Solid State Theory

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Sheet 2: return on: Wednesday, Oct 31, 2012, 16:00 (SR THP)

Exercise 1: reciprocal lattice

a) A three-dimensional triangular lattice can be defined in the following way:

$$L = \{\vec{R}_{\vec{n}} | n_i \in \mathbb{Z}\} \ , \ \text{with } \vec{R}_{\vec{n}} = \sum_i n_i \vec{a}_i \ ,$$

and the primitive vectors

$$\vec{a}_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \ , \ \vec{a}_2 = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{3} \\ 0 \end{pmatrix} \ , \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \ .$$

Determine the reciprocal lattice vectors $\vec{b}_i$ and the volume of the unit cells of both direct and reciprocal lattice. (2 points)

b) Given an arbitrary Bravais lattice L, show that $(L_\mathrm{r})_\mathrm{r}$ equals L up to a common factor. (The reciprocal lattice of the reciprocal lattice is again the direct lattice.) (3 points)

c) The body-centered cubic lattice L_bcc has been defined in exercise 1, sheet 1. Show that the reciprocal lattice of L_bcc is the face-centered cubic lattice L_fcc. (2 points)

Exercise 2: adiabatic approximation

The Hamiltonian of a quantum-mechanical two-particle system is given by

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + \frac{1}{2}k_1 x_1^2 + \frac{1}{2}k_2 (x_1 - x_2)^2 \ .$$

The variables x_1, x_2 correspond to the positions of the ion (mass M) and the electron (mass m) respectively.

a) Show that the (exact) eigenenergies of the system are given by

$$E_{n_1,n_2} = \hbar\omega_1 \left(n_1 + \frac{1}{2}\right) + \hbar\omega_2 \left(n_2 + \frac{1}{2}\right) \ ,$$

where

$$\omega_{1,2}^2 = \frac{1}{2}\left(\frac{k_1+k_2}{M}+\frac{k_2}{m}\right) \pm \sqrt{\frac{1}{4}\left(\frac{k_1+k_2}{M}-\frac{k_2}{m}\right)^2+\frac{k_2^2}{Mm}}$$

and $n_1, n_2 \in \mathbb{N}_0$. (4 points)

b) Within the adiabatic approximation (Born-Oppenheimer approximation), one first solves the problem for a fixed position x_1 of the ion. Calculate the eigenenergies of the resulting electronic problem as a function of x_1. (3 points)

c) The electronic energies calculated in b) correspond to the effective potential for the ion. Calculate the eigenenergies of this effective model for the ion. (2 points)

d) Compare the results of a) and c) by expanding the exact eigenenergies up to first order in m/M. (4 points)