1}{2}a^\dagger\sigma_0 a = \frac{1}{2}\left(a_1^\dagger a_1 + a_2^\dagger a_2\right)$$

$$J_x = \frac{1}{2}a^\dagger\sigma_x a = \frac{1}{2}\left(a_1^\dagger a_2 + a_2^\dagger a_1\right)$$

$$J_y = \frac{1}{2}a^\dagger\sigma_y a = \frac{i}{2}\left(-a_1^\dagger a_2 + a_2^\dagger a_1\right)$$

$$J_z = \frac{1}{2}a^\dagger\sigma_z a = \frac{1}{2}\left(a_1^\dagger a_1 - a_2^\dagger a_2\right)$$

HW20

- 得到：

$$[J_x, J_y] = iJ_z, \quad [J_y, J_z] = iJ_x, \quad [J_z, J_x] = iJ_y$$

$$\begin{aligned} J^2 &= J_x^2 + J_y^2 + J_z^2 \\ &= \frac{n_1 + n_2}{2}(\frac{n_1 + n_2}{2} + 1) \\ &= \frac{n}{2}(\frac{n}{2} + 1) \end{aligned}$$

HW21

- $H = bS^\dagger + b^* S^- + b_z S^z$, 代入 HP 变换
  $S^\dagger = a^\dagger\sqrt{2S - a^\dagger a}, S^- = \sqrt{2S - a^\dagger a}a, S^z = a^\dagger a - S$，求解自由能。
- 考虑 $S = \frac{1}{2}$，则 $H = ba^\dagger\sqrt{1-n} + b^*\sqrt{1-n}a + b_z(n - \frac{1}{2})$, 基矢 $|0\rangle, |1\rangle$

$$H|0\rangle = b|1\rangle - \frac{1}{2}b_z|0\rangle$$

$$H|1\rangle = b^*|0\rangle + \frac{1}{2}b_z|1\rangle$$

$$H = \begin{pmatrix} -b_z/2 & b \\ b^* & b_z/2 \end{pmatrix}$$

能级 $E = \pm\frac{1}{2}\sqrt{4|b|^2 + |b_z|^2}$
配分函数 $Z = \sum_n e^{-\beta E_n}$
自由能 $F = -\beta^{-1}\ln Z = -\frac{\ln[2\cosh\left(\frac{1}{2}\beta\sqrt{4|b|^2+|b_z|^2}\right)]}{\beta}$

HW22

- 计算 $\sum_{nm}\left(\Delta a_n^\dagger b_n^\dagger + \Delta b_n^\dagger a_m^\dagger + h.c.\right)$ 的色散关系。
- FT:

$$a_n = \frac{1}{\sqrt{N}}\sum_k a_k e^{ikn}, \quad b_n = \frac{1}{\sqrt{N}}\sum_k b_k e^{-ikn}$$

$\Rightarrow$

$$H = \Delta\Sigma_{k\delta}\left(a_k^\dagger b_k^\dagger + b_k^\dagger a_k^\dagger e^{-ik\delta} + \mathrm{h.c.}\right), \quad \delta = m - n$$

Let $\gamma_k = \sum_\delta e^{-ik\delta} \Rightarrow H = \Delta\Sigma_k\left[(1+\gamma_k)\, a_k^\dagger b_k^\dagger + \mathrm{h.c.}\right]$

- Bogoliubov 变换

$$a_k = u_k\alpha_k + v_k\beta_k^\dagger$$

$$b_k = u_k\beta_k + v_k\alpha_k^\dagger$$

$$u_k^2 - v_k^2 = 1$$

对角化：

$$H = \Delta\Sigma_k i\,(1+\gamma_k)\left(\alpha_k^\dagger\alpha_k + \beta_k^\dagger\beta_k + 1\right)$$

$$E_k = i\Delta(1+\gamma_k)$$

HW23

作业23 $H = E_1 a_1^\dagger a + E_2 a_2^\dagger a_2 + U_1 n_1(n_1-1) + U_2 n_2(n_2-1) + J(a_1^\dagger a_2 + h.c.)$

方法一：(1). 利用Schwinger-Boson变换，用自旋算符J_x, J_y, J_z表示以上哈密顿量

(2). 在（1）结果上进行HP变换得到$H(a, a^\dagger)$，求运动方程

(3). Josephson变换：$a = e^{-i\theta}\sqrt{\rho},\ a^\dagger = \sqrt{\rho}e^{i\theta}$

方法二：$a_1 = e^{-i\theta_1}\sqrt{N_1},\ a_2 = e^{-i\theta_2}\sqrt{N_2} \Rightarrow i\dot{a}_1 = [a_1, H], i\dot{a}_2 = [a_2, H]$

