PROBLEM SET 1 Solutions

Physics 140A– WINTER 2013

[1.] Sidebottom Problem 1.1 Show that the volume of the primitive cell of a BCC crystal lattice is $a^3/2$ where a is the lattice constant of the conventional cell.

The primitive lattice vectors are

$$\begin{aligned}\vec{a}_1 &= \frac{a}{2}(-\hat{x}+\hat{y}+\hat{z}) \\ \vec{a}_2 &= \frac{a}{2}(+\hat{x}-\hat{y}+\hat{z}) \\ \vec{a}_3 &= \frac{a}{2}(+\hat{x}+\hat{y}-\hat{z})\end{aligned}$$

The volume of the unit cell is $V_c = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$. You can compute this either by "brute force" using the rules for cross and dot products of the basis vectors ($\hat{x} \times \hat{y} = \hat{z}, \quad \hat{x} \cdot \hat{y} = 0$, etc) or the identity from your linear algebra class which says the result is the determinant of the matrix formed by choosing the components of the three vectors as the three rows of the matrix.

Let's do it by "brute force". We first get

$$\begin{aligned}\vec{a}_2 \times \vec{a}_3 = \frac{a^2}{4}(+\hat{z}+\hat{y}+\hat{z}+\hat{x}+\hat{y}-\hat{x}) &= \frac{a^2}{2}(+\hat{z}+\hat{y}) \\ \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3) &= \frac{a^3}{2}\end{aligned}$$

The determinant method also yields $a^3/2$.

[2.] Sidebottom Problem 1.4 Show that the packing fraction of a FCC crystal lattice is $\sqrt{2}\,\pi/6$.

The centers of the nearest neigbor atoms in an FCC crystal are $a/\sqrt{2}$ apart. Spheres centered at this separation will touch when their radii are $R = a/(2\sqrt{2})$. There are four atoms per unit cell, so the packing fraction is $4(4/3)\pi[\,a/(2\sqrt{2})\,]^3/a^3 = \pi/(3\sqrt{2}) = 0.740$.

[3.] Sidebottom Problem 1.7 For the HCP structure, show that the ideal c/a ratio is 1.633.

In the HCP crystal there are layers of atoms with centers arranged in a triangular lattice, with atom centers in succeeding layers sitting above the centers of the triangles of the layer below. The centers of the three atoms forming a triangle in one layer, together with the center of the atom above them, forms an equilateral pyramid (tetrahedron). The height of such a tetrahedron h is obtained from the Pythagorean theorem, applied to a triangle of hypotenuse a and base $a/\sqrt{3}$ (distance from vertex of equilateral triangle to its center) $a^2 = h^2 + (a/\sqrt{3})^2 \rightarrow h = \sqrt{2/3}\,a$. The c axis distance is twice this height: $c = 2\sqrt{2/3} = 1.633$.

[4.] Sidebottom Problem 1.9

A "tetragonal" structure is one made up of rectangular boxes two sides of which have equal length. ("Cubic" has all sides equal length and "orthorhombic" has all sides different length. One of the interesting facts about the structure of cuprate superconductors of Problem 1-6 is that they have a tetragonal to orthorhombic structural phase transition in proximity to their superconducting phase transition. There was considerable discussion whether this change in structure had anything to do with the superconductivity.) Clearly the structure in this problem is tetragonal, and because of the atom in the center, it is body-centered tetragonal.

