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PHYS 7450: Advanced Solid State Physics

Homework Set 1

Issued January 13, 2015
Due January 27, 2015

Reading Assignment: J. Solyoms, Solids 1

1. Band structure

   Consider a tight-binding model of an electron described by a Hamiltonian,

   $$H = -t \sum_{\langle \mathbf{R}, \mathbf{R}' \rangle} c^\dagger_{\mathbf{R}} c_{\mathbf{R}'},$$

   with a hopping matrix element t.

   Compute the electronic band structure, the spectrum $E_{\mathbf{k},n}$ (n band index and $\mathbf{k}$ crystal momentum) for

   (a) honeycomb lattice

   (b) kagome lattice

   and plot it in the 2d BZ and as a one-dimensional cut through the Γ ($\mathbf{k} = 0$) point.

   Hint:

   - These lattices have 2- and 3- atom basis, that needs to be carefully taken into account as independent intra-cell degrees of freedom.
   - As usual use momentum states $\mathbf{k}$ (with the crystal momentum confined to the 1st Brillouin zone), Fourier transforming to momentum operators $c_{\mathbf{k},s}$, with $c_{\mathbf{R}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} c_{\mathbf{k},s} e^{i\mathbf{k}\cdot\mathbf{R}}$ and $s = 1, \ldots, p$ the basis label for intra-cell atoms, to diagonalize these single particle problems.

2. A diatomic crystal 1d chain

   Consider a one-dimensional array of atoms, with Hamiltonian

   $$H = \sum_i \frac{p_i^2}{2m} + \frac{1}{2} \sum_i B_i (u_{i+1} - u_i)^2$$

in which every mass m is the same, but the *harmonic* springs alternate in spring-constant strength B_i on every other site between values of B_0 and B_1. Take the lattice period to be $2a$ and spacing between atoms within the cell to be c. This problem simulates a crystal chain of a diatomic molecule such as H_2.

(a) By diagonalizing the Newton's equation of motion for atoms in this 1d crystal with 2-atom basis (using Fourier series) show that there is one optical and one acoustic mode, and compute and plot their dispersions $\omega_o(k)$ and $\omega_a(k)$, respectively.

To get full credit, on your graph please indicate all the relevant frequency and wavevector scales (e.g., $\omega_{o/a}(k=0)$, $\omega_{o/a}(k=1\text{BZ}-\text{boundary})$, $k_{1\text{BZ}-\text{boundary}}$,...) characterizing these two dispersions.

(b) Find the eigenmodes for (a) and show that they correspond to in-phase (acoustic mode) and out-of-phase (optical mode) motion of the two atoms within the unit cell.

(c) Repeat parts (a,b) by working with a Hamiltonian and diagonalizing it (i.e., by transforming to its eigenmode basis in terms of which H becomes a sum of Hamiltonians for independent harmonic oscillators for each mode k) and then simply reading off the eigenfrequencies $\omega_o(k)$ and $\omega_a(k)$.

(d) Compute the gap between these optical and acoustic branches.

(e) Show that for $B_0 = B_1$, and $c = a$, (after taking advantage of the periodicity of the k-modes by a shift by a reciprocal lattice vector) your results reduce to that of a single-atom Bravais lattice chain studied in class.

(f) Working with the decoupled Hamiltonian form above treat this elastic chain quantum mechanically. Introducing bosonic (commuting) creation and annihilation operators, $a_k, a_k^\dagger$, (as you would for a single harmonic oscillator through their relation to operators x and p) derive the corresponding phonon spectrum and the total zero point energy.

Hints:

- Approximate the problem with (only) nearest neighbors harmonic springs.
- Use periodic boundary conditions.
- As discussed in class, it is convenient to think of such non-Bravais crystal as a periodic array of identical units, each of which consists of two atoms, with atoms labeled by a basis: x_n^α, where $n \in \{1, \ldots, N/2\}$ (N total number of atoms) labels repeated units and $\alpha \in \{0, 1\}$, labels the two atoms in each unit cell. Whether you work with the Newton's equation or the Hamiltonian, you will end up with a 2×2 matrix (describing coupling between displacements u_0 and u_1 of the two atoms comprising the unit cell) that you will need to diagonalize to answer above questions.

