HW3 solution

MTLE-6120: Spring 2017

Due: Feb 23, 2017

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.

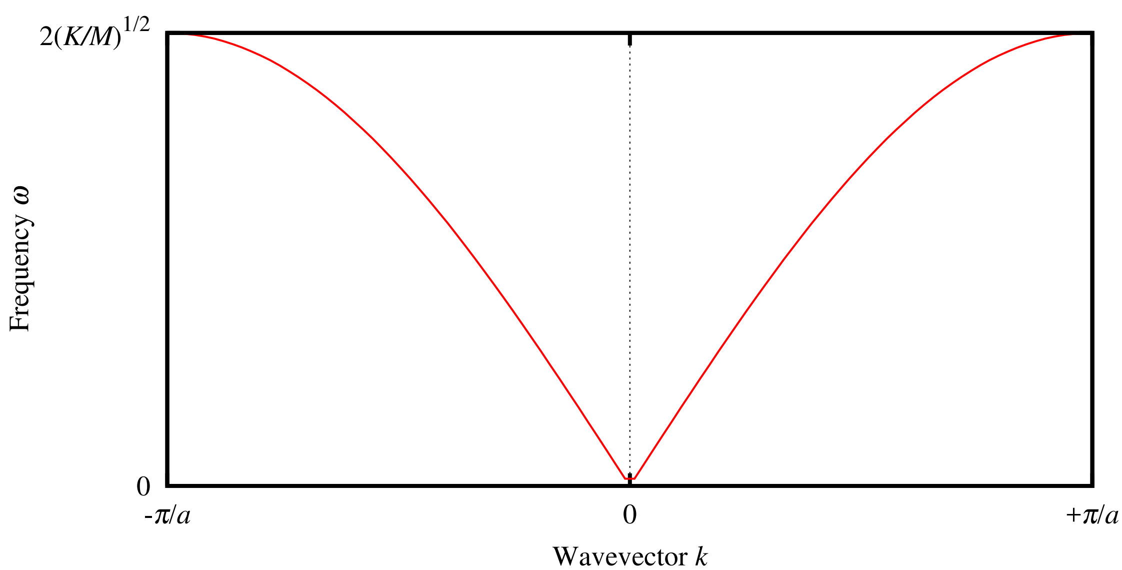
   In class, we had two types of springs; those with constant k that connected the masses to a fixed point in space, and coupling springs K that coupled the masses to each other. There, we found

$$M\omega^2 = k + 2K - 2K\cos ka$$

   Now, we only have the coupling springs K, and so we get instead

$$\begin{aligned} M\omega^2 &= 2K - 2K\cos ka \\ &= 2K(1-\cos ka) \\ &= 4K\sin^2\frac{ka}{2} \\ \Rightarrow \qquad \omega &= 2\sqrt{K/M}\left|\sin\frac{ka}{2}\right| \end{aligned}$$

   Note $\omega > 0$, so we only take the positive solution above.



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

The lowest frequency mode is $\omega = 0$ corresponding to $k = 0$. Since $k = 0$, all atoms move together. This pattern involves no extension of the springs, hence there is no restoring force and this has zero oscillation frequency.

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

The highest frequency mode is $\omega = 2\sqrt{K/M}$ corresponding to $k = \pm\pi/a$ Since $k = \pi/a$, adjacent atoms move opposite to each other. This causes maximum compression / extension of the springs: equal in magniude to twice that of the atom displacements, and there are two such springs acting on each atom. Therefore the net restoring force is four times that of the isolated oscillator with spring K, and correspondingly the resonant frequency is twice that of the isolated oscillator ($\sqrt{K/M}$).

(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.

