6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 5

Issued: 3-16-99 Due: 4-7-99, at the beginning of class.

Readings:
PSSA Chapter 7
Ashcroft and Mermin, Chapter 10

Problem 5.1 PSSA Problem 7.1

Problem 5.2 PSSA Problem 7.2

Problem 5.3 PSSA Problem 7.3

Problem 5.4 *Phase of the Bloch wave function*
SSS Exercises 8.4, 8.7, and 8.10

Problem 5.5 *Nearly Free Electron Model*
This problems is based on the exercises in Section 8.5 of SSS.

(a) Load `bloch` of SSS and select PRESET 1. On the show button, select PSI-SQUARED. Change the POTENTIAL WIDTH to $0.1\,\text{Å}$ and the POTENTIAL DEPTH to $-20\,\text{eV}$. Click on CALCULATE BANDS and CALCULATE PSI. Obtain the widths of the first four bands gaps from the data in the BAND LIST. Why are the gaps nearly the same?

(b) Click on the energies for the first and then the second band at the Brillouin zone edge on the graph to the right. Print out the PSI-SQUARED graph and comment on the relative shapes of the wave functions, with respect to each other and to the potential. Repeat this for the states at the zone center between the second and third bands.

(c) Repeat part (a) for the pairs of points (POT. WIDTH, POT. DEPTH) equal to $(0.2\,\text{Å}, -10\,\text{eV})$ and $(0.4\,\text{Å}, -5\,\text{eV})$.

Show that the potentials considered in parts (a) and (b) all give nearly the same energy gaps. Why is this true? When do you expect these potentials to give different energy gaps?