6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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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 $\Psi(\mathbf{r})$ 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 *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 votage V as the variable and write the Hamiltonian in the form

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

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

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

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

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 100nm $\times$ 100nm and have a specific capacitance of about 50 fF/μm^2. The circuit loop can be about 5 μm in diameter p. Assume $L \approx \mu_o p$. 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 negligiblely small at low temperatures.)

Problem 1.5 *Quantum LC Circuit II.*

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

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

where Φ is the flux in the inductor.

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

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

Find M_Φ 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 Φ in terms of creation and annihilation operators.

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

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

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