3. Elastic chain in a continuum limit

   (a) Show that for long wavelengths the equation of motion for a one-dimensional chain of identical atoms of mass m, spacing a and elastic constant B reduces to a continuum elastic wave equation

$$\frac{\partial^2 u}{\partial t^2} = v_s^2 \frac{\partial^2 u}{\partial x^2} \tag{1}$$

   (b) What is the sound velocity v_s in terms of B, m, and a?

   (c) Find the eigenfrequencies of vibration of such sound, i.e., find the dispersion $\omega(k)$ and compare it to the full solution $\omega_{\text{full}}(k)$ (no continuum-limit approximation) that we found in class and in (e) above.

   (d) Repeat this exercise of taking a continuum limit at the level of the Hamiltonian and by decoupling it via Fourier modes, show that it reduces to independent harmonic oscillators whose natural frequencies $\omega(k)$ can be simply read off.

4. "Isotropic" crystal

   Consider a higher ($d > 1$) dimensional crystal. Recall from our discussion in class (also see Solyom and any text on elasticity, e.g., Landau and Lifshits or Chaikin and Lubensky) that a generic crystal is characterized by an elastic Hamiltonian (Einstein's summation convention over repeated indices is implied)

$$H = \int d^d x \left[\frac{\boldsymbol{\pi}^2}{2\rho} + \frac{1}{2} C_{ijkl} u_{ij} u_{kl} \right],$$

   where $\boldsymbol{\pi} = \rho \partial_t \mathbf{u}$ is the canonical momentum of the ion displacement (phonons) field $\mathbf{u}(\mathbf{r})$, ρ is the mass density, C_{ijkl} is the matrix of elastic constants that is determined by the symmetry of the crystal, and

$$u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$$

   is the symmetric strain tensor characterizing arbitrary lattice distortion.

   For some crystals, (e.g., a very common 2d hexagonal lattice) to harmonic order $C_{ijkl} = \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda \delta_{ij}\delta_{kl}$, characterized by just two elastic constants, the so-called Lamé coefficients μ,λ, and the elastic Hamiltonian reduces to

$$H = \int d^d x \left[\frac{\boldsymbol{\pi}^2}{2\rho} + \mu u_{ij} u_{ij} + \frac{\lambda}{2} u_{ii} u_{jj} \right].$$

   (a) Treating this Hamiltonian classically, use Fourier representation of the phonon fields $\mathbf{u}(\mathbf{r}) = \int \frac{d^d k}{(2\pi)^d} \mathbf{u}_k e^{i\mathbf{k}\cdot\mathbf{r}}$ to decouple H into a sum of independent Hamiltonians, one for each mode $\mathbf{k}$.

(b) Use canonical statistical mechanics to compute the phonon-phonon correlator $\langle u_i(\mathbf{k}) u_j(\mathbf{k}')\rangle$, that is a crucial quantity characterizing ions' fluctuations, and in turn deviation from perfect crystalline order as measured by x-rays.

Hint:

(a) In classical statistical mechanics the canonical coordinate and momentum are treated independently, so $\langle u^2\rangle = \frac{1}{Z}\int du d\pi e^{-\beta H[u,\pi]}$, where Z is the partition function and $\beta = 1/(k_B T)$.

(b) You should find that the elastic part of the Hamiltonian will take the form $\Gamma_{ij}(\mathbf{k}) u_i(-\mathbf{k}) u_j(\mathbf{k})$, where your job is to find the dynamical matrix $\Gamma_{ij}(\mathbf{k})$, whose inverse is directly related to the phonon correlator that we are after. To this end it is convenient to express Γ_{ij} in terms of longitudinal $P^L_{ij} = k_i k_j/k^2$ and transverse $P^T_{ij} = \delta_{ij} - k_i k_j/k^2$ projection operators with respect to $\mathbf{k}$, as in $\Gamma_{ij} = A P^L_{ij} + B P^T_{ij}$. Once you have this, the inverse of Γ_{ij} is simple (as transverse and longitudinal modes are independent), given by

$$\Gamma^{-1}_{ij} = \frac{1}{A} P^L_{ij} + \frac{1}{B} P^T_{ij}.$$

(c) In class we will discuss how to generalize this result to the full quantum treatment of phonons.