Physics 861 { Fall 01 Problem set 6 - Due Tuesday, Oct 23

Problem 1.

Look at the fcc free electron energy levels (empty lattice plot) of Figure 9.5, Ashcroft and Mermin.

(a) Give the coordinates of the points X, W, L, K in units of 2¹/₄=a:

(b) What are the degeneracies of all the levels with energy less or equal to 3, in the units of the \neg gure?

(c) These degeneracies are lifted by a periodic potential V, which has Fourier coefcients V_G . Note that V_G depends only on the magnitude of the vector G. List the rst 5 non-zero values of G^2 (this is the familiar problem of reciprocal lattice point shells).

(d) Using the lowest order of perturbation theory as in Figure 9.4, \neg nd the magnitude of the energy gaps that open up at the lowest level of point X (unperturbed energy = 1), of point L, and of point K. That is, relate these gaps to speci⁻c coe±cients V_G. Compare Figure 11.9.

Problem 2.

Recall that in an earlier problem set you wrote down the operations of the group C_{4v} . Divide these operations into classes and identify these classes with those listed on the top line of Table III, page 22, of Callaway's book (on reserve). You can make reasonable guesses, knowing that operations of the same type belong to the same class (Note that JC_4^2 is simply a specular re[°] ection, more commonly denoted as $\frac{3}{h}$. Similarly for JC_2). However, if two operations A and B belong to the same class, check that there is a C such that $B = CAC^{\frac{1}{1}}$, or BC = CA. How many operations are in each class?

Problem 3.

(a) Consider the 6 functions x^2 , y^2 , z^2 , xy, yz, zx. Using Table III, page 22, of Callaway's book (on reserve), project out combinations that belong to the 5 irreducible representations listed in that table. One or more irreps may not be contained in this set. All the results, except one, are given in the Table itself.

(b) Do the same for the 4 functions exp(ik:r) for $k = (k_x; \S1; \S1)$.