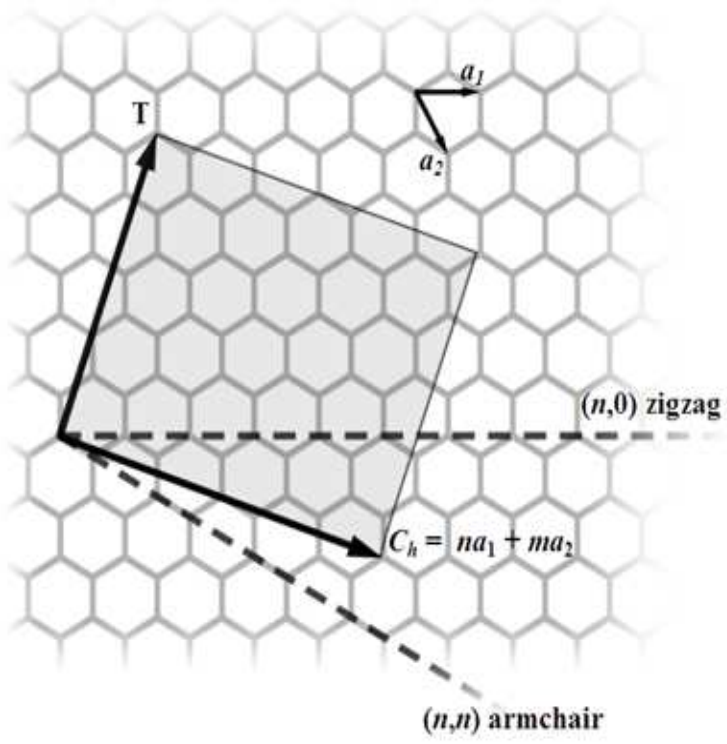
To get the packing fraction we put the largest possible non-overlapping spheres in place of all the atoms and ask what portion of the volume these fill up. We need to figure out when the spheres first touch. Two spheres at the corners of the cell separated by $3\mathring{A}$ will touch when their radii are $r = 1.5\mathring{A}$. This is of course more restrictive than touching along the $4\mathring{A}$ direction. But what about contact between atoms at the corners and the one in the center? The diagonal of the cell has length $\sqrt{3^2+3^2+4^2} = \sqrt{34} = 5.831\mathring{A}$. The maximum radius is one-fourth of this, $1.46\mathring{A}$. So this is a slightly more restrictive condition than touching along the $3\mathring{A}$ distance.

There are two balls per unit cell (one at the center and eight balls at the corners which are one eighth in the cell). So the ratio of the maximal ball volume to the unit cell volume, the packing fraction, is

$$\mathrm{PF} = \frac{2\,(\,\frac{4}{3}\,\pi(1.46)^3\,)}{3\times 3\times 4} = 0.724.$$

[5.] What is "graphene" and what is its structure? What is a "carbon nanotube" and how does it relate to graphene? What do "armchair," "zigzag," and "chiral" mean in referring to a nanotube?

Graphene is a two dimensional sheet of carbon atoms arranged in a hexagonal (honeycomb) structure. The carbon atoms are 0.142 nm apart. If graphene sheets are stacked to form graphite, the intersheet separation is 0.335 nm. (For perspective, recall the Bohr radius of the H atom is 0.0529 nm.)

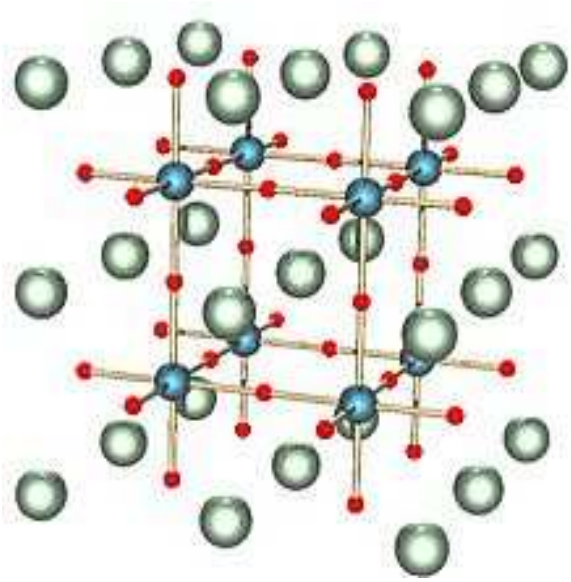


Rolling up a graphene sheet yields a nanotube. The different types of nanotubes formed are classified by two integers n, m which define the vector C_h giving the two points which coincide when the graphene sheet is rolled up. A zig-zag nanotube has $m = 0$ and an armchair nanotube has $m = n$.

[6.] The "family" of high temperature (cuprate) superconductors contains many compounds. $La_{2-x}Sr_xCuO_4$ is one example. The "parent" compound, La_2CuO_4 is an antiferromagnetic insulator. What is the lattice structure of La_2CuO_4? What is a "perovskite"?

