6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 1

Issued: 2-3-99 Due: 2-10-99, at the beginning of class.

Readings:
PSSA Chapter 1. (overview)
PSSA Chapter 2. (bonding)
6.728 Course Notes, Lectures 12 (The Quantum LC Circuit))
6.728 Course Notes, Lectures 24—26 (Statistical Physics Review))
Aschroft and Mermin: Chapters 19 and 20 (bonding)
Aschroft and Mermin: Chapter 2 (Sommerfeld Model)

Problem 1.0

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Problem 1.1 *Homonuclear Diatomic Molecule* **PSSA problem 2.1**

This problem reviews the bonding and antibonding states that were developed in class.

Problem 1.2 *Finite Basis Set Expansion* **PSSA Problem 2.3**

This is an important problem and forms the backbone for much of the band structure calculations that we will do in Chapter 7 as well as other approximations for quantum states. See Lecture 16 of 6.728. Rather than use Lagrange mulitpliers, it is simplier to minimize $E = <\psi|\hat{H}|\psi> / <\psi|\psi>$ and setting $<\psi|\psi> = 1$ only at the end of the minimization procedure. Make sure you are confortable with the results of this problem. (See Morrison *et al.*, *Understanding More Quantum Physics*, pp. 99—101 for guidance if you need a hint.)

Problem 1.3 *sp-Valent dimers* **PSSA Problem 2.4**, parts a and b only, and parts (e) and (f) listed below.

This problem tests your understanding of the next level of approximation for a molecule when more atomic function states are included in the basis set expansion. Note that you only have to set up the problem and interpret what a typical result might be. We will encounter problems of this nature throughout the class.

(e) How many eigen energies and eigen values result form this problem?

(f) Write out $\Psi(\mathbf{r})$ in terms of $\phi_s(\mathbf{r}-\mathbf{r}_1), \phi_{pz}(\mathbf{r}-\mathbf{r}_1), \phi_s(\mathbf{r}-\mathbf{r}_2)$ and $\phi_{pz}(\mathbf{r}-\mathbf{r}_2)$ if the eigen vector $\mathbf{c}$ is

$$\mathbf{c} = A \begin{pmatrix} c_1 \\ c_2 \\ c_1 \\ -c_2 \end{pmatrix}$$

What is the value of the normalization constant A?

Problem 1.4 *Molecular crystals.* **PSSA Problem 2.5**, but do it only for a cubic and face-centered cubic crystal. Also compare your results with Table 20.2 in Aschcroft and Mermin, which is reprinted below. Attach your .m files from `matlab`. (Note that the notes have this problem labled mistakenly as 2.4.)

You should use `matlab` to numerically evaluate the lattice sums. Later on in the class you will be gives programs in `matlab` to write or to modify . So this problem is meant to familarize you both with crystal structures and with `matlab`.