固体物理大作业：能带计算

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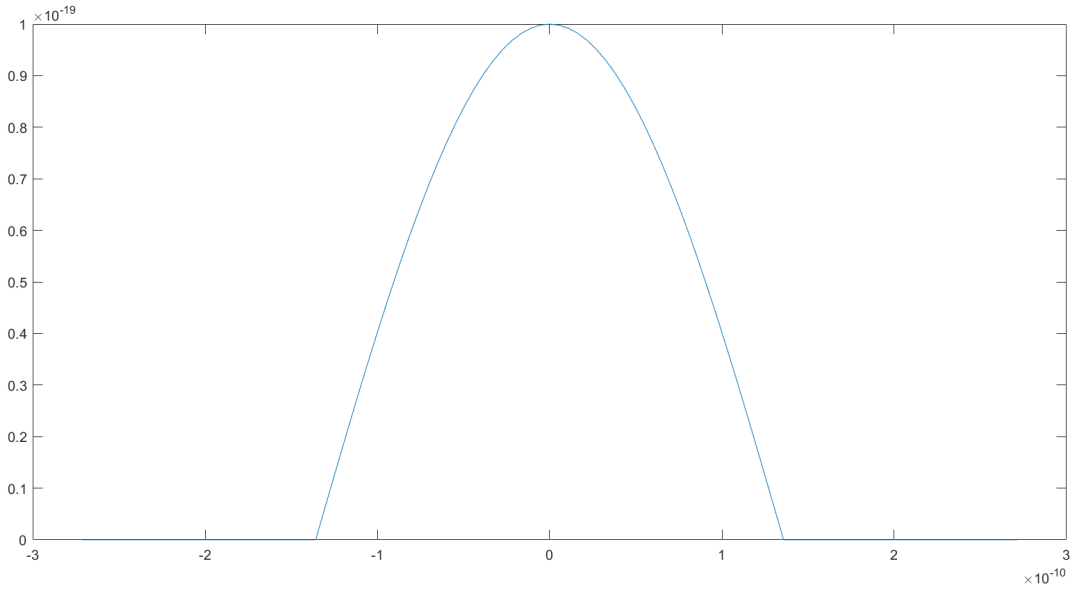
势能分布曲线如下图所示，图中仅为1个周期中的势能



利用特征根方法求解第一布里渊区的E-k关系思路如下：

求解能量本征值即求解如下无穷维方程组：

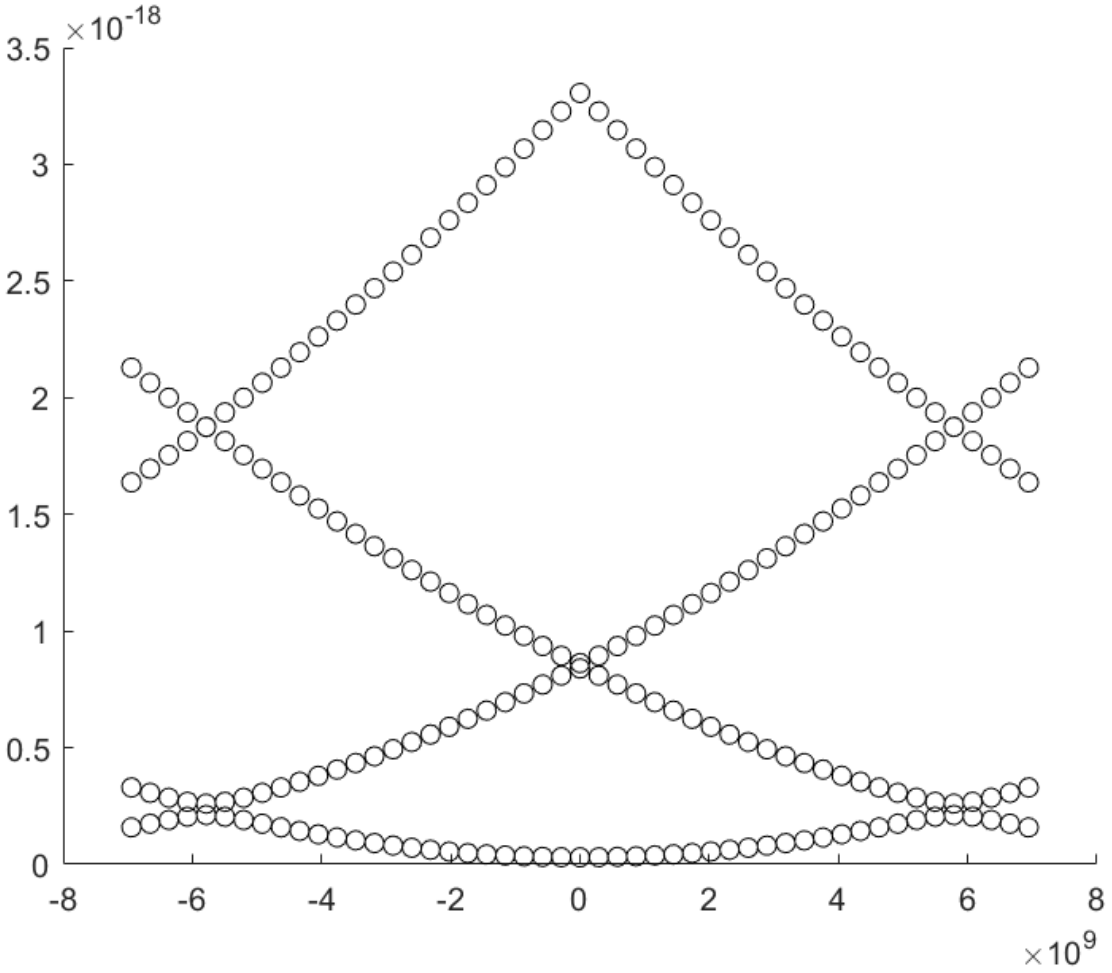
$$\begin{bmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right)^2+V_0-E & V_{-1} & V_{-2} & \cdots \\ \cdots & V_1 & \frac{\hbar^2}{2m}k^2+V_0-E & V_{-1} & \cdots \\ \cdots & V_2 & V_1 & \frac{\hbar^2}{2m}\left(k+\frac{2\pi}{a}\right)^2+V_0-E & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix} \begin{bmatrix} \cdots \\ u_{-1} \\ u_0 \\ u_1 \\ \cdots \end{bmatrix} = 0$$