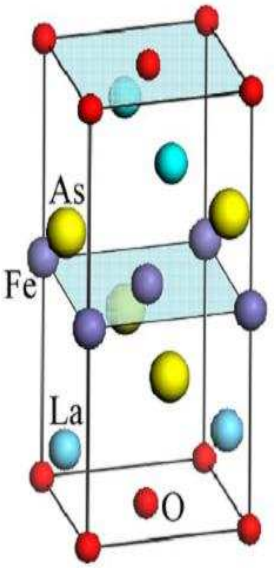
The La_2CuO_4 crystal structure is composed of CuO_2 sheets in which the Cu atoms are at the vertices of a square, with an O atom at the center of each bond. The La atoms, and additional O atoms, lie between these sheets. The CuO_2 sheets are the common feature of the whole family of cuprates (whilst there are many variants in which La is replaced by other rare earths), suggesting that they must be crucial to the phenomenon of high temperature superconductivity. The additional intersheet O atoms are arranged so that each Cu atom is surrounded by a tetrahedron of O. (See perovskite structure below.)

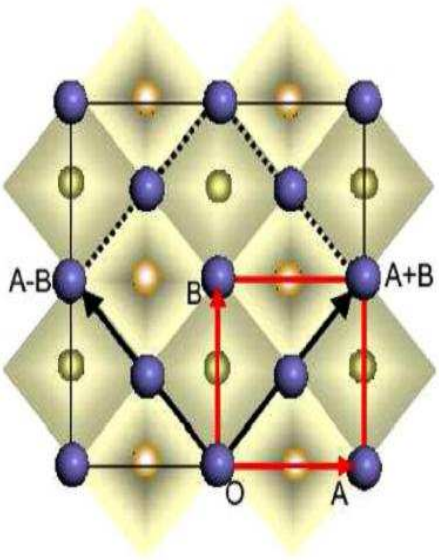
I really meant to ask what is the perovskite structure as opposed to what is a perovskite.



The perovskite structure is illustrated at left. The red spheres are typically O, whilst the blue spheres are often a smaller metal atom and the green spheres are larger metal atoms. In the case of the cuprate superconductor, the blue spheres are copper and the green spheres might be, for example, La. Notice the CuO_2 sheets and the O tetrahedra surrounding each Cu.

[7.] Another "family" of superconductors are the iron pnictides. What is the structure of the "1111" material LaOFeAs?





The structure of LaOFeAs is shown at left. As with the cuprates, the 'iron superconductors' are highly layered. The electrons tend to move in the FeAs layers. The Fe atoms form a square lattice in these layers.

The problems below are *numeric*. I will be available in the computer lab, room 106, Wednesday 10:00 am - noon to help with these problems, or with general background on writing C programs, compiling them, etc.

[8.] We often encounter transcendental equations in physics. For example, in the quantum problem of the energy levels of a particle in a finite square well, you need to solve,

$$\tan z = \sqrt{(z_0/z)^2 - 1}$$

Write a bisection program (do *not* use some canned root-finding software) and find the solution to this equation for $z_0 = 2.5$. Looking at the figure 2.18 in Griffiths will help you pick a good set of initial values to bracket the solution. (For this problem you can just treat z_0 as number. However, for completeness, let me remind you of the connection of z_0 to the physics: $z_0 = (a/\hbar)\sqrt{2mV_0}$ where $2a$ is the well width, V_0 is the well depth, and m is the particle mass. For $z_0 = 2.5$ it turns out there is just a single bound state.)

C programs to solve problems 8,9 are at the end of this solutions set. If you take a peak at Griffiths you see that the expected solution is between $z = 0$ and $z = \pi/2 \approx 1.57$. So I will choose $z_0 = 0.1$ and $z_1 = 1.5$ as my initial bracket points. When I do so, the program output is:

```
[rts@sherlock p140a]$ finitesqwell.e
Enter N
15
Enter z1,z2,z0
0.1 1.5 2.5

 z1=    0.80000  z2=    1.50000
 z1=    0.80000  z2=    1.15000
 z1=    0.97500  z2=    1.15000
 z1=    1.06250  z2=    1.15000
 z1=    1.10625  z2=    1.15000
 z1=    1.10625  z2=    1.12812
 z1=    1.10625  z2=    1.11719
 z1=    1.10625  z2=    1.11172
 z1=    1.10898  z2=    1.11172
 z1=    1.11035  z2=    1.11172
 z1=    1.11035  z2=    1.11104
 z1=    1.11035  z2=    1.11069
 z1=    1.11035  z2=    1.11052
 z1=    1.11044  z2=    1.11052
 z1=    1.11048  z2=    1.11052
```

So the solution (to four decimal places) is $z = 1.1105$.

