PHYS 516 Assignment 5
Tight Binding Model of Electronic Structures **Cathie Tsz Yan SO**

1.

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#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include "tb_util.c"
#include "eigen.c"

int n4;

/* For periodic boundary condition ******************************************/
double RegionH[3];
double SignR(double v, double x) {if (x>0) return v; else return -v;}

void Hamiltonian(){
    double **h; /* Hamiltonian matrix */
    double *d; /* Eigenvalues */
    double *e; /* Work array for matrix diagonalization */
    n4 = 4*nAtom;
    h = dmatrix(1,n4,1,n4);
    d = dvector(1,n4);
    e = dvector(1,n4);
    double r0=2.360352;
    double Es=-5.25,Ep=1.20;
    double h_lambda0[]={-2.038,1.745,2.75,-1.075};
    double h_lambda[4];
    double n_lambda[]={9.5,8.5,7.5,7.5};
    double r_lambda[]={3.4,3.55,3.7,3.7};
    double unit_r_relative[3];
    double length_r_relative;

    int i,j,k;

    for(i=1;i<=n4;i++){
        for(j=1;j<=n4;j++){
            h[i][j]=0;
        }
    }
    for(i=0;i<nAtom;i++){
        h[4*i+1][4*i+1]=Es;
        h[4*i+2][4*i+2]=Ep;
        h[4*i+3][4*i+3]=Ep;
        h[4*i+4][4*i+4]=Ep;
    }
    for(i=0;i<nAtom;i++){
        for(j=i+1;j<nAtom;j++){
            length_r_relative=0;
            for(k=0;k<3;k++){
                RegionH[k] = 0.5*LCNS*InitUcell[k];
                unit_r_relative[k]=r[i][k]-r[j][k];
                //Boundary condition ---->
                unit_r_relative[k] = unit_r_relative[k]
                -SignR(RegionH[k],unit_r_relative[k]-RegionH[k])
                -SignR(RegionH[k],unit_r_relative[k]+RegionH[k]);
                // <----
                length_r_relative+=pow(unit_r_relative[k],2);
            }
            length_r_relative=sqrt(length_r_relative);
            for(k=0;k<3;k++){
                unit_r_relative[k]/=length_r_relative;
            }
            //At this point unit_r_relative is the unit vector from atom i to j.
```

```
            for(k=0;k<4;k++){
                h_lambda[k]=h_lambda0[k]*pow(r0/length_r_relative,2)*
                exp(2*(-pow(length_r_relative/r_lambda[k],n_lambda[k])+
pow(r0/r_lambda[k],n_lambda[k])));
            }

            h[4*i+1][4*j+1]=h_lambda[0];
            h[4*i+1][4*j+2]=unit_r_relative[0]*h_lambda[1];
            h[4*i+1][4*j+3]=unit_r_relative[1]*h_lambda[1];
            h[4*i+1][4*j+4]=unit_r_relative[2]*h_lambda[1];

            h[4*i+2][4*j+1]=-unit_r_relative[0]*h_lambda[1];
            h[4*i+2][4*j+2]=unit_r_relative[0]*unit_r_relative[0]*h_lambda[2]
            + (1-unit_r_relative[0]*unit_r_relative[0])*h_lambda[3];
            h[4*i+2][4*j+3]=unit_r_relative[0]*unit_r_relative[1]*(h_lambda[2]-
h_lambda[3]);
            h[4*i+2][4*j+4]=unit_r_relative[0]*unit_r_relative[2]*(h_lambda[2]-
h_lambda[3]);

            h[4*i+3][4*j+1]=-unit_r_relative[1]*h_lambda[1];
            h[4*i+3][4*j+2]= unit_r_relative[0]*unit_r_relative[1]*(h_lambda[2]-
h_lambda[3]);
            h[4*i+3][4*j+3]=unit_r_relative[1]*unit_r_relative[1]*h_lambda[2]
            + (1-unit_r_relative[1]*unit_r_relative[1])*h_lambda[3];
            h[4*i+3][4*j+4]=unit_r_relative[1]*unit_r_relative[2]*(h_lambda[2]-
h_lambda[3]);

