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St Hilda's College - Michaelmas 2009

B2: Condensed Matter Physics and Photonics

Tutorial 2 - Lattice Dynamics

Please leave your work in my Keble pigeon hole by 5pm on Friday of 3rd week.
Suggested reading: Hook & Hall 2; Kittel 4, 5; Ashcroft/Mermin 22, 23. There is also some useful information on scattering in Dove: Structure and Dynamics.

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1 Boundary Conditions and the Density of States

1. What are Born - von Karman boundary conditions? What is the philosophy behind their use? Based solely on the assumption of Born - von Karman boundary conditions, what are the allowed **k**-states in an ideal crystal? Show that the number of **k**-states in the first Brillouin zone is equal to the number of primitive unit cells in the crystal.

   What is the meaning of the term *density of states*? Find expressions, both in **k**-space and in terms of the energy, for the density of states of a free system in 1, 2 and 3 dimensions.

2 Lattice Vibrations / Phonons - Theory and Measurement

2. Please attempt B2 2005 q2 from the online past papers. As well as the dispersion, please also sketch the group velocity as a function of wavenumber, and explain why it is important.

3. How many solutions to the phonon wave equation (i.e. the number of phonon branches) are there for a particular value of the wavevector for the following crystals;

   (a) Solid argon - f.c.c. unit cell, with 4 Ar atoms per unit cell.

   (b) NaCl

   (c) CsCl

   (d) Silicon

   Discuss in each case whether optical absorption or scattering techniques would be appropriate for the study of phonons.

   A monatomic primitive cubic crystal with lattice spacing 0.318nm has a longitudinal sound velocity of 5000ms^{-1}. Estimate the maximum phonon frequency, ν_m, for this solid.

3 Thermal Properties of the Lattice

4. Please attempt B2 2006 Q2 from the online exam papers.

4 Quantum Approach

5. So far we have talked about vibrations from a classical, Newtonian standpoint. However, all we have really done is find a transformation into normal coordinates - this transformation holds equally well for the quantum mechanical operators. The following problem leads you through the quantisation of lattice vibrations in one dimension.

   The Hamiltonian for the 1-D monatomic chain is a sum of coupled harmonic oscillators:

$$H = \sum_j \Big(\frac{p_j^2}{2m} + \frac{m\omega_0^2}{2}(x_{j+1} - x_j)^2 \Big)$$

   Show that the following Fourier decomposition decouples them;

$$x_j = N^{-1/2} \sum_k e^{-ikja} X_k \qquad p_j = N^{-1/2} \sum_k e^{ikja} P_k$$

   into the from:

$$H = \sum_k \Big(\frac{P_{-k}P_k}{2m} + \frac{m\omega_0^2}{2}(4\sin(ka/2))X_{-k}X_k \Big) \tag{1}$$

   where N is the number of atoms in the chain and a is the equilibrium atomic spacing.

   Hint: use the identity $\sum_j \exp(i(k' + k)ja) = N\delta_{k,-k'}$. What are the allowed values of k?

   So far we have made no assumptions about whether we are dealing with a quantum or a classical system. In the classical case, we could use this form of H to derive the same dispersion as in question 2 (don't worry about the details of how to do this - the easiest way is with Hamiltonian mechanics). In the quantum case, we need to explicitly consider the observables a operators.

   (a) Show that $[X_k, P_q] = i\hbar\delta_{k,q}$, and that $X_k^\dagger = X_{-k}$ (and similarly for $P_k^\dagger$). To do this you will need to use the hermitian property of x_j: $x_j^\dagger = x_j$.

   (b) Define the operator a_k by:

$$a_k = \Big(\frac{m\omega_k}{2\hbar}\Big)^{1/2}(X_k + \frac{i}{m\omega_k}P_k^\dagger), \tag{2}$$

   where $\omega_k = 2\omega_0|\sin(ka/2)|$. Show that $[a_k, a_q^\dagger] = \delta_{k,q}$, and hence that the Hamiltonian simplifies to the form:

$$H = \sum_k \hbar\omega_k(a_k^\dagger a_k + 1/2) \tag{3}$$

   We have now decoupled the system into independent quantum oscillators. What is the energy spectrum? Explain what each of the new operators means physically. Referring to your answer, or otherwise, explain what a phonon is.

5 Summary

6. Bringing together everything you've done this week, describe (in half a page or so) how we've moved from ions connected to each other with harmonic potentials to a description of the thermal properties of the lattice. Your answer should include references to normal modes and how the relate to the phonons.