
Exercise 8 for Theoretical Solid State Physics in Summer 2023

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1. Born-Oppenheimer approximation (8 points)

A heavy particle M and a light particle $m \ll M$ move inside an infinitely high potential well of width L . The particles experience an attractive potential interaction described by the potential $W(r - R) = -\lambda\delta(r - R)$, where $\lambda > 0$ and R and r are the positions of the heavy and light particle, respectively.

Calculate the spectrum of the corresponding Hamiltonian

$$H = -\frac{\hbar^2}{2m}\partial_r^2 - \frac{\hbar^2}{2M}\partial_R^2 - \lambda\delta(r - R)$$

in Born-Oppenheimer-approximation.

- (a) In step one transform the Hamiltonian into a dimensionless form and neglect the kinetic energy of the heavy particle. Determine the unnormalized eigenfunctions and an equation for the eigenvalues $\epsilon_n(R)$ of the light particle. Consider only the case $\epsilon > 0$.
- (b) What is the meaning of $\epsilon_n(R)$ and how should we include qualitatively the heavy particle into our picture?

2. Density of states (8 points)

Calculate and plot (for $d = 1, 2, 3$ in part (c)) the density of states $D(\omega)$ in the following cases:

- (a) the monoatomic harmonic chain (lattice constant a , mass m , spring constant k) with dispersion relation

$$\omega^2(q) = \frac{4k}{m} \sin^2 \frac{qa}{2}, \quad -\frac{\pi}{a} \leq q < \frac{\pi}{a},$$

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- (b) the diatomic harmonic chain (lattice constant a , masses m and M , spring constant k) with dispersion relation

$$\omega^2(q) = \frac{k}{m} + \frac{k}{M} \pm k \sqrt{\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4}{mM} \sin^2(qa)}, \quad -\frac{\pi}{a} \leq q < \frac{\pi}{a},$$

- (c) the acoustic branch in d dimensions in the Debye model, i. e. $\omega(\vec{q}) = e|\vec{q}|$.