            h[4*i+4][4*j+1]=-unit_r_relative[2]*h_lambda[1];
            h[4*i+4][4*j+2]=unit_r_relative[0]*unit_r_relative[2]*(h_lambda[2]-
h_lambda[3]);
            h[4*i+4][4*j+3]=unit_r_relative[1]*unit_r_relative[2]*(h_lambda[2]-
h_lambda[3]);
            h[4*i+4][4*j+4]=unit_r_relative[2]*unit_r_relative[2]*h_lambda[2]
            + (1-unit_r_relative[2]*unit_r_relative[2])*h_lambda[3];

        }
    }

    for(i=1;i<n4;i++){
        for(j=i+1;j<n4;j++){
            h[j][i]=h[i][j];
        }
    }
    tred2(h,n4,d,e);

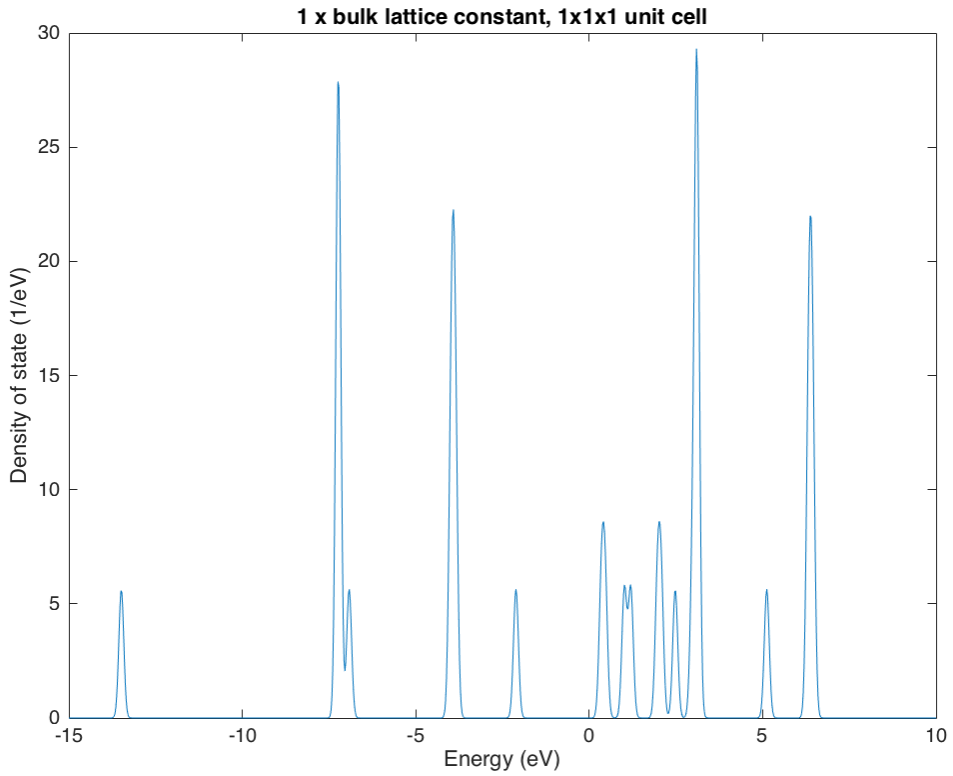
    tqli(d,e,n4,h);