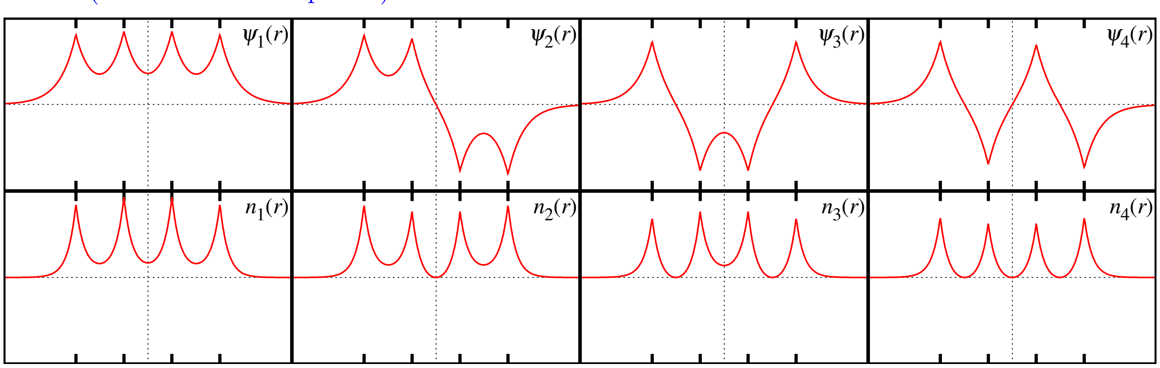
The sound velocity is

$$\begin{aligned} v_g &= \lim_{k\to 0} \frac{\partial \omega}{\partial k} \\ &= \lim_{k\to 0} \frac{\partial}{\partial k} 2\sqrt{K/M} \left| \sin \frac{ka}{2} \right| \\ &= \lim_{k\to 0} 2\sqrt{K/M} \frac{a}{2} \cos \frac{ka}{2} \\ &= a\sqrt{\frac{K}{M}} \\ &= \sqrt{\frac{Ka}{M/a}} \end{aligned}$$

The last form is written suggestively as the ratio of the elastic modulus Ka and mass density M/a, which is the 1D analog of the relation $v_g = \sqrt{B/\rho}$, where B is the bulk modulus and ρ is the mass density, for longitudinal sound waves in 3D.

2. **Kasap 4.2**

Each orbital is proportional to $e^{-r/a}$, which looks like $e^{-|x|/a}$ on the x-axis. (Same as the δ-atom!) Overall the wavefunctions must be symmetric or antisymmetric about the center. For each, there are two possibilities in the relative phase between adjacent atoms, resulting in the following possibilities overall (densities in lower panels):



The wavefunctions have already been sorted in ascending order of number of nodes going from left to right, so they would have increasing order of energies.

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.

The space in now divided in three segments, $x < -a/2$, $-a/2 < x < a/2$ and $x > a/2$. In each segment, the wavefunction must be of the form $e^{\pm\kappa x}$ for the bound states. On the left end, only $e^{+\kappa x}$ is allowed so that $\psi(x) \to 0$ as $x \to -\infty$, and similarly on the right end, only $e^{-\kappa x}$ is allowed so that $\psi(x) \to 0$ as $x \to +\infty$. Therefore:

$$\psi(x) = \begin{cases} Ae^{\kappa x}, & x < -a/2 \\ Be^{\kappa x} + Ce^{-\kappa x}, & |x| < a/2 \\ De^{-\kappa x} & x > a/2 \end{cases}$$

As usual, we next impose the matching conditions (continuity and derivative discontinuity) at $x = \pm a/2$:

$$\begin{aligned} Ae^{-\kappa a/2} &= Be^{-\kappa a/2} + Ce^{\kappa a/2} && \left(x = -\frac{a}{2} \text{ continuity}\right) \\ De^{-\kappa a/2} &= Be^{\kappa a/2} + Ce^{-\kappa a/2} && \left(x = +\frac{a}{2} \text{ continuity}\right) \\ -q\left[Ae^{-\kappa a/2}\right] &= \left[\kappa Be^{-\kappa a/2} - \kappa Ce^{\kappa a/2}\right] - \left[\kappa Ae^{-\kappa a/2}\right] && \left(x = -\frac{a}{2} \text{ derivative}\right) \\ -q\left[De^{-\kappa a/2}\right] &= \left[-\kappa De^{-\kappa a/2}\right] - \left[\kappa Be^{\kappa a/2} - \kappa Ce^{-\kappa a/2}\right] && \left(x = +\frac{a}{2} \text{ derivative}\right) \end{aligned}$$

