Long problem 1

Show all your calculations. Write in pen, not in pencil, otherwise I can't read it.

For a Kronig-Penney model with delta-function potential

$$U(x) = aU_0\delta(x-na)$$

Assume the wavefunction for wavevector k is of the form

$$\psi_k(x) = Ae^{iqx} + Be^{-iqx}$$

in the interval

$$0 \le x \le a$$

and that it satisfies the Bloch condition

$$\psi_k(x+a) = e^{ika}\psi_k(x)$$

(a) Give an expression for the energy in terms of either k or q or both.
(b) Find an equation for A and B by requiring that the wavefunction is continuous at x=0.
(c) Find a second equation for A and B by integrating the Schrodinger equation for this wavefunction between –δ and δ with δ →0.
(d) By setting the determinant=0, find an algebraic equation relating k (Bloch wavevector) to q..

Assume units so that a=1, hbar^2/m=1. In these units, assume U_0=3*pi/4.

(e) Make a graph of the energy versus k relation for the three lowest energy bands.

(f) Give the numerical values of the bandwidth of the three lowest bands.

(g) Give the numerical values of the energy gaps between the first and second, and between the second and third bands.

(h) Find numerical values of m*/m at the bottom and top of the first and second bands (m*=effective mass, m=bare mass).

(i) Make graphs of the electron charge density versus x in the interval 0<x<2a, normalized so that the total charge in the interval 0<x<a is 1, for:
(1) state at the bottom of the lowest band
(2) state at the top of the lowest band
(3) state at the bottom of the second band
(4) state at the top of the second band