

Condensed Matter Physics (I): Homework 3

Due: November 11, 2019

Exercises in Ashcroft/Mermin

22-1, 22-5, 22-4, 23-3, 25-3(a)

Ex.1 10% Evaluate number of independent elastic constants for orthorhombic and tetragonal lattice systems.

Ex.2 Discrete rotations and isotropy of tensors

A rank- n tensor in 2-dimension, $T^{\alpha_1\alpha_2\cdots\alpha_n}$, $\alpha_i = 1, 2$, is an object which transforms under rotations via the rule

$$(R_\theta T)^{\alpha_1\alpha_2\cdots\alpha_n} = \sum_{\beta_1, \dots, \beta_n} R(\theta)^{\alpha_1\beta_1} \cdots R(\theta)^{\alpha_n\beta_n} T^{\beta_1\cdots\beta_n} \quad (1)$$

where

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \quad (2)$$

is the rotation by angle θ . T is isotropic if

$$T^{\alpha_1\alpha_2\cdots\alpha_n} = \int_0^{2\pi} \frac{d\theta}{2\pi} (R_\theta T)^{\alpha_1\cdots\alpha_n}, \quad (3)$$

while it has discrete p -fold symmetry if

$$T^{\alpha_1\alpha_2\cdots\alpha_n} = \frac{1}{p} \sum_{j=0}^{p-1} \left(R_{\frac{2\pi j}{p}} T \right)^{\alpha_1\cdots\alpha_n}. \quad (4)$$

(a) 10% Show that T is isotropic if and only if $R_\theta T = T$ for any angle θ and it is a p -fold symmetric if and only if $R_{\frac{2\pi j}{p}} T = T$.

(b) 10% Show that if $n < p$, a p -fold symmetric tensor is isotropic. Hint: You may use the identity $\frac{1}{p} \sum_{j=-\infty}^{\infty} \delta(\theta - \frac{2\pi j}{p}) = \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} e^{ikp\theta}$ to show that, for $l + m < p$,

$$\int_0^{2\pi} \cos^l(\theta) \sin^m(\theta) \frac{d\theta}{2\pi} = \frac{1}{p} \sum_{j=0}^{p-1} \cos^l\left(\frac{2\pi j}{p}\right) \sin^m\left(\frac{2\pi j}{p}\right). \quad (5)$$

Ex.3 20% Consider a linear chain of atoms with only nearest neighboring interaction

$$U = \sum_{n=0}^{n=N} \frac{1}{2} m \omega^2 |u_n - u_{n+1}|^2, \quad (6)$$

where m is the mass of the atom, ω is some characteristic frequency, and $u_n = u(na)$ with a being the lattice constant. The linear chain is fixed to a wall at $x = 0$ and $x = (N + 1)a$.

- (a) Find normal modes and determine all possible frequencies ω_k of normal modes.
- (b) Express the Hamiltonian in terms of phonon operators.
- (c) Evaluate $\langle e^{ik u_n} \rangle$ in terms of a summation over number of phonons. Here k is a wavevector.

Ex.4 10% Assuming that the change of the phonon mode of frequency $\omega_{\mathbf{k}}$ due to the change of volume is given by $\delta\omega_{\mathbf{k}}/\omega_{\mathbf{k}} = -\gamma\Delta$ with γ being independent of \mathbf{k} (Grüneisen constant) and Δ being the fractional volume change, find Δ in terms of γ , total thermal energy due to phonons $U(T)$, and the bulk modulus B . Hint: consider the contribution due to the volume change to the free energy up to $O(\Delta^2)$.

Ex.5 10% A simple, monoatomic, two-dimensional square lattice is modelled by balls and springs. The lattice constant is a , the mass of the balls is m , the spring constant of the nearest-neighbor springs is k_1 , and the spring constant between the next nearest neighbors (along the diagonal of the squares) is k_2 . All other interactions can be neglected. Find the frequencies of phonons at $\mathbf{k} = (\pi/a, 0)$. (Hint: you do not need to find the complete solutions to find the answer.)

Ex.6 10% Wick's theorem for classical Gaussian averages

- (a) Show that if Y is a Gaussian variable (i.e., its probability density is given by $P(Y) = \frac{e^{-Y^2/2\sigma_y^2}}{\sqrt{2\pi}\sigma_y}$ for some σ_y) then $\langle e^{tY} \rangle = e^{\frac{1}{2}t^2\langle Y^2 \rangle}$ where t is an arbitrary (possibly complex) constant.
- (b) Show that if Y_1, Y_2, \dots, Y_n are Gaussian (that is, they have a joint probability density $N^{-1} \exp(-\frac{1}{2} \sum_{i,j=1}^n a_{ij} Y_i Y_j)$, where N is the normalization constant and a_{ij} is a symmetric positive definite matrix), then $Y = t_1 Y_1 + \dots + t_n Y_n$ is also Gaussian. Find $\langle Y_i Y_j \rangle$.
- (c) Using part (a), expanding both sides as a Taylor series in the t 's, derive the Wick's theorem:

$$\langle Y_1 Y_2 Y_3 \cdots Y_n \rangle = \sum_{\text{all possible pairing}} \langle Y_{i_1} Y_{j_1} \rangle \langle Y_{i_2} Y_{j_2} \rangle \cdots \langle Y_{i_p} Y_{j_p} \rangle \quad (7)$$