We can simplify the last two equations to

$$\begin{aligned} \left(1 - \frac{q}{\kappa}\right) Ae^{-\kappa a/2} &= Be^{-\kappa a/2} - Ce^{\kappa a/2} \\ \left(1 - \frac{q}{\kappa}\right) De^{-\kappa a/2} &= -Be^{\kappa a/2} + Ce^{-\kappa a/2} \end{aligned}$$

We can now add and subtract the first and second equations from the two sets above to write B and C in terms of A as well as D

$$\begin{aligned} B &= \left(1 - \frac{q}{2\kappa}\right) A \\ C &= \frac{q}{2\kappa} Ae^{-\kappa a} \\ C &= \left(1 - \frac{q}{2\kappa}\right) D \\ B &= \frac{q}{2\kappa} De^{-\kappa a} \end{aligned}$$

We can equate B/C obtained from the first two and last two equations to get:

$$\frac{\left(1 - \frac{q}{2\kappa}\right) A}{\frac{q}{2\kappa} Ae^{-\kappa a}} = \frac{\frac{q}{2\kappa} De^{-\kappa a}}{\left(1 - \frac{q}{2\kappa}\right) D}$$

$$\Rightarrow \qquad \left(1 - \frac{q}{2\kappa}\right)^2 = \left(\frac{q}{2\kappa}\right)^2 e^{-2\kappa a}$$
$$\Rightarrow \qquad \frac{2\kappa}{q} - 1 = \pm e^{-\kappa a}$$
$$\Rightarrow \qquad \kappa = \frac{q}{2}\left(1 \pm e^{-\kappa a}\right)$$
$$\Rightarrow \qquad \frac{q}{2\kappa} = \frac{1}{1 \pm e^{-\kappa a}}$$

This is a transcendental equation in κ that we cannot solve explicitly. But we can substitute this form back into the wavefunction coefficients:

$$B = \left(1 - \frac{q}{2\kappa}\right) A = \frac{\pm 1}{e^{\kappa a} \pm 1} A$$
$$C = \frac{q}{2\kappa} A e^{-\kappa a} = \frac{1}{e^{\kappa a} \pm 1} A$$
$$D = \frac{C}{1 - \frac{q}{2\kappa}} = \pm A$$

Thus the wavefunctions are:

$$\psi_\pm(x) = A \begin{cases} e^{\kappa x}, & x < -a/2 \\ \frac{1}{e^{\kappa a} \pm 1}\left(\pm e^{\kappa x} + e^{-\kappa x}\right), & |x| < a/2 \\ \pm e^{-\kappa x} & x > a/2 \end{cases}$$

Writing the two cases separately, we have

$$\psi_+(x) = A \begin{cases} e^{\kappa x}, & x < -a/2 \\ \frac{1}{e^{\kappa a} + 1}\left(e^{\kappa x} + e^{-\kappa x}\right), & |x| < a/2 \\ e^{-\kappa x} & x > a/2 \end{cases} = A \begin{cases} e^{-\kappa |x|}, & |x| > a/2 \\ \frac{2\cosh \kappa x}{e^{\kappa a} + 1}, & |x| < a/2 \end{cases}$$

and

$$\psi_-(x) = A \begin{cases} e^{\kappa x}, & x < -a/2 \\ \frac{1}{e^{\kappa a} - 1}\left(-e^{\kappa x} + e^{-\kappa x}\right), & |x| < a/2 \\ -e^{-\kappa x} & x > a/2 \end{cases} = -A \begin{cases} \text{sign}(x) e^{-\kappa |x|}, & |x| > a/2 \\ \frac{2\sinh \kappa x}{e^{\kappa a} - 1}, & |x| < a/2, \end{cases}$$

which are odd and even functions of x respectively.

(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.

