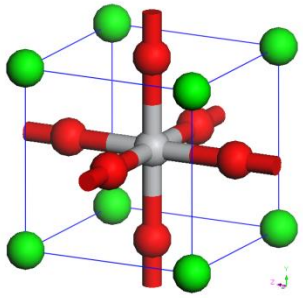
PHY 392K (57710) Solid State Physics I, Spring 2019

Homework 5 (Due May 9th)

Problem 1: This is a cell of a perovskite crystal ABO_3, let's say $BaTiO_3$. Corner (green) atom is Ba ($6s^2$), center atom (grey) is Ti ($3d^24s^2$), and oxygen atoms (red) are in the middle of each face ($2s^2p^4$). The valence configuration of each atom is given in parenthesis.

a) How many Bloch LCAO functions you might want to use in a minimum basis tight-binding calculation? Write them down.
b) What would be the size of your secular matrix?



Problem 2: Take the paper by J. Chadi and M. Cohen, phys. stat. sol. (b) **68**, 405 (1975), and construct the tight binding Hamiltonian for crystalline Si. Calculate the band structure along the usual high symmetry directions of the *fcc* Brillouin zone: **L** to **Γ** to **X**.

Calculate and plot the band structure of Si from **Γ** to **X**. Find the lowest energy state of the lowest conduction band (give the coordinates). This is your **band minimum**. Find the effective mass at this point along the **ΓX** direction.

Please note that is there a typo in the red box below about tight binding matrix of this paper, by using which you cannot get the band structure shown in the paper.

	s_0	s_1	x_0	y_0	z_0	x_1	y_1	z_1
s_0	$E_{s_0}-E(\boldsymbol{k})$	$V_{ss}g_0$	0	0	0	$V_{s_0p}g_1$	$V_{s_0p}g_2$	$V_{s_0p}g_3$
s_1	$V_{ss}g_0^*$	$E_{s_1}-E(\boldsymbol{k})$	$-V_{s_1p}g_1^*$	$-V_{s_1p}g_2^*$	$-V_{s_1p}g_3^*$	0	0	0
x_0	0	$-V_{s_1p}g_1$	$E_{p_0}-E(\boldsymbol{k})$	0	0	$V_{xx}g_0$	$V_{xy}g_3$	$V_{xy}g_2$
y_0	0	$-V_{s_1p}g_2$	0	$E_{p_0}-E(\boldsymbol{k})$	0	$V_{xy}g_3$	$V_{xx}g_0$	$V_{xy}g_1$
z_0	0	$-V_{s_1p}g_3$	0	0	$E_{p_0}-E(\boldsymbol{k})$	$V_{xy}g_1$	$V_{xy}g_2$	$V_{xx}g_0$
x_1	$V_{s_0p}g_1^*$	0	$V_{xx}g_0^*$	$V_{xy}g_3^*$	$V_{xy}g_1^*$	$E_{p_1}-E(\boldsymbol{k})$	0	0
y_1	$V_{s_0p}g_2^*$	0	$V_{xy}g_3^*$	$V_{xx}g_0^*$	$V_{xy}g_2^*$	0	$E_{p_1}-E(\boldsymbol{k})$	0
z_1	$V_{s_0p}g^*$	0	$V_{xy}g_1^*$	$V_{xy}g_1^*$	$V_{xx}g_0^*$	0	0	$E_{p_1}-E(\boldsymbol{k})$

You can use the following matrix after I correct and test it.

H :=

Es0	Vss * g0	0	0	0	Vs0p * g1	Vs0p * g2	Vs0p * g3
Vss * (g0)*	Es1	-Vs1p * (g1)*	-Vs1p * (g2)*	-Vs1p * (g3)*	0	0	0
0	-Vs1p * g1	Ep0	0	0	Vxx * g0	Vxy * g3	Vxy * g2
0	-Vs1p * g2	0	Ep0	0	Vxy * g3	Vxx * g0	Vxy * g1
0	-Vs1p * g3	0	0	Ep0	Vxy * g2	Vxy * g1	Vxx * g0
Vs0p * (g1)*	0	Vxx * (g0)*	Vxy * (g3)*	Vxy * (g2)*	Ep1	0	0
Vs0p * (g2)*	0	Vxy * (g3)*	Vxx * (g0)*	Vxy * (g1)*	0	Ep1	0
Vs0p * (g3)*	0	Vxy * (g2)*	Vxy * (g1)*	Vxx * (g0)*	0	0	Ep1

This is should give you the correct results.

Bonus question: Now calculate the band structure along a vector starting from the band minimum but pointing at 90° to the **ΓX** direction. Calculate the effective mass at the band minimum along this new direction.

Problem 3: Consider the electron energy dispersion in the vicinity of the band minimum so that E(k) is approximately parabolic:

$$E(\vec{k}) = E_c + \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} + \frac{k_z^2}{m_z}\right)$$

For simplicity, assume the mass is isotropic. Show that the density of states D(E) is proportional to $(E-E_c)^{1/2}$ around the gamma point (***k*** = (0,0,0)).

Problem 4

Compute the band structure of Si using the empirical pseudopotential method (EPM). Use the parameters published in M. Cohen and T.K. Bergstresser, Phys. Rev. **141**, 789 (1966). Plot the band structure along the high symmetry directions.

Set the potential to zero and compute the band structure in the empty-lattice approximation. Compare to the EPM result.