也等价于求以下无穷阶矩阵的特征值：

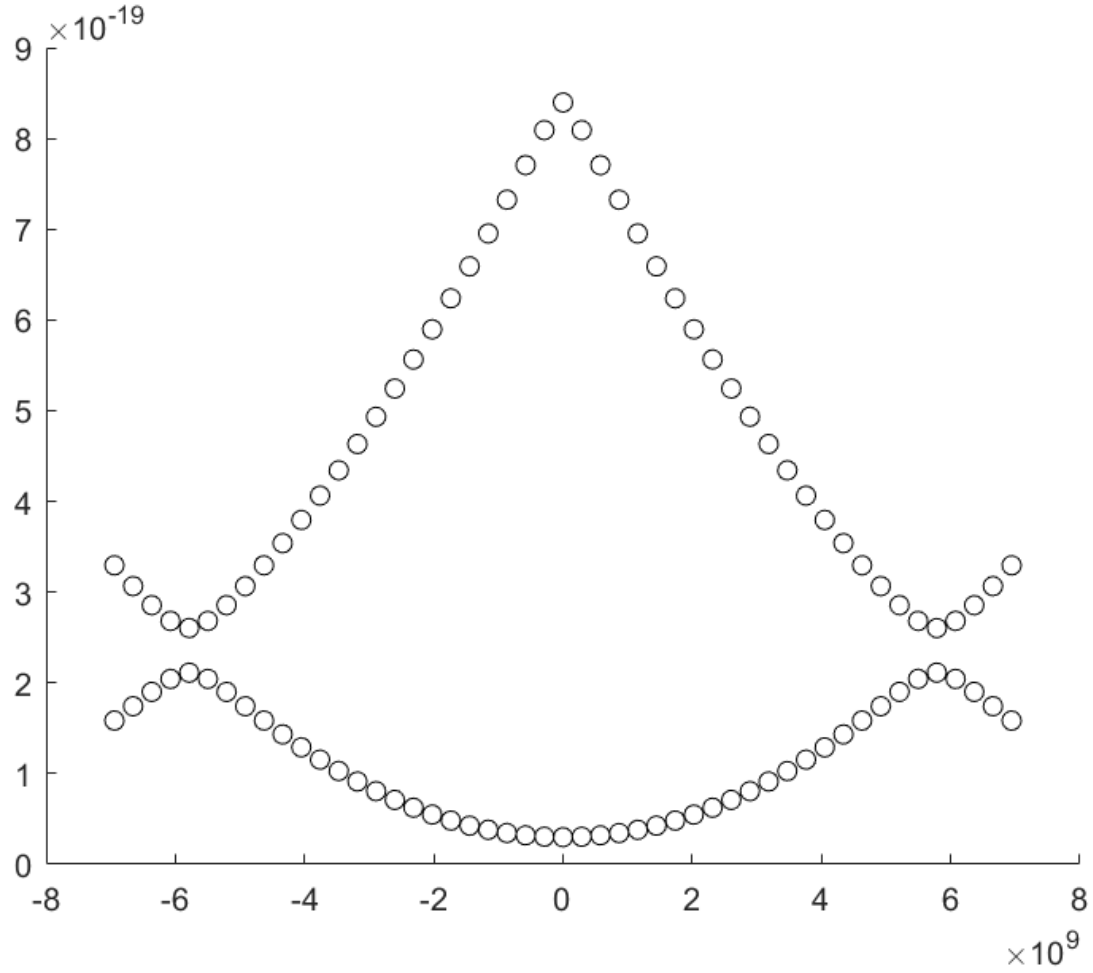
$$\begin{bmatrix} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \frac{\hbar^2}{2m}\left(k-\frac{2\pi}{a}\right)^2+V_0 & V_{-1} & V_{-2} & \cdots \\ \cdots & V_1 & \frac{\hbar^2}{2m}k^2+V_0 & V_{-1} & \cdots \\ \cdots & V_2 & V_1 & \frac{\hbar^2}{2m}\left(k+\frac{2\pi}{a}\right)^2+V_0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}$$

