Háskóli Íslands
Raunvísindadeild
Eðlisfræði

Haust 2015

Eðlisfræði þéttefnis I

Dæmablað 9

Skilafrestur 3. November 2015 kl. 15:00

1. **Empty lattice or free electron model** (15)

   (a) Construct the first, second and third Brillouin zones for a two dimensional square lattice crystal of lattice constant a. In the free electron approximation, what is the number of electrons per unit cell needed for the third Brillouin zone to start being filled ?

   (b) Consider a monovalent simple cubic crystal and calculate the fraction of substitutions with bivalent atoms required for the Fermi surface to touch the boundary of the first Brillouin zone.

   (c) In a FCC crystal with conventional lattice constant $a = 0.4$ nm, what is the energy difference between the lowest and next lowest bands at the center of the first Brillouin zone.

   (d) Determine if the Fermi surface of a monovalent BCC crystal lies within the first Brillouin zone.

2. **van Hove singularities** (15)

   (a) In a linear harmonic chain with only nearest-neighbor interactions, the normal-mode dispersion relation has the form $\omega(q) = \omega_0|\sin(qa/2)|$, where the constant ω_0 is the maximum frequency (assumed when q is on the zone boundary). Show that the density of normal modes in this case is given by

$$D(\omega) = \frac{2}{\pi a\sqrt{\omega_0^2 - \omega^2}}.$$

The singularity at $\omega_0 - \omega$ is called a van Hove singularity.

(b) In three dimensions the van Hove singularities are infinities not in the normal mode density itself, but in its derivative. Show that the normal modes in the neighborhood of a maximum of $\omega(q)$, for example, lead to a term in the normal mode density that varies as $(\omega_0 - \omega)^{1/2}$.