LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Fakultät für Physik im WiSe 2023/24
TA1: Condensed matter physics
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https://www2.physik.uni-muenchen.de/lehre/vorlesungen/wise_24_25/TA1_theoretical_condensed_matter/index.html

Problem set 4

Problem 1 The Born-Oppenheimer approximation: Ménage à trois

In the lecture we introduced the adiabatic approximation (also known as Born-Oppenheimer approximation) to decouple the electronic degrees of freedom from the nuclei, such that they only act as an effective potential between the nuclei. In this exercise, we want to illustrate this mechanism at the example of a one-dimensional toy model for a molecule composed of a single electron with mass m and two nuclei with masses M_1, M_2, imposing $m \ll M_1, M_2$. We assume that a good approximation for the potential of this 3-body problem is given by

$$V(X_1, X_2, x) = -\frac{K_1}{2}(X_1 - X_2)^2 + \frac{K_2}{2}\left[(x - X_1)^2 + (x - X_2)^2\right], \tag{1}$$

where X_1, X_2 denote the coordinates of the nuclei and x the coordinate of the electron. Note that the first summand describes a repulsion between the nuclei while the second describes an attraction between the electron and the nuclei (why?).

(1.a) Use the adiabatic approximation to derive the effectve potential $U(X_1, X_2)$ between the nuclei and find the stability condition on the effective coupling constants K_1, K_2 such that the molecule is stable.

(1.b) Assuming that the stability condition holds true, derive the classical oscillation frequency of the coupled nuclei.

(1.c) This three-body Hamiltonian can actually be solved exactly because it is nothing else but coupled harmonic oscillators. Find the corresponding frequency in the exact solution, and show that it is identical to what you found in (ii), for the special case of $M_1 = M_2$. For $M_1 \neq M_2$, show that the exact frequency approaches the result in (ii) in the limit $m \ll M_1, M_2$. Give a physical explanation why the adiabatic approximation is exact (in this toy model) when $M_1 = M_2$.

Problem 2 Phonons in a diatomic chain

We consider a one-dimensional chain with a two-site basis of harmonically coupled nuclei with mass M and alternating spring constants K_1, K_2. We denote the lattice constant spanning the unit cell by a.

(2.a) Solve the classical equations of motions using the plane-wave ansatz discussed in the lecture and determine the dispersion relation $\omega(q)$.

(2.b) Consider the limit $q \ll \pi/a$ and expand the dispersion relation to the first non-trivial order. Show that you obtain an acoustic and a gapped optical branch.

(2.c) Now assume that $K_2 \gg K_1$. Expand the dispersion relation to the first non-trivial order in K_1/K_2 and show that you obtain an acoustic branch corresponding to a chain of diatomic molecules with mass $2M$ and spring constant K_1.

Problem 3 The Debye-Waller factor of an acoustic phonon and what we can learn from it

In this problem we want to compute the Debye-Waller factor $\mathrm{e}^{-2\Gamma_{\vec{k}}}$ introduced in the lecture explicitly for a d-dimensional system with a single acoustic phonon mode with dispersion relation $\hbar\omega(\vec{k}) = \hbar v_s|\vec{k}|$.

(3.a) We begin by computing

$$\Gamma_{\vec{k}} = \frac{1}{2}\langle\!\langle (\vec{k}\cdot\hat{\vec{X}}_j)^2 \rangle\!\rangle \,, \tag{2}$$

where $\hat{\vec{X}}_j$ denotes the displacement operator of the jth atom at $\vec{R}_j$ and is given in terms of the ladder operators $\hat{a}^{(\dagger)}_{\vec{k}}$ of the harmonic oscillator by

$$\hat{\vec{X}}_j = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \vec{\epsilon} \sqrt{\frac{\hbar}{2m\omega(\vec{k})}} \left(\hat{a}_{\vec{k}} + \hat{a}^\dagger_{-\vec{k}}\right) \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{R}_j} \,. \tag{3}$$

Show that

$$\Gamma_{\vec{k}} = (\vec{\epsilon}\cdot\vec{k})^2 \frac{\hbar}{4m} \int_{(1.BZ)} \frac{\mathrm{d}^d\vec{k}}{(2\pi)^d} \frac{\coth(\beta\hbar\omega(\vec{k})/2)}{\omega(\vec{k})} \,. \tag{4}$$

(3.b) Determine the Debye-Waller factor for the case $d = 3$. For that purpose, replace the integration domain (first Brillouin zone) by a sphere with radius k_d. Expand your result for the case of high temperatures $\beta\hbar v_s k_d \ll 1$ and low temperatures $\beta\hbar v_s k_d \gg 1$ to the first non-trivial order.

(3.c) Show that the Debye-Waller factor diverges in $d = 2$ dimensions. Explain how and why this is consistent with the Hohenberg-Mermin theorem stating that in a system with short-ranged interactions, continuous symmetries can not be broken spontaneously at any finite temperature if $d \leq 2$.