A sample MATLAB code is included below (you will need to edit it), but you can write your own.

The EPM MATLAB file:

```
%%%%  Program EPM (based on the Cohen-Bergstresser 1966 paper)
%%%%
%%%%  Read in G vectors included in the calculation
fid=fopen('g.txt','r');
G=fscanf(fid,'%d',[3,65]);
G';
%%%% read in K-pts
fid=fopen('k.txt','r');
K=fscanf(fid,'%f',[3,3]);
K';
status=fclose('all')
fid=fopen('epm_out.txt','w')
fprintf(fid,' EPM OUPUT\n')
%%%  set parameters
%  form factors
%  lattice constant
v3=-0.115 ;
v8=0.005 ;
v11=0.030 ;
a= 5.65 /0.529;
con=(2*pi/a)^2;
% cut offs (k+G)^2 and potential
qcut=11.1;
gcut=11.1;
%%% Loop over k-vectors
for nk=1:3
   xk=K(1,nk);
   yk=K(2,nk);
   zk=K(3,nk);
%%% Sort out the (k+G) space
n=0;
for j=1:65
   test=(xk+G(1,j))^2+(yk+G(2,j))^2+(zk+G(3,j))^2;
   if test < gcut
      n=n+1;
      GK(1,n)=xk+G(1,j);
      GK(2,n)=yk+G(2,j);
      GK(3,n)=zk+G(3,j);
      H(n,n)=0.5*con*(GK(1,n)^2+GK(2,n)^2+GK(3,n)^2);
   end
end
H';
n;
%%% Construct H matrix for off diagonal
```

```
%%
for j1=1:n
   m=j1+1;
for j2=m:n
   gx=GK(1,j1)-GK(1,j2);
   gy=GK(2,j1)-GK(2,j2);
   gz=GK(3,j1)-GK(3,j2);
   sg=cos(0.25*pi*(gx+gy+gz));
   gtest=gx^2+gy^2+gz^2;
   v=0.;
   if abs(gtest-3) < 0.01   v=v3; end
   if abs(gtest-8) < 0.01   v=v8; end
   if abs(gtest-11) <0.01   v=v11; end
   H(j1,j2)=sg*v;
   H(j2,j1)=H(j1,j2);
end
end
%%  Find eigenvalues
E=eig(H);
E=27.2.*E-9.5623;
fprintf(fid,'\n \n  k-point %5.1f   %5.1f   %5.1f', xk,yk,zk);
for jj=1:8
fprintf(fid,'\n %8.3f',E(jj));
end
clear H
end
status=fclose('all');
```

The G-file:

```
     0     0     0
     1     1     1
     1     1    -1
     1    -1     1
    -1     1     1
     1    -1    -1
    -1     1    -1
    -1    -1     1
    -1    -1    -1
     2     0     0
     0     2     0
     0     0     2
    -2     0     0
     0    -2     0
     0     0    -2
     2     2     0
     2     0     2
     0     2     2
    -2     2     0
```

```
 2   -2    0
-2    0    2
 2    0   -2
 0   -2    2
 0    2   -2
-2   -2    0
-2    0   -2
 0   -2   -2
 3    1    1
 3   -1    1
 3    1   -1
 3   -1   -1
-3    1    1
-3   -1    1
-3    1   -1
-3   -1   -1
 1    3    1
 1    3   -1
-1    3    1
-1    3   -1
 1     -3    1
 1     -3   -1
-1   -3    1
-1   -3   -1
 1    1    3
 1   -1    3
-1    1    3
-1   -1    3
 1      1   -3
 1     -1   -3
-1    1   -3
-1   -1   -3
 2    2    2
 2    2   -2
 2   -2    2
-2    2    2
 2   -2   -2
-2    2   -2
-2   -2    2
-2   -2   -2
 4    0    0
-4    0    0
 0    4    0
 0   -4    0
 0    0    4
 0    0   -4
```

The k-space file

```
0.    0.   0.
1.    0.   0.
0.5   0.5  0.5
```

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     1    -1    -1
    -1     1    -1
    -1    -1     1
    -1    -1    -1
     2     0     0
     0     2     0
     0     0     2
    -2     0     0
     0    -2     0
     0     0    -2
     2     2     0
     2     0     2
     0     2     2
    -2     2     0
```

```
 2   -2    0
-2    0    2
 2    0   -2
 0   -2    2
 0    2   -2
-2   -2    0
-2    0   -2
 0   -2   -2
 3    1    1
 3   -1    1
 3    1   -1
 3   -1   -1
-3    1    1
-3   -1    1
-3    1   -1
-3   -1   -1
 1    3    1
 1    3   -1
-1    3    1
-1    3   -1
 1     -3    1
 1     -3   -1
-1   -3    1
-1   -3   -1
 1    1    3
 1   -1    3
-1    1    3
-1   -1    3
 1      1   -3
 1     -1   -3
-1    1   -3
-1   -1   -3
 2    2    2
 2    2   -2
 2   -2    2
-2    2    2
 2   -2   -2
-2    2   -2
-2   -2    2
-2   -2   -2
 4    0    0
-4    0    0
 0    4    0
 0   -4    0
 0    0    4
 0    0   -4
```

The k-space file

```
0.    0.   0.
1.    0.   0.
0.5   0.5  0.5
```