6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 1

Issued: 2-4-04 Due: 2-13-04, at the beginning of class.

Readings:
PSSA Chapter 1. (overview)
PSSA Chapter 2. (bonding)

Problem 1.1 *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.)

Problem 1.2 *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 1.3 *Two Dimensional Electron Gas.* **PSSA Problem 3.2**

Problem 1.4 *Classical Limit of Fermi-Dirac Statistics* **PSSA Problem 3.1 parts a—d**

This problem shows how if one assumes the Boltzmann factor (Eqn. 3.77), then the classical results that we quote many times in class follow.

Problem 1.5 *Perturbation Theory. This problem explores the accuracy of perturbation theory when applied to a finite quantum well.*

Consider an infinitely deep quantum well of width a and situated from $x = 0$ to $x = a$. This is the usual one-dimensional particle in the box problem with confining potential

$$V_0(x) = \begin{cases} 0 & \text{if } 0 < x < a \\ \infty & \text{otherwise} \end{cases}$$

which has eigen energies given by

$$E_n^{\infty} = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Now consider a new potential which is given by

$$V(x) = \begin{cases} 0 & \text{if } 0 < x < a/2 \\ E_1^{\infty}/10 & \text{if } a/2 < x < a \\ \infty & \text{otherwise} \end{cases}$$

(a) Calculate the first order energy shift of the nth eigen state due to the perturbation $V(x) - V_0(x)$.
(b)Calculate the new ground state wave function. Use only the first three non-vanishing terms in the perturbation expansion.
(c) Use a finite difference representation of Schrödinger's equation to calculate the energy of the ground state in the perturbed quantum well. The finite difference representation can be written as a matrix operation as shown on the next page. The matlab code will be sent to you. Assume a quantum well thickness of 10 nm.