NANO 705
Homework 4
Due: M-3/20, 10:00 AM

Show all work and discuss results.

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1) Using a particular representation, an arbitrary state can be written as $|\psi\rangle = c_1|\phi_1\rangle + c_2|\phi_2\rangle + c_3|\phi_3\rangle$,

where the basis vectors are orthonormal: $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. In matrix form, the state can be written:

$$\{\psi\} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

The hamiltonian matrix in this basis appears as

$$[H] = \begin{pmatrix} 3a & 0 & 0 \\ 0 & 3a & -a \\ 0 & -a & 3a \end{pmatrix}$$

where a is a constant.

a) Find the three energy eignvalues E_i ($i = 1, 2, 3$).

b) Find the eigenvector $|\psi_i\rangle$ ($i = 1, 2, 3$) for each eigenvalue.

c) Write the hamiltonian matrix $[H']$ in the diagonal representation.

d) Given a chemical potential μ at some temperature *T*, write the equilibrium density matrix $[\rho']$ in the diagonal representation. [Abbreviate the Fermi functions $f_i = f_0(E_i - \mu)$ ($i = 1, 2, 3$).]

e) Write the transformation matrix $[V]$, such that $[H] = [V] \cdot [H'] \cdot [V]^\dagger$.

f) Find the equilibrium density matrix $[\rho]$ in the original representation.

g) Write an expression for the equilibrium carrier concentration $n(x)$ in terms of the basis wave functions $\phi_i(x)$ ($i = 1, 2, 3$).

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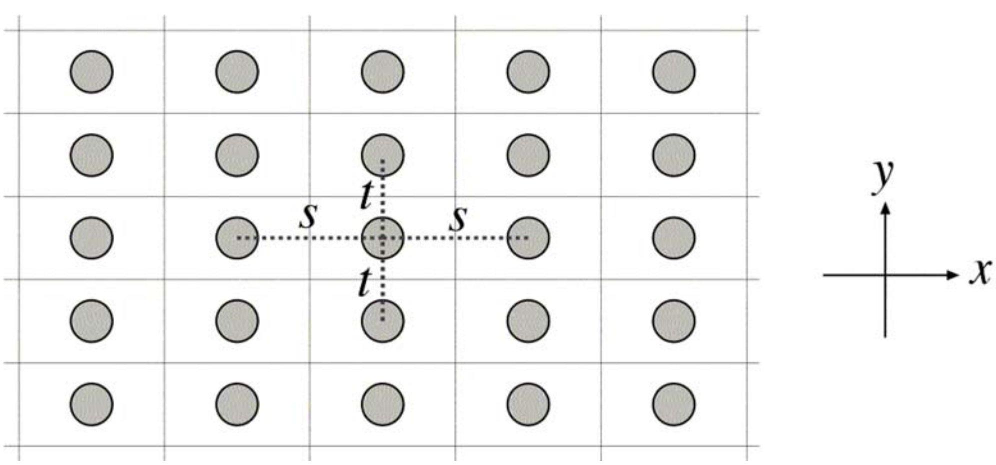
2) A 2-D crystal with a one-atom basis on a rectangular lattice is shown below. The matrix matrix elements coupling neighboring atoms are indicated by the letters *s* and *t*.



Find a general expression for the dispersion relation $E(k_x, k_y)$.