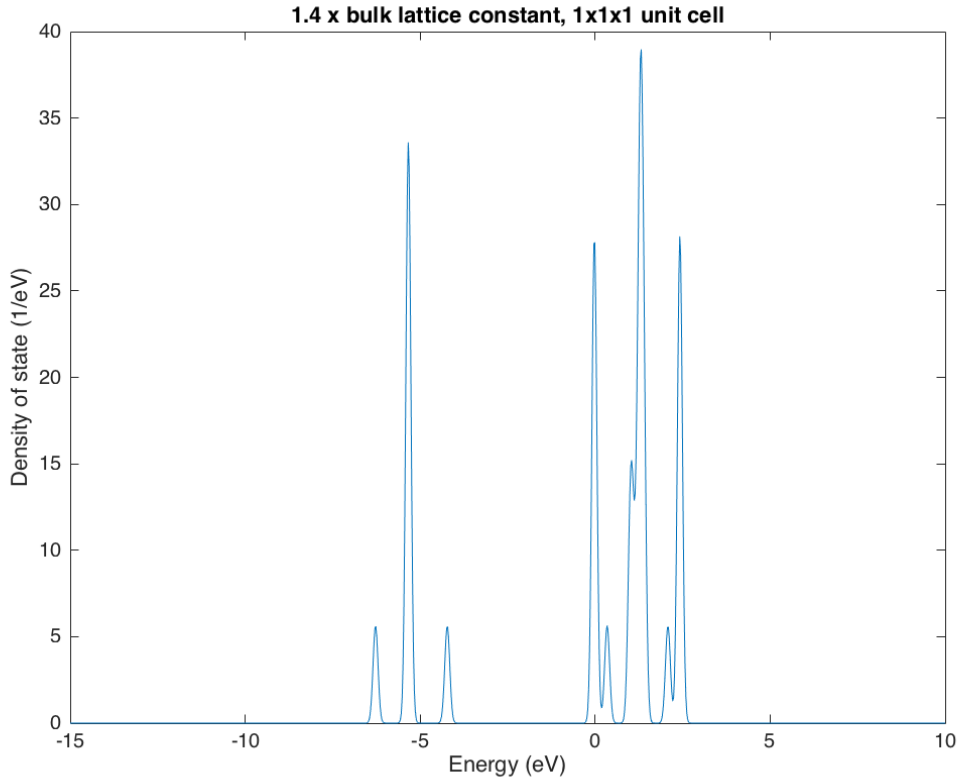
    for(i=1;i<=n4;i++){
        printf("%le ",d[i]);
    }

