Physics 518
Final Exam — Tuesday, April 30

1. The primitive translation vectors of a Bravais lattice are

$$\begin{aligned}\vec{t}_1 &= (a, 0, 0)\\ \vec{t}_2 &= (a/3, b, 0)\\ \vec{t}_3 &= (0, 0, c)\end{aligned} \tag{1}$$

where $a = 2.0\mathring{A}$, $b = 2.3\mathring{A}$ and $c = 3.0\mathring{A}$. Calculate:
(a) the volume of the primitive cell
(b) the primitive translation vectors of its reciprocal lattice
(c) the volume of the first Brillouin zone in reciprocal space

2. A newly discovered one-dimensional crystal has the structure of a *ladder*. It has two parallel lines of atoms with each atom bonded to its two intrachain neighbors at lattice constant a_1 and to one interchain neighbor, separated by distance a_2. This problem concerns the electronic spectrum, band filling and specific heat of this crystal.

(a) A tight binding Hamiltonian for this system describes the tunneling motion of electrons from each lattice site to its two neighbors on the same chain and to a single neighbor on the other chain. Let's label the chains A and B, and the basis states $|m, A(B)\rangle$ denotes an orbital on the m-th lattice site of the $A(B)$-th chain. Using this basis the Hamiltonian can be expressed

$$\begin{aligned}\mathcal{H} = \sum_m -|t_A| \quad & (\quad |m+1, A\rangle\langle m, A| + |m-1, A\rangle\langle m, A| + |m, A\rangle\langle m+1, A| + |m, A\rangle\langle m-1, A|)\\ +|t_B| \quad & (\quad |m+1, B\rangle\langle m, B| + |m-1, B\rangle\langle m, B + |m, B\rangle\langle m+1, B| + |m, B\rangle\langle m-1, B|)\\ t_2 \quad & (\quad |m, A\rangle\langle m, B| + |m, B\rangle\langle m, A|)\end{aligned} \tag{2}$$

Notice the signs of the various terms in this equation: the intrachain hopping amplitudes are negative on the A chain and positive on the B chain. The interchain amplitudes are positive. For definiteness let's take $t_A = 0.5\,\mathrm{eV}$ and $t_B = 0.2\,\mathrm{eV}$.

If $t_2 = 0$ plot the dispersion relation $E(k)$ for electronic states of the ladder. Note that there will be two branches, so be careful to identify the maximum and minimum energies of these branches, and the positions of any possible crossing points.

(b) Setting $t_2 = 0.05\,\mathrm{eV}$, calculate the minimum energy gap between the two branches obtained in (a), and replot the dispersion relation.

(c) If each lattice site contributes one electron, what is the energy of the highest filled state.

(d) A plot of the logarithm of the low temperature specific heat $\ln(c_V)$ versus $1/kT$ is approximately linear at low temperature. What is the slope of this line.

(e) (5 points extra credit) Using $a_1 = 4\mathring{A}$ and $a_2 = 6\mathring{A}$, calculate the effective masses for electrons at the two band edges that bound the minimum band gap for this system.

3. A one dimensional monatomic crystal consists of atoms of mass M ordered on a lattice of lattice constant a. It has a phonon dispersion relation:

$$\omega^2(k) = \frac{4K_1}{M}\sin^2(ka/2) + \frac{4K_2}{M}\sin^2(ka) \tag{3}$$

(a) Sketch this dispersion relation in the first Brillouin zone (you should assume both K's are positive and that $K_1 > K_2$).
(b) Calculate the sound velocity for modes propagating along this linear chain.
(c) What is the phonon contribution to the specific heat of this crystal when $kT >> 2\hbar\sqrt{K_1/M}$.
(d) What is the specific heat of this crystal when $kT << 2\hbar\sqrt{K_1/M}$. (Hint: Your answer can contain as a factor a dimensionless integral of the form $I_n = \int_0^\infty dx \frac{x^n}{e^x - 1}$, but be sure to clearly indicate the prefactors and temperature dependence of your result.)

4. Give a one line descriptive setence identifying each of the following items

Debye Temperature

Cooper Instability

Reciprocal Lattice

Pauli Paramagnetism

$h/2e^2$

Miller Indices

Meissner Effect

Bravais Lattice

Fermi Surface

Debye Waller Factor