6.730 PHYSICS FOR SOLID STATE APPLICATIONS

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PROBLEM SET 7

Issued: 4-3-96 Due: 4-10-96, at the beginning of class.

Readings:
Central Equation: Chapter 7.3—7.4 in the 6.730 notes, and Chapter 10 in Ashcroft and Mermin.
1D Band Structures: Chapter 7.4 in the 6.730 notes.
Weak Periodic Potential Approximation: Chapter 7.5 in the 6.730 notes, and Chapter 9 in Ashcroft and Mermin.
Properties of Bloch functions: Chapter 7.6 in the 6.730 notes, and Chapter 8 in Ashcroft and Mermin.

Problem 7.1 Set up a $M \times M$ central equation matrix for a particle in a periodic potential with $a = 4\,\text{Å}$,

$$V = 1\text{eV}\cos\frac{2\pi x}{a} - 0.5\text{eV}\cos\frac{4\pi x}{a}\,.$$

You may use a truncated matrix.
(a) Let $M = 16$, plot E versus k for all the eigenvalues found. Also plot it for the first 4 bands. Put energy in terms of electron volts and k in units of $2\pi/a$. Restrict yourself to the first Brillouin Zone.

(b) Plot the velocity $v_{k,N}$ as a function of k in the first Brillouin zone for the first 4 bands.

Problem 7.2 For the potential in Problem 7.1, write a program to find the eigen energies and eigen vectors.

(a) For each of the crystal momenta k and band indices n given below make the following four plots. (You can use the `subplot` command to get them all on one page.)

- Plot the eigen wave functions $a_{k,n}(q)$, by ploting $u_{k,n}[K_i]$ at each $q = k + K_i$ as done in the notes.
- Plot the real and imaginary parts of the real space eigen function $\psi_{k,n}(x)$.

- Plot the real and imaginary part of $u_{k,n}(x)$.
- Plot $|\psi_{k,n}(x)|^2$.

Do the above for the series of points given by

$$(k, n) = (\pi/a, 1); (\pi/a, 2); (\pi/2a, 1); (0, 2); (0, 3); (\pi/2a, 3);$$

(b) Use the weak potential approximation to find the energy gaps bewteen the band up to $N = 4$. How does this approximation compare with part (a). Also explain the nature of the wave functions at each point.

Hint: The command

[A,D]=eig(H)

puts the eigenvectors as columns in the matrix A, and the corresponding eigenvalues along the diagonal matrix D. The command

[E,n]=sort(diag(D)); A=A(:,n)

sorts the eigenvales and eigenvectors.

Quiz 2 is Friday, April 19, 1996.