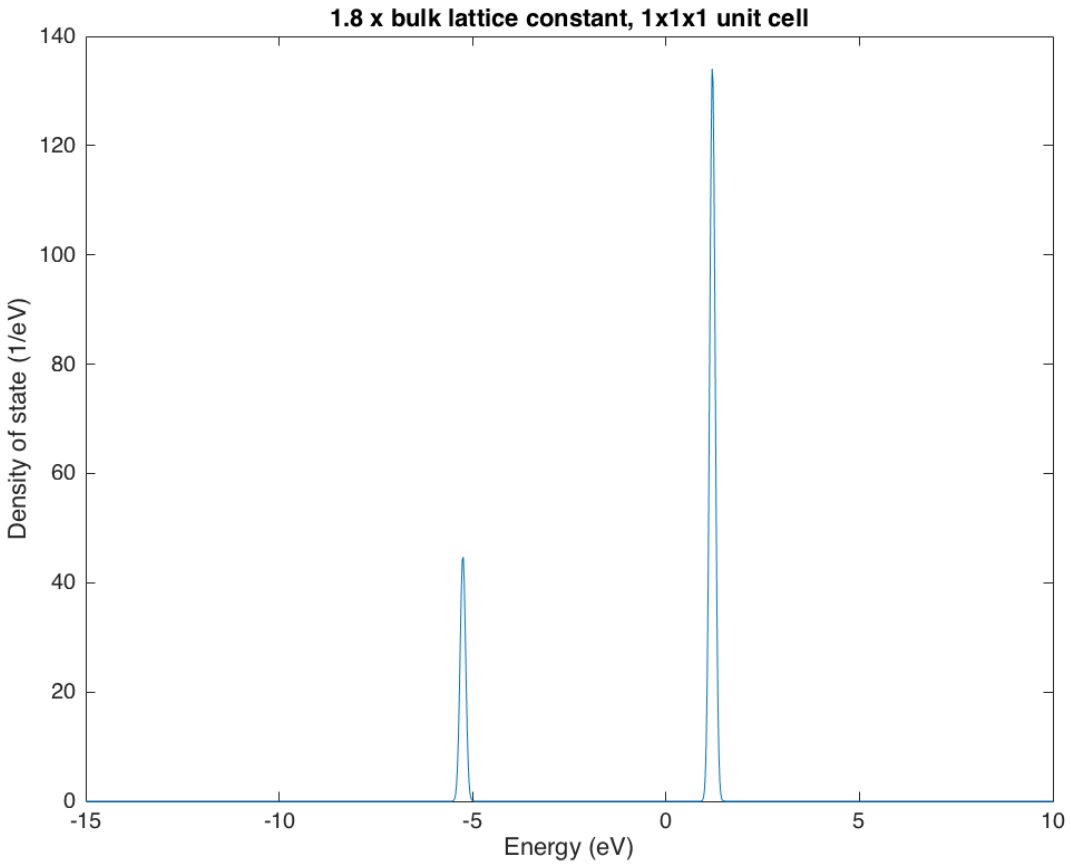
}

int main()
{
    InitConf();
    Hamiltonian();
    return 0;
}
```

2.

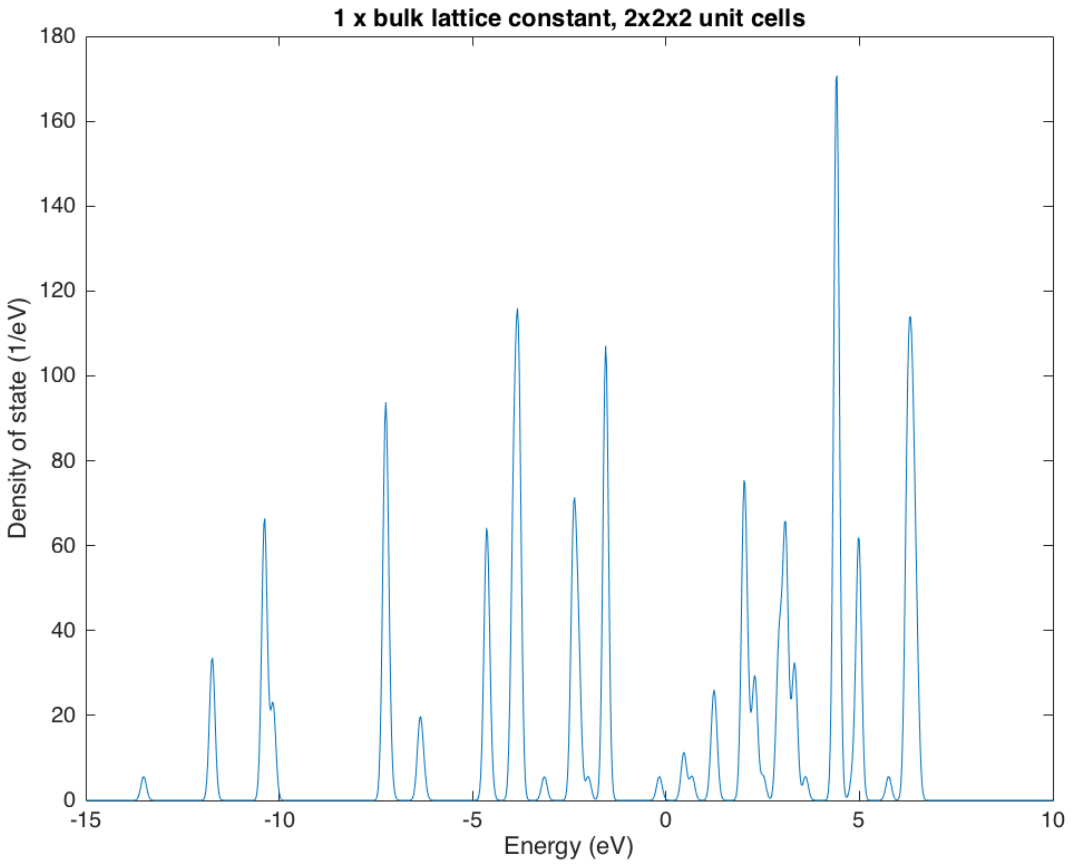

1 x bulk lattice constant, 1x1x1 unit cell
Density of state (1/eV)
Energy (eV)
30
25
20
15
10
5
0
-15
-10
-5
0
5
10


1.4 x bulk lattice constant, 1x1x1 unit cell
Density of state (1/eV)
Energy (eV)
40
35
30
25
20
15
10
5
0
-15
-10
-5
0
5
10



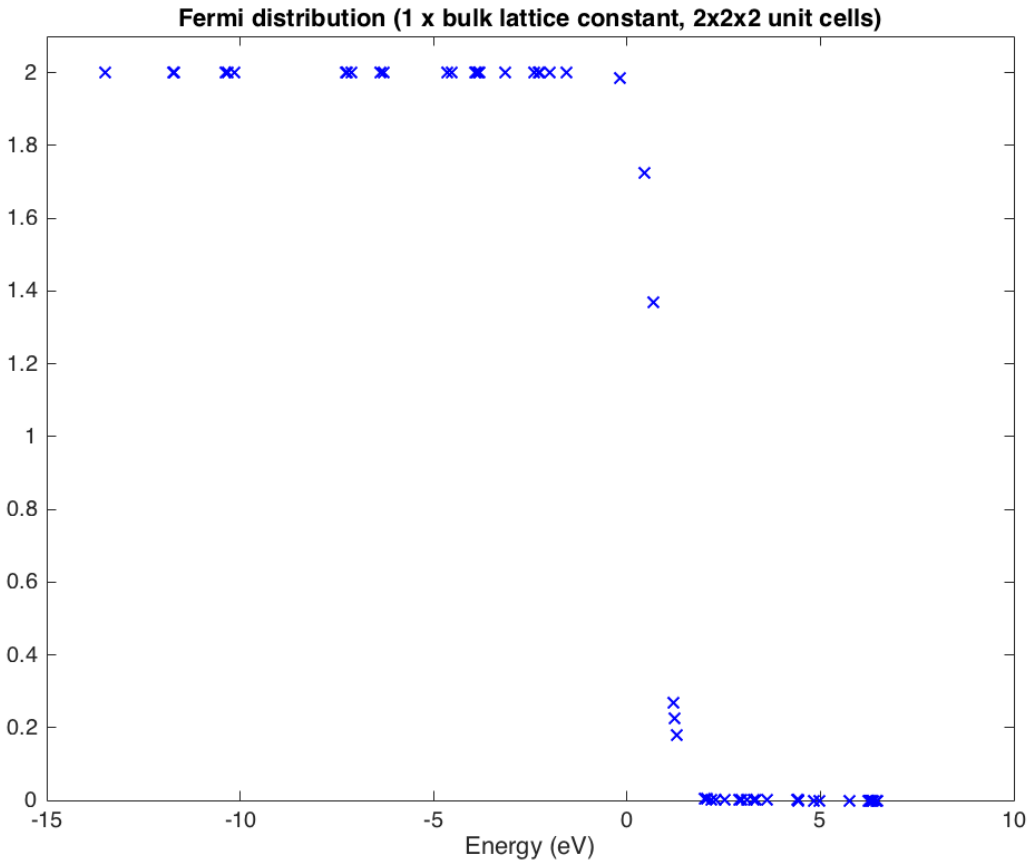
Effect of lattice constant on the density of states: Eigen-energies tends to be more spread out when the lattice constant is smaller. As the lattice constant increases, the density of state concentrates and peaks mostly at E_p = 1.20 eV and some at E_s = -5.25 eV.

3.



Difference from the 8-atoms case: The peak at E_s = -5.25 eV is more apparent while more values of eigen-energies are present.

4.


Fermi distribution (1 x bulk lattice constant, 2x2x2 unit cells)
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-15
-10
-5
0
5
10
Energy (eV)