The conditions on κ are

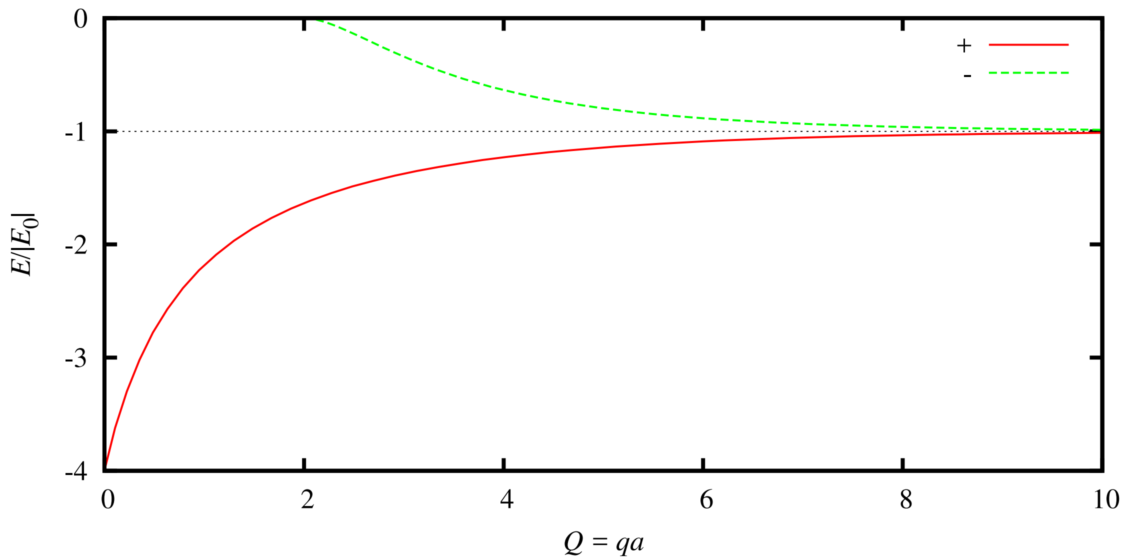
$$\frac{q}{2\kappa} = \frac{1}{1 \pm e^{-\kappa a}}$$

$$\Rightarrow \qquad \frac{qa}{2\kappa a} = \frac{1}{1 \pm e^{-\kappa a}}$$

$$\Rightarrow \qquad Q = \frac{2K}{1 \pm e^{-K}}$$

$$\frac{E}{|E_0|} = \frac{-4K^2}{Q^2}$$

Now we have both Q and $E/|E_0|$ as a function of K, and we can plot them (parametrically):



The symmetric-wavefunction (or even) + case has a lower energy compared to the antisymmetric-wavefunction (or odd) − case. The energy difference increases when Q decreases, i.e. when either the potential q gets weaker or when the atoms get closer (a reduces).

When $a \to \infty$ i.e. $Q \to \infty$, $E/|E_0| \to -1$ i.e. $E \to E_0$, the energy of the isolated δ-atom, which makes sense because the two atoms no longer interact,

When $a \to 0$ i.e. $Q \to 0$, $E/|E_0| \to -4$ i.e. $E \to 4E_0$, because this is effectively now two coincident δ-atoms, which is exactly the same as a single δ-atom with potential of strength $2q$. The energy $\propto q^2$, and hence $E \to 4E_0$. Note that this is only the electronic energy. If these were real atoms, the nuclear-nuclear repulsion would grow as the atoms get closer, which is not a piece captured here.

(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).

The matching conditions in general yield

$$\kappa = \frac{q}{2}\left(1 \pm e^{-\kappa a}\right)$$

In the limit $qa \to \infty$ of isolated δ-atoms, $\kappa \to q/2$. Substituting that in the RHS, we get an approximate expression for large qa,

$$\kappa \approx \frac{q}{2}\left(1 \pm e^{-qa/2}\right)$$

and hence for the energies

$$E = \frac{-\hbar^2\kappa^2}{2m} \approx \frac{-\hbar^2 q^2}{8m}\left(1 \pm e^{-qa/2}\right)^2 \approx E_0 \mp 2|E_0|e^{-qa/2}$$

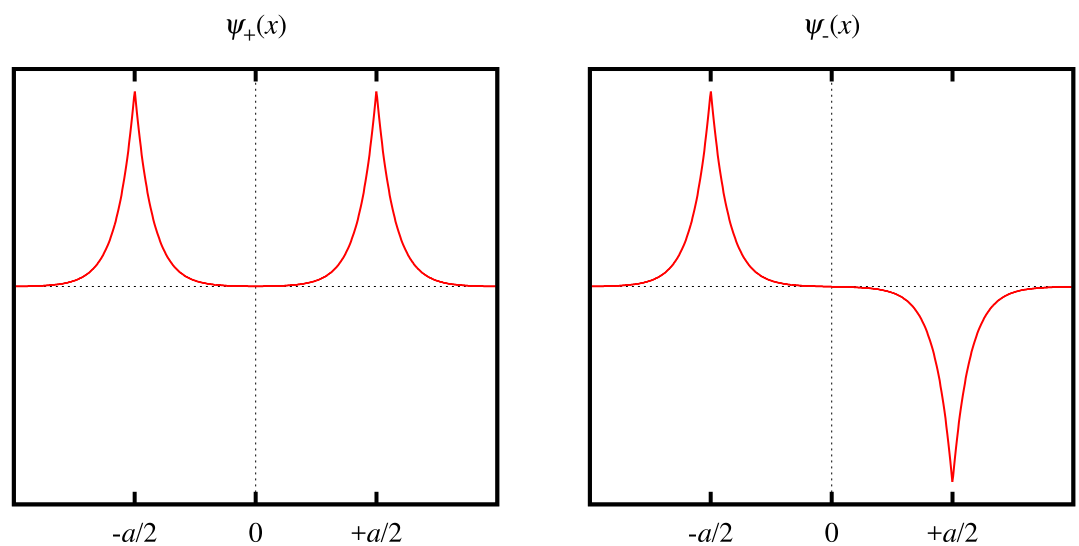
where $E_0 - \hbar^2 q^2/(8m)$ is the energy of the isolated δ-atom.
As for the wavefunctions $\kappa a \approx qa/2 \gg 1$, which means that $e^{\kappa a} \gg 1$. Therefore the wavefunctions simplify to:

$$\begin{aligned}
\psi_+(x) &= A \begin{cases} e^{-\kappa|x|}, & |x| > a/2 \\ 2\cosh \kappa x e^{-\kappa a}, & |x| < a/2 \end{cases} \\
&\approx A e^{-\kappa a/2} \begin{cases} e^{-\kappa(|x|-a/2)}, & |x| > a/2 \\ e^{\kappa(x-a/2)} + e^{\kappa(-x-a/2)}, & |x| < a/2 \end{cases} \\
&\propto e^{-\kappa(|x+a/2|} + e^{-\kappa(|x-a/2|}
\end{aligned}$$

and

$$\begin{aligned}
\psi_-(x) &= -A \begin{cases} \text{sign}(x) e^{-\kappa|x|}, & |x| > a/2 \\ 2\sinh \kappa x e^{-\kappa a}, & |x| < a/2, \end{cases} \\
&\approx -A e^{-\kappa a/2} \begin{cases} \text{sign}(x) e^{-\kappa(|x|-a/2)}, & |x| > a/2 \\ e^{\kappa(x-a/2)} - e^{\kappa(-x-a/2)}, & |x| < a/2, \end{cases} \\
&\propto e^{-\kappa(|x+a/2|} - e^{-\kappa(|x-a/2|}
\end{aligned}$$

by examining the exponentials in each segment. Essentially these correspond to isolated δ-atom wavefunctions added and subtracted from each other, as sketched below.



In analogy with the two-spring system, the two eigen-states / normal modes correspond to the wavefunctions on the two atoms are exactly in phase or out of phase with each other. The in-phase case, corresponding to the springs moving together, has the lower energy, while the out-of-phase case has the higher energy. The split between the energies is proportional to the coupling strength, which is proportional to $e^{-\kappa a} \sim e^{-qa/2}$, which for the molecule is related to the wavefunction overlap between the two atoms.