(1). 推导 $\begin{cases} \dot{z} & = -\sqrt{1-z^2}\sin\phi \\ \dot{\phi} & = \Lambda z + \frac{z}{\sqrt{(1-z^2)}}\cos\phi + \Delta E \end{cases}$ 其中 $\begin{cases} z & = \frac{N_1 - N_2}{N_1 + N_2} \\ \phi & = \theta_2 - \theta_1 \end{cases}$

(2). 数值计算

(3). 比较两种方法

- Schwinger-Boson

$$\begin{cases} S^+ = a_1^\dagger a_2 \\ S^- = a_2^\dagger a_1 \\ S_z = \left(a_1^\dagger a_1 - a_2^\dagger a_2\right)/2 \end{cases}$$

$$N = a_1^+ a_1 + a_2^+ a_2$$

$$H = S_z^2 (U_1 + U_2) + S_z [E_1 - E_2 + (U_1 - U_2)(N-1)] + J\left(S^+ + S^-\right)$$
$$+ \left[(E_1 + E_2) + (U_1 + U_2)\left(\frac{N}{2} - 1\right)\right] \frac{N}{2}$$

HW23

- (2) HP 变换

$$\begin{cases} S^{+} = \sqrt{2S-n}a \\ S^{-} = a^{\dagger}\sqrt{2S-n} \\ S_z = S - n \end{cases}$$

运动方程：

$$i\dot{a} = [a, H] = a(U_1 + U_2)(2n - 1 - 2S) - a\left[E_1 - E_2 + (U_1 - U_2)(N-1)\right]$$
$$+ J\{a^2[\sqrt{2S-(n-1)} - \sqrt{2S-(n-2)}]$$
$$+ \sqrt{2S-n} + [\sqrt{2S-n} - \sqrt{2S-(n-1)}]n\}$$

$$i\dot{a}^{\dagger} = [a^{\dagger}, H]$$

- (3) Josephson 变换

$$\begin{cases} a = e^{-i\theta}\sqrt{\rho} \\ a^{\dagger} = \sqrt{\rho}e^{i\theta} \end{cases}$$

假设 $S \gg \rho$

$$\dot{\rho} = 2\sqrt{2S\rho}\sin\theta$$

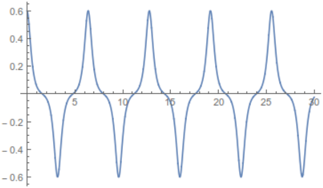
$$\dot{\theta} = -[2(U_1 + U_2)S + E_1 - E_2 + (U_1 - U_2)(N-1)] + J\sqrt{2S/\rho}\cos\theta$$

HW23

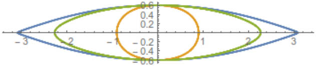
- 方法二 (2)

```
eqs = {z'[t] == -√(1 - z[t]²) Sin[ϕ[t]], ϕ'[t] == Λ z[t] + z[t]/√(1 - z[t]²) Cos[ϕ[t]] + dE,
                          正弦                                               余弦
   z[0] == 0.6, ϕ[0] == 0};
Eq = NDSolve[eqs /. {dE → 0., Λ → 9.99}, {z[t], ϕ[t]}, {t, 0, 30}] ;
     数值求解微分方程组

Plot[Evaluate[z[t]] /. Eq, {t, 0, 30}, PlotRange → All]
绘图  计算                          绘制范围     全部
```




```
ParametricPlot[{Evaluate[{ϕ[t], z[t]} /. Eq],
绘制参数图        计算
  Evaluate[{ϕ[t], z[t]} /. NDSolve[eqs /. {dE → 0., Λ → 1}, {z[t], ϕ[t]}, {t, 0, 30}]],
  计算                      数值求解微分方程组
  Evaluate[{ϕ[t], z[t]} /. NDSolve[eqs /. {dE → 0., Λ → 8}, {z[t], ϕ[t]}, {t, 0, 30}]]},
  计算                      数值求解微分方程组
 {t, 0, 30}]
```



HW24

- 对于上文 Dicke model 经典方法, 定义 $Y = (x_1, p_1, x_2, p_2)$，求 $\dot{Y} = AY$
- 利用

$$\dot{p}_i = -\frac{\partial H}{\partial x_i}, \quad \dot{x}_1 = \frac{\partial H}{\partial p_1}$$

$$H = \frac{p_1^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{p_2^2}{2m} + \frac{1}{2}m\omega_0^2 x_2^2 + \sqrt{2}gm\sqrt{\omega\omega_0}x_1x_2 + \sqrt{2}g\frac{p_1p_2}{m\sqrt{\omega w_0}}$$