[9.] Given a normalized vector $\vec{v}$ with components v_n, $n = 1, 2, \cdots N$, the participation ratio

$$\mathcal{P} = \Big(\sum_n v_n^4 \Big)^{-1}$$

provides an estimate of the number of components of $\vec{v}$ which are of significant size. When we study lattice vibrations and the effects of defects, it will be useful for us to compute $\mathcal{P}$. Write a C program to compute $\mathcal{P}$, for vectors $\vec{v}$ with components

$$v_n = A \exp\Big(- \frac{(n - N/2)^2}{\xi^2} \Big)$$

Here ξ is a free parameter. You need to normalize $\vec{v}$, that is, choose A so that $\sum_n v_n^2 = 1$. By looking at the form of v_n what would you guess should be a reasonable result for $\mathcal{P}$? That is, how would you expect $\mathcal{P}$ to depend on ξ? Does your program conform to this expectation?

C programs to solve problems 8,9 are at the end of this solutions set. The Gaussian function given has center at $N/2$ and width ξ. Thus, if the participation ratio does what it is supposed to do, we might expect $\mathcal{P} \approx 2\xi$. The numerical values I get conform to this expectation. Some examples are the following:

```
[rts@sherlock p140a]$ participation.e
Enter N
500
Enter xi
2

 P=  3.544541

[rts@sherlock p140a]$ participation.e
Enter N
500
Enter xi
10

 P=  17.724539
```

C program to solve Problem 1-8.

```
#include <stdio.h>
#include <math.h>

int main(void)

{

int i,N;
double z0,z1,z2,f1,f2,zm,fm;

printf("Enter N");
printf("\n");
scanf("%d",&N);
printf("Enter z1,z2,z0");
printf("\n");
scanf("%lf %lf %lf",&z1,&z2,&z0);

f1=tan(z1)-sqrt( (z0/z1)*(z0/z1) - 1.0 );
f2=tan(z2)-sqrt( (z0/z2)*(z0/z2) - 1.0 );

for (i=0; i<N; i=i+1)
{
  zm=(z1+z2)/2.0;
  fm=tan(zm)-sqrt( (z0/zm)*(z0/zm) - 1.0 );
  if (fm<0.0)
  {
  z1=zm;
  }
  else
  {
  z2=zm;
  }
  printf("\n z1=  %9.5lf  z2=  %9.5lf",z1,z2);

}

printf("\n");

return 0;
}
```

C program to solve Problem 1-9.

```
#include <stdio.h>
#include <math.h>

int main(void)

{

int j,N,N2;
double v[1000],A,P,xi;

printf("Enter N");
printf("\n");
scanf("%d",&N);
printf("Enter xi");
printf("\n");
scanf("%lf",&xi);

N2=N/2;

A=0.;
for (j=0; j<N; j=j+1)
{
v[j]=exp( -(j-N2)*(j-N2)/(xi*xi) );
A=A+v[j]*v[j];
}
A=sqrt(A);

P=0.;
for (j=0; j<N; j=j+1)
{
v[j]=v[j]/A;
P=P+v[j]*v[j]*v[j]*v[j];
}
P=1./P;
printf("\n P=  %lf",P);

printf("\n");

return 0;
}
```

Comments: I have not tried to be super-efficient in writing this program. If we were interested in speed, we would define a new variable to store the square of ξ so that it is not computed over and over in the loop. (A good compiler might realize this by itself and do it, especially if you choose a high optimization value.) I also might consider defining a new variable for the inverse of the normalization constant and multiply by that number instead of dividing. It used to be (I have not checked recently) that computers wer substantially faster at multiplication than division, so replacing divisions by multiplications was advantageous. In fact, the same was true of exponentiation: it was better to compute x^2 via $x * x$ than via $\mathrm{pow}(x, 2)$.