HW4

MTLE-6120: Spring 2019

Due: Feb 18, 2019

1. **Phonons in 1D**

   Consider an infinite chain of identical atoms of mass M each, with each pair of nearest neighbours separated by distance a, and connected by springs of spring constant K. This is the simplest model of describing the vibrations of atoms in a solid. Quantum mechanically, each vibration mode (a wave) corresponds to a particle called the phonon which is a boson, exactly analogous to how EM waves correspond to photons.

   (a) Find and plot the phonon frequency ω as a function of the wave-vector $k \in [-\pi/a, +\pi/a]$ of atom displacements. Hint: no complicated math required! We have already solved a more general case in class; this time we only have coupling springs. Also remember that $\omega \geq 0$ by definition.

   (b) What is the minimum oscillation frequency? What is the pattern of atom displacements of this mode?

   (c) What is the maximum oscillation frequency? What is the pattern of atom displacements of this mode?

   (d) What is the group velocity of waves with low wave-vectors $k \to 0$? Note that this wave of lattice vibrations is sound, this group velocity is therefore the sound velocity, and this type of $\omega \to 0$ phonons are therefore called acoustic phonons.

2. **Kasap 4.2**

3. **The δ-molecule**

   Consider two δ atoms separated by distance a, located symmetrically about the origin at $x = \pm a/2$, so that the net potential for the electrons is

   $$V(x) = -V_0 \delta(x + a/2) - V_0 \delta(x - a/2).$$

   As before, use $q = 2mV_0/\hbar^2$ for convenience.

   (a) Find the wavefunctions $\psi(x)$ with energies $E < 0 = -\hbar^2\kappa^2/(2m)$ for the bound states of the electrons in this potential.

   Hint: there are exactly two such states, one symmetric and the other antisymmetric about $x = 0$. You will end up with a transcendental equation for κ, which you will not be able to solve exactly, but you can still find a neat form for the wavefunctions. Also, there is no need to normalize the wavefunctions.

   (b) The conditions on κ for both the symmetric and antisymmetric cases are not analytically solvable for κ, but they do directly give q in terms of κ. Rewrite the conditions in terms of dimensionless variables $K = \kappa a$ and $Q = qa$.

   Using this form, plot Q on the x-axis versus the dimensionless energy given by

   $$\frac{E}{|E_0|} = \frac{-\hbar^2\kappa^2/(2m)}{\hbar^2 q^2/(8m)} = \frac{-4K^2}{Q^2}$$

   on the y-axis, for both the symmetric and antisymmetric wavefunctions. (Above, E_0 is the energy of the isolated δ-atom.)

Which wavefunction has a lower energy? How does the energy difference between the two wavefunctions depend on the strength of the potential q and the spacing between atoms a?

Calculate and explain the $a \to 0$ and $a \to \infty$ limits of the lower (ground state) energy.

(c) Now consider the weakly-interacting limit $qa \gg 1$. Sketch / plot the two bound state wavefunctions in this limit, and find an approximate expression for their energies. Explain the analogy with the two spring system considered in class (i.e. identify the isolated energies and the coupling strength).