PROBLEM SET 1
Issued: 2-7-01 Due: 2-14-01, at the beginning of class.

Readings:
PSSA Chapter 1. (overview)
PSSA Chapter 2. (bonding)
6.728 Course Notes, Lectures 9, 10 and 12 (SHO and The Quantum LC Circuit))
Aschroft and Mermin: Chapters 19 and 20 (bonding)
Aschroft and Mermin: Chapter 2 (Sommerfeld Model)

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 \( \Psi(r) \) in terms of \( \phi_s(r - r_1), \phi_{p_z}(r - r_1), \phi_s(r - r_2) \) and \( \phi_{p_z}(r - r_2) \) 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 Quantum LC Circuit I.**

Consider an inductor $L$ and a capacitor $C$ connected in parallel. The Hamiltonian for this circuit is

$$H = \frac{1}{2}LI^2 + \frac{1}{2}CV^2$$

where $I$ is the current flowing through the inductor and $V$ is the voltage across the capacitor.

(a) Take the voltage $V$ as the variable and write the Hamiltonian in the form

$$H = \frac{P^2_V}{2M_V} + \frac{1}{2}M_V\omega^2V^2$$

where $\omega = \sqrt{1/LC}$ is the resonant frequency of the circuit. Find $M_V$ and $P_V = M_VdV/dt$.

(b) By analogy with the Simple Harmonic Oscillator, define the creation and annihilation operators such that

$$\hat{V} = \sqrt{\frac{\hbar}{2C}}(a + a^\dagger) \quad \text{and} \quad \hat{P}_V = L\hat{\omega} = -i\sqrt{\frac{\hbar LC^2}{2}}(a - a^\dagger)$$

and show that $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$.

(c) The Uncertainty Relation can be written as $\Delta V \Delta I \geq A$. What is $A$?

(d) Capacitors of niobium can be made $100\text{nm} \times 100\text{nm}$ and have a specific capacitance of about $50 \text{fF}/\mu\text{m}^2$. The circuit loop can be about $5 \mu\text{m}$ in diameter $p$. Assume $L \approx \mu_{op}$. At what temperature would you have to operate to see the circuit behave quantum mechanically. (Note niobium is a superconductor and the resistance can be made negligibly small at low temperatures.)

**Problem 1.5 Quantum LC Circuit II.**

(a) The Hamiltonian of the $LC$ circuit can also be written as

$$H = \frac{1}{2}CV^2 + \frac{1}{2}\Phi^2$$

where $\Phi$ is the flux in the inductor.

(b) Show that the Hamiltonian can be written with the flux as the variable as

$$H = \frac{P^2_\Phi}{2M_\Phi} + \frac{1}{2}M_\Phi\omega^2\Phi^2$$

Find $M_\Phi$ and $P_\Phi = M_\Phi d\Phi/dt$ and show that $P_\Phi = Q$, where $Q$ is the charge on the capacitor.

(c) Express $Q$ and $\Phi$ in terms of creation and annihilation operators.

(d) Show that the uncertainty principle can be written as

$$\Delta Q \Delta \Phi \geq \frac{\hbar}{2}$$