为了能够进行数值计算，考虑到实际上 n 很大时，傅里叶展开系数 V_n 很小，可以对矩阵进行截断进行计算。因此利用 fft 获得周期势场 V(x) 的傅里叶展开系数，针对第一布里渊区的波矢 k，构造如上矩阵，然后求解特征值，取最小的 Ne 个特征值即可获得 Ne 条能带。

最终获得的前 4 条能带如图所示



几乎看不出来带隙，原因是带隙宽度相对于能带宽度过小，仅显示前两条能带时如下图所示



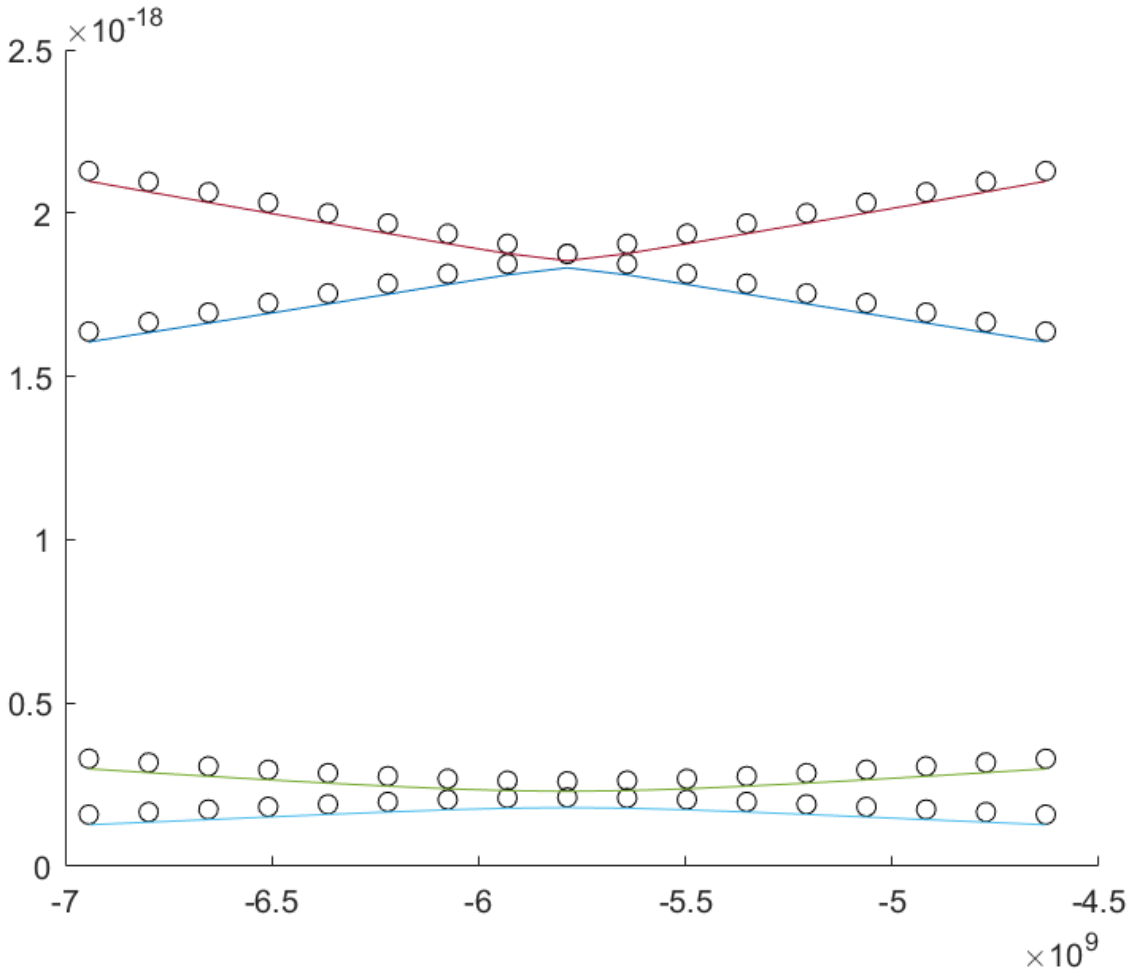
数值计算得到的带隙与近自由电子近似计算得到的前 3 个带隙对比如下，前两个带隙两者误差较小，第三个有较大误差，这应该与计算过程中对矩阵进行截断有关。

