

1. **Zinc in copper**

Copper is a monovalent fcc nearly-free electron metal. Zinc is an fcc divalent metal. In small quantities, zinc mixes substitutionally with copper, its main effect being to increase the electron concentration.

- a) Find the relationship between electron density and the Fermi wave vector within the nearly free electron approximation.
- b) Still working in the nearly free electron approximation, assume that the zinc-copper mixture will undergo a phase transition to bcc as soon as the Fermi sphere first touches some point on the edge of the Brillouin zone. Show that the transition occurs at 36 % zinc. Remember that in an fcc conventional unit cell there are four ions.
- c) As the concentration of zinc further increases, another phase transition next occurs when the Fermi sphere intersects the Brillouin zone of the bcc lattice. What is the second concentration of zinc?

2. **Wannier functions**

- a) Show that matrix elements of the Hamiltonian between Wannier functions coming from different bands must vanish.
- b) Show that the matrix element $\langle \vec{R} | \hat{\mathcal{H}} | \vec{R}' \rangle$ depends only upon $\vec{R} - \vec{R}'$, where $\langle \vec{R} |$ is a Wannier function centered at lattice site $\vec{R}$.

3. **Tight-binding model, part 1**

Consider a tight-binding Hamiltonian that acts upon a single band of localized states in one dimensions,

$$\hat{\mathcal{H}} = 2t \sum_l \frac{1}{2} (|l\rangle \langle l+1| + |l\rangle \langle l-1|) + \cos(2\pi l \tau_3) |l\rangle \langle l|$$

with $\tau_3 = \frac{5}{3}$. The integer l should be thought of as indexing sites along a chain of atoms; the state $|l\rangle$ locates an electron on atom l .

- a) What is the periodicity of the Hamiltonian?
- b) Use Bloch's theorem to reduce the eigenvalue problem associated with the Hamiltonian to the solution of a small finite matrix equation.

4. **Tight-binding model, part 2**

Compute and plot the bands of the previous problem for k throughout the Brillouin zone. (Needs to be done numerically. In Mathematica, the 'Eigenvalues[M]'-command computes the eigenvalues of the matrix M.)