得到

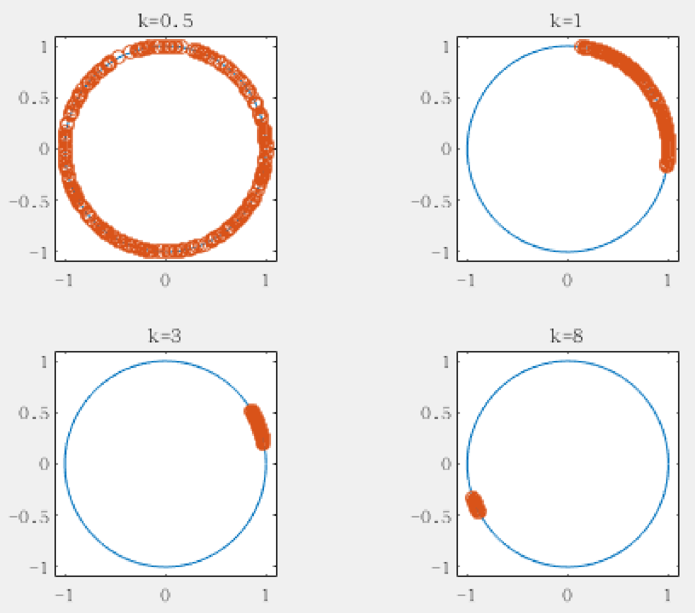
$$A = \begin{pmatrix} 0 & -m\omega^2 & 0 & -\sqrt{2}gm\sqrt{\omega\omega_0} \\ \frac{1}{m} & 0 & \frac{\sqrt{2}g}{m\sqrt{\omega\omega_0}} & 0 \\ 0 & -\sqrt{2}gm\sqrt{\omega\omega_0} & 0 & -m\omega_0 \\ \frac{\sqrt{2}g}{m\sqrt{\omega\omega_0}} & 0 & \frac{1}{m} & 0 \end{pmatrix}$$

HW25

- Kuramoto model $\dot{\theta}_i = \omega_i + \frac{K}{N}\sum_j^N \sin(\theta_j - \theta_i)$ 数值求解，$N = 200 \sim 500$ 左右。

```
func=@(w,K,N,theta) (w+(K/N)*sum(sin(theta*ones(1,N)-ones(N,1)*theta'),1)');
x=0:0.01:2*pi;
T=600;
N=300;
K=8;
theta0=2*pi*rand(N,1);
w=rand(N,1);
[t,y]=ode45(@(t,y)func(w,K,N,y),[0 T],theta0);
subplot(2,2,4)
plot(cos(x),sin(x),cos(y(end,:)),sin(y(end,:)),'o')
axis square
axis([-1.1 1.1 -1.1 1.1])
title('K=8')
```

HW25



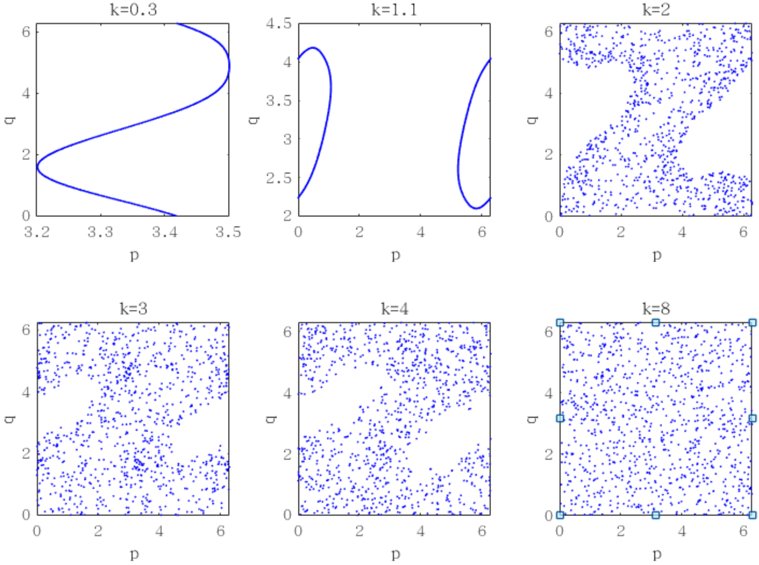
HW26

- 求 Standard map 相图，扫描 k

$$p_{n+1} = p_n + k\sin q_n, \quad q_{n+1} = q_n + p_{n+1}$$

```
N=1000;
k = 8;
subplot(2,3,6)
hold on
p=2*pi*rand(1);
q=2*pi*rand(1);
for i=1:N
    p=p+k*sin(q);
    p=mod(p,2*pi);
    q=q+p;
    q=mod(q,2*pi);
    plot(p,q,'b.','MarkerSize',4)
end
title('k=8')
xlabel('p')
ylabel('q')
axis square
box on
```