命令行窗口

```
Fourier series
   1.0e-19 *

    0.4975    0.2159    0.0038

Numerical calculation
   1.0e-19 *

    0.4908    0.2307    0.0111
```

在**第一布里渊区边界附近**（$k=-\frac{\pi}{a}\pm\frac{1}{10}\cdot\frac{2\pi}{a}$）的对比如图所示，其中散点图代表数值求解，实线代表利用简并微扰法按照如下公式获得的能带曲线

$$E_{\pm} = \frac{1}{2}\left\{ \left(E_k^0 + E_{k^*}^0\right) \pm \left[\left(E_k^0 - E_{k'}^0\right)^2 + 4|V_n|^2 \right]^{2/2} \right\}$$



附：源代码

```
clear all; close all;  clc;
%% predefine
h = 6.63e-34;   % plank constant
m0 = 9.1e-31;   % mass of electronic
a = 5.43e-10;   % lattice constant
x = linspace(-a/2, a/2, 101);
V = x>=-a/4 & x<=a/4;
V = V .* cos(x*2*pi/a) * 1e-19;  % potential field
% plot(x,V);
k = linspace(-pi/a * 1.2 , pi/a * 1.2 , 97);
%% compute enerfy band
N = length(V);
fs = fft(V) / N;          % Fourier Series of peoriodic potential
disp('Fourier series');
disp(abs(fs(2:4))*2);
v = flip([fs, fs]);        % v is Conjugate symmetric
L = 9;                   % get L eigen roots
```

```
Hamilton = zeros(L, L);
t = -floor(L/2):floor(L/2);
for m = 1:L
    Hamilton(m,:) = v(N+ceil(L/2)-m+t);
end
t = t * 2*pi / a;
t = t' * ones(1,length(k));
K = ones(L,1) * k;
K = (K + t).^2 * h.^2 / (8 * pi.^2 * m0);
figure;
hold on;
Ne = 4;          % num of band
E = zeros(length(k),Ne);
gap = zeros(1,3);
for s = 1:length(k)
    H = Hamilton + diag(K(:,s));
    e = eig(H);
    e = sort(e);
    E(s,:) = e(1:Ne);
    temp = k(s)*ones(1,Ne);
    scatter(temp, e(1:Ne),'ko');
end
gap(1) = E(5,2) - E(5,1);
gap(3) = E(5,4) - E(5,3);
gap(2) = E(25,3) - E(25,2);
disp('Numerical calculation');
disp(gap);
%% compare
k =linspace(-pi/a * 1.2 , pi/a * 1.2 , 97);
tempk = k(5:13);
Ek = h.^2/(8*pi.^2*m0)*k.^2;
e1 = Ek(5:13);
e2 = Ek(85:93);
E1 = (e1+e2 + sqrt((e1-e2).^2 + 4 * abs(fs(2)).^2))/2;
E2 = (e1+e2 - sqrt((e1-e2).^2 + 4 * abs(fs(2)).^2))/2;
Ek = h.^2/(8*pi.^2*m0)*(k-2*pi/a).^2;
e1 = Ek(5:13);
Ek = h.^2/(8*pi.^2*m0)*(k+2*pi/a).^2;
e2 = Ek(85:93);
E3 = (e1+e2 + sqrt((e1-e2).^2 + 4 * abs(fs(3)).^2))/2;
E4 = (e1+e2 - sqrt((e1-e2).^2 + 4 * abs(fs(3)).^2))/2;
figure;
hold on;
scatter(tempk,E(5:13,1),'ko');
scatter(tempk,E(5:13,2),'ko');
scatter(tempk,E(5:13,3),'ko');
scatter(tempk,E(5:13,4),'ko');
plot(tempk,E1);
plot(tempk,E2);
plot(tempk,E3);
plot(tempk,E4);
```