Theorie der Kondensierten Materie I WS 2012/2013

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1. Elasticity of harmonic square lattice (15 + 10 + 10 + 15 + 10 = 60 Punkte)

Consider a square lattice of mass points m. The unit vectors read $\boldsymbol{a}_1 = a(1,0)$, $\boldsymbol{a}_2 = a(0,1)$.

(a) Assume that only nearest neighbors are connected by central force harmonic springs with spring constant k. Calculate the harmonic elasticity matrix

$$\Phi^{k,k'}_{n-n';\alpha,\beta} = \frac{\partial^2 V_{ii}}{\partial u^k_{n,\alpha} \partial u^{k'}_{n',\beta}} ,$$

where k, k' labels the basis sites of the lattice, n, n' refer to the Bravais lattice vectors $\boldsymbol{R}^{(0)}_n$ (and $\boldsymbol{R}^{(0)}_{n'}$) and $\alpha, \beta = x, y$.

(b) Calculate the tensor of elasticiy $K_{\alpha\beta\gamma\delta}$ with $\alpha, \beta, \gamma, \delta = x, y$ for the setup of part (a). It is defined as

$$K_{\alpha\beta\gamma\delta} = -\frac{1}{8v} \sum_n \Big\{ \boldsymbol{R}^{(0)}_{n,\beta} \boldsymbol{R}^{(0)}_{n,\delta} \Phi_{n;\alpha\gamma} + \boldsymbol{R}^{(0)}_{n,\alpha} \boldsymbol{R}^{(0)}_{n,\delta} \Phi_{n;\beta\gamma} + \boldsymbol{R}^{(0)}_{n,\beta} \boldsymbol{R}^{(0)}_{n,\gamma} \Phi_{n;\alpha\delta} + \boldsymbol{R}^{(0)}_{n,\alpha} \boldsymbol{R}^{(0)}_{n,\gamma} \Phi_{n;j\gamma} \Big\} ,$$

where v denotes the volume of the unit cell and $\boldsymbol{R}^{(0)}_{n,\alpha}$ refers to spatial component α of the Bravais lattice vector $\boldsymbol{R}^{(0)}_n$.

(c) What is the response of this model to a shear stress ?

(d) Now add central force springs connecting next nearest neighbors on the lattice with spring constant k'. Again calculate $\Phi^{k,k'}_{n-n';\alpha,\beta}$ and $K_{\alpha\beta\gamma\delta}$.

(e) Is the response to a shear stress different from part (a), and why ?

2. Thermal expansion. (5 + 25 + 10 = 40 Punkte)

Thermal expansion of crystals can be studied using the model of a diatomic molecule. It deals with two atoms interacting via a 1D anharmonic potential, $U(x) = \beta x^2 + \delta x^3 + \gamma x^4$, where x is the relative shift of the atoms from the equilibrium at T=0. The cubic term is responsible for the thermal expansion, while the quartic term prevents the molecule from flying apart and smoothens the oscillations at large amplitudes.

(a) Assuming that the interactions come from the electrons in the atoms, make order-of-magnitude estimates of constants δ and γ, i.e. express them in terms of the fundamental constants.

(b) Evaluate the coefficient of linear thermal expansion $\alpha = l^{-1}(dl/dT)$ in the temperature interval $(\beta/m)^{1/2} \ll T \ll \beta a^2$, where m and a are respectively the mass of one atom and the equilibrium distance between the atoms.

(c) Find $\langle x \rangle$ by averaging the classical equations of motion of the atoms and using the equipartition theorem.