KARLSRUHER INSTITUT FÜR TECHNOLOGIE

INSTITUT FÜR THEORIE
DER KONDENSIERTEN MATERIE

Theorie der Kondensierten Materie I WS 2018/2019

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1. Phonons in Graphene: (40 Punkte)

Consider the honeywell lattice in graphene. Find the phonon specrum of graphene assuming that the carbon atoms move only within the two-dimensional plane.

Hint Consider only nearest-neighbor couplings within harmonic approximation.

2. Debye-Waller factor: (60 Punkte)

In the lecture the following expression for the structure factor of phonons for a mono-atomic crystal was derived

$$S(\boldsymbol{q},\omega) = e^{-2W}\int \frac{dt}{2\pi} e^{i\omega t}\sum_{\boldsymbol{R}} e^{-i\boldsymbol{q}\boldsymbol{R}} \exp\langle[\boldsymbol{q}\boldsymbol{u}(0)][\boldsymbol{q}\boldsymbol{u}(\boldsymbol{R},t)]\rangle,$$

where $\boldsymbol{u}(\boldsymbol{R},t)$ is the atomic displacement, $\boldsymbol{R}$ denotes the vectors of the Bravais lattice, and W is the Debye-Waller factor, given by the expression

$$W = \frac{1}{2}\langle[\boldsymbol{q}\boldsymbol{u}(0)]^2\rangle.$$

(a) Show, that the Debye-Waller factor can be written as

$$W = \frac{V}{2}\int \frac{d^dk}{(2\pi)^d}\sum_s \frac{[\boldsymbol{q}\boldsymbol{\epsilon}_s(\boldsymbol{k})]^2}{2M\omega_s(\boldsymbol{k})}\coth\frac{\omega_s(\boldsymbol{k})}{2T}.$$

Here V is the appropriate cell volume ans s denotes the phonon branch.

(b) Show that $e^{-2W} = 0$ in one and two dimensions. What are the implications of this result for the possible existence of one- and two-dimensional crystalline ordering?

Hint Consider the behavior of the integrand for small k.

(c) Estimate the size of the Debye-Waller factor for a monoatomic three-dimensional crystal. Analyze your result for the limiting cases of temperatures low and high as compared to the Debye temperature.

(d) Evaluate the one-phonon contribution to the structure factor. Interpret the result in terms of absorbtion and emission of phonons.

Hint The one-phonon contribution corresponds to the linear term in the expansion of the last exponential in the above expression for the structure factor.