HW26



HW27

作业27 $H = \frac{p^2}{2} + k\cos q \sum_n [\delta(t-nT) + \delta(t-nT+T_0)]$

(1). 求出standard map方程(eq1)

(2). 画出相图(fig1)

- $$\dot{p} = k \sin q \sum [\delta(t-nT) + \delta(t-nT+T_0)]$$
  $$\dot{q} = p$$

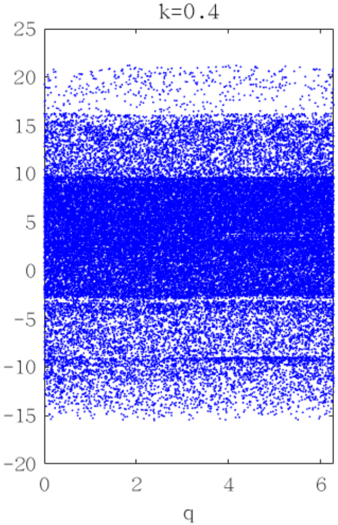
时间段：$[(n-1)T, nT-T_0], [nT-T_0, nT]$, Let $T=1$, $0 < T_0 < 1$

$$p_{N+1} = p_N + K_\epsilon \sin x_N; \quad p_{N+2} = p_{N+1} + K_\epsilon \sin x_{N+1}$$
$$x_{N+1} = x_N + p_{N+1}; \quad x_{N+2} = x_{N+1} + p_{N+2}\tau_\epsilon$$

$$K_\epsilon = k\epsilon, \quad \tau_\epsilon = (T-\epsilon)/\epsilon$$

HW27

```
N=50000;
k = 0.4;
tau = 24;
hold on
p=2*pi*rand(1);
q=2*pi*rand(1);
for i=1:N
    p=p+k*sin(q);
    q=q+p;q=mod(q,2*pi);
    p=p+k*sin(q);
    q=q+p*tau;q=mod(q,2*pi);
    Q(i)= q; P(i) = p;
end
plot(Q,P,'b.','MarkerSize',4)
title('k=0.4')
xlabel('q')
ylabel('p')
box on
```



HW28

作业28 已知$H = T(x) + V(x), T = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$, Time-evolution equation, $\psi(x, t+\Delta t) = e^{-i\Delta t H/\hbar}\psi(x,t)$,
证明: $e^{-i\Delta t H/\hbar} \approx e^{-i\Delta t V/(2\hbar)}e^{-i\Delta t T/\hbar}e^{-i\Delta t V/2\hbar}\psi$ holds the error $(\mathcal{O}(\Delta t^3))$

$$
\begin{aligned}
e^{-i\Delta t H/\hbar} =& 1 - i\Delta t(V+T)/\hbar - \frac{\Delta t^2}{2}(V+T)^2/\hbar^2 + \frac{i\Delta t^3}{6}(V+T)^3/\hbar^3 \\
=& 1 - \frac{i}{\hbar}(V+T)\Delta t - \frac{\Delta t^2}{2\hbar^2}\left(V^2 + T^2 + VT + TV\right) + \\
& \frac{i\Delta t^3}{6\hbar^3}\left(V^3 + T^3 + V^2T + TV^2 + VTV + VT^2 + TVT + T^2V\right)
\end{aligned}
$$

$$
\begin{aligned}
\text{right} =& \left(1 - \frac{i\Delta t}{2\hbar}V - \frac{\Delta t^2}{8\hbar^2}V^2 + \frac{i\Delta t^3}{48\hbar^3}V^3\right)\left(1 - \frac{i\Delta t}{2\hbar}T - \frac{\Delta t^2}{2\hbar^2}T^2 + \frac{i\Delta t^3}{46\hbar^3}T^3\right) \\
& \left(1 - \frac{i\Delta t}{2\hbar}V - \frac{\Delta t^2}{8\hbar^2}V^2 + \frac{i\Delta t^3}{48\hbar^3}V^3\right) \\
=& 1 - \frac{i\Delta t}{\hbar}(V+T) - \frac{\Delta t^2}{2\hbar^2}\left(V^2 + T^2 + VT + TV\right) \\
& + \frac{i\Delta t^3}{6\hbar^3}\left(V^3 + T^3 + \frac{3}{4}\left(V^2T + TV^2\right) + \frac{3}{2}\left(VT^2 + T^2V + VTV\right)\right)
\end{aligned}
$$

HW29

作业29 已知Time-Dependent Gross-Pitaevskii Equation

$i\hbar\frac{\partial}{\partial t}\psi(\mathrm{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathrm{x},t)+g|\psi(\mathrm{x},t)|^2\right]\psi(\mathrm{x},t)$, 其中$V(x)=\frac{1}{2}m\omega^2(x^2-a^2)$,数值求解基态能量和波函数。