PHYSICS 141A – Problem Set 4

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Exercise 1 - Simon 9.4

We have defined our vibrational nodes as

$$\delta x_n = A e^{i\omega t} e^{-ikna} \tag{1}$$

while we have the dispersion relation

$$\omega(k) = \sqrt{\frac{\kappa}{m}} \left| \sin\left(\frac{ka}{2}\right) \right| = \omega_{max} \left| \sin\left(\frac{ka}{2}\right) \right|$$

We observe that if we set ω larger than ω_{max}, we will obtain a complex k, as sin doesn't output values larger than 1 for real arguments. Let us set $\omega = \sigma\omega_{max}$, $\sigma > 1$, such that

$$\sigma = \frac{\omega}{\omega_{max}} = \left| \sin\left(\frac{ka}{2}\right) \right| \tag{2}$$

Now, considering a complex $k = k_r + ik_c$, we can write equation 1 as

$$\delta x_n = A e^{i\omega t} e^{-ik_r na} e^{k_c na}$$

The last term, containing k_c, will either blow up as for large n, if $k_c > 0$, or disappear for large n, if $k_c < 0$.

We can write this as a decay-relation

$$\delta x_n = C(t,k) e^{-qa}, \quad q = -k_c a$$

where $C(t,k)$ is some harmonic planewave solution.

Writing out 2 using the $\sin(x) = \frac{i}{2}\left(e^{-ix} - e^{ix}\right)$, we get

$$\sigma = \sin\left(\frac{ka}{2}\right) = \frac{i}{2}\left(e^{-ika/2} - e^{ika/2}\right)$$

Multiplying each side by $2ie^{ika/2}$, we get

$$2i\sigma e^{ika/2} = e^{ika} - 1$$

which can be written as

$$x^2 - 2i\sigma x - 1 = 0, \qquad x = e^{ika/2}$$

which is a 2nd degree polynomial eqn with solutions

$$e^{ika/2} = x = \sigma i \pm \sqrt{1-\sigma^2}$$

Now, we have defined that $\sigma > 1$, such that $\sigma^2 > 1$, and we can define $\sqrt{1-\sigma^2} = \gamma i$, where γ must be real. This gives

$$\begin{aligned} e^{ika/2} &= \sigma i \pm \gamma i \\ \frac{ika}{2} &= \ln(\sigma i \pm \gamma i) = \ln(i) + \ln(\sigma \pm \gamma) = \frac{\pi}{2} i + \ln(\sigma \pm \gamma) \\ k &= \frac{\pi}{a} + \frac{2}{a} i \ln(\sigma \pm \gamma) = k_r + ik_c \end{aligned}$$

where we have that $k_c = \ln(\sigma \pm \gamma)$, as we know both σ and γ must be real. Inserting gives

$$k_c = \ln\left(\sigma \pm \frac{\sqrt{1-\sigma^2}}{i}\right)$$

which is real. Remember that $\sigma = \omega/\omega_{max}$.

Exercise 2 - Simon 9.6

Given the mode

$$\delta x_n = Ae^{i\omega t}e^{q|n|a} \tag{3}$$

We have the double time derivative:

$$\delta\ddot{x}_n = A\omega^2 e^{i\omega t}e^{q|n|a}$$

From Simon eqn (9.1), we have Newtons equation of motion written out for neighboring nodes:

$$m\delta\ddot{x}_n = \kappa(\delta x_{n+1} + \delta x_{n-1} - \ 2\delta x_n)$$

Inserting for equation 3 on the left hand side, and the derivative on the right, we get

$$\begin{aligned} Am\omega^2 e^{i\omega t}e^{q|n|a} &= \kappa Ae^{i\omega t}\Big[e^{q|n+1|a} + e^{iq|n-1|a} - 2e^{q|n|a}\Big] \\ \omega^2 m &= \kappa\Big[e^{qa(|n+1|-|n|)} + e^{qa(|n-1|-|n|)} - 2e^{qa(|n|-|n|)}\Big] \end{aligned}$$

Now, for $n \geq 1$, we have $|n| = n$, $|n-1| = n-1$ and $|n+1| = n+1$, giving

$$\omega^2 m = \kappa\big[e^{qa} + e^{-qa} - 2\big], \qquad n \geq 1$$

For $n \leq -1$, we have $|n| = -n$, $|n-1| = -n+1$, and $|n+1| = -n-1$, giving

$$\omega^2 m = \kappa\big[e^{-qa} + e^{qa} - 2\big], \qquad n \leq -1$$

which turns out to be the same thing.

At $n = 0$, we end up getting the same story. This could also have been seen due to symetry, as swithcing n-direction only switches $|n-1|$ and $|n+1|$, leaving the same expression.

We regocnize this as

$$m\omega^2 = 2\kappa[1 - \cosh(qa)]$$

where we can rewrite $2[\cosh(qa) - 1] = 4\sinh^2(qa/2)$, giving

$$\omega = 2\sqrt{\frac{k}{m}}\sinh\left(\frac{qa}{2}\right)$$

In constrast to exercise 9.4, where having $\omega > \omega_{max}$ would require a complex k, which in turn would lead to a decaying wave, $\sinh(qa/2)$ offers values larger than 1 without requiring q to be complex, which in turn doesn't it require to decay.

Exercise 3

From Simon eq. (10.3) and (10.4) have the planewave solutions to both atoms as

$$\begin{aligned} \delta x_n &= A_x e^{i\omega t - ikna} \\ \delta y_n &= A_y e^{i\omega t - ikna} \end{aligned}$$

which we plug into the equations of motion, described in Simon eq (10.1) and (10.2) as (with consideration of the differing masses):

$$\begin{aligned} m_x\delta\ddot{x}_n &= \kappa(\delta y_n - \delta x_n) + \kappa(\delta y_{n-1} - \delta x_n) \\ m_y\delta\ddot{y}_n &= \kappa(\delta x_{n+1} - \delta y_n) + \kappa(\delta x_n - \delta y_n) \end{aligned}$$

giving

$$
\begin{aligned}
-\omega^2 m_x A_x e^{i\omega t - ikna} &= \kappa(\delta y_n - \delta x_n) + \kappa(\delta y_{n-1} - \delta x_n) \\
-\omega^2 m_y A_y e^{i\omega t - ikna} &= \kappa(\delta x_{n+1} - \delta y_n) + \kappa(\delta x_n - \delta y_n)
\end{aligned}
$$

Inserting for δx_n and δy_n, as done is Simon, results in

$$
\begin{aligned}
-\omega^2 m_x A_x &= \kappa A_y + \kappa A_y e^{ika} - 2\kappa A_x \\
-\omega^2 m_y A_y &= \kappa A_x e^{-ika} + \kappa A_x - 2\kappa A_y
\end{aligned}
$$

which can be written as the eigenvalue equation

$$
\omega^2 \begin{pmatrix} A_x \\ A_y \end{pmatrix} = \begin{pmatrix} 2\kappa/m_x & (-\kappa - \kappa e^{ika})/m_x \\ (-\kappa - \kappa e^{-ika})/m_y & 2\kappa/m_y \end{pmatrix} \begin{pmatrix} A_x \\ A_y \end{pmatrix}
$$

$$
0 = \begin{vmatrix} 2\kappa/m_x - \omega^2 & (-\kappa - \kappa e^{ika})/m_x \\ (-\kappa - \kappa e^{-ika})/m_y & 2\kappa/m_y - \omega^2 \end{vmatrix}
$$

which becomes

$$
\begin{aligned}
0 &= \frac{4\kappa^2}{m_x m_y} - \omega^2 2\kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] + \omega^4 - \frac{\left(\kappa + \kappa e^{-ika}\right)^2}{m_x m_y} \\
&= \omega^4 - \omega^2 2\kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] + \frac{4\kappa^2 - \left(\kappa + \kappa e^{-ika}\right)^2}{m_x m_y}
\end{aligned}
$$

which is a is a second order polynomial equation for (ω^2) with solutions

$$
\omega^2 = 2\kappa\left[\frac{1}{2m_x} + \frac{1}{2m_y}\right] \pm \sqrt{\kappa^2\left[\frac{1}{m_x} + \frac{1}{m_y}\right]^2 + 4\frac{\kappa^2 + \left(\kappa + \kappa e^{-ika}\right)^2}{m_x m_y}}
$$

where we can simplify

$$
\begin{aligned}
\left|\kappa + \kappa e^{ika}\right| &= \sqrt{\left(2\kappa e^{ika}\right)\left(\kappa + \kappa e^{-ika}\right)} \\
&= \sqrt{2\kappa^2(1 + \cos(ka))}
\end{aligned}
$$

giving

$$
\begin{aligned}
x &= \kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] \pm \sqrt{\kappa^2\left(\left[\frac{1}{m_x} + \frac{1}{m_y}\right]^2 - \frac{4}{m_x m_y}\right) + 4\frac{\kappa^2 + \kappa\cos(ka)}{m_x m_y}} \\
&= \kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] \pm \sqrt{\kappa^2\left(\frac{1}{m_x^2} + \frac{1}{m_y^2} - \frac{2}{m_x m_y}\right) + 4\frac{\kappa^2 + \kappa\cos(ka)}{m_x m_y}} \\
&= \kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] \pm \sqrt{\kappa^2\left(\frac{1}{m_x^2} + \frac{1}{m_y^2}\right) - \frac{6\kappa^2 + 4\kappa\cos(ka)}{m_x m_y}}
\end{aligned}
$$

giving

$$
\omega_\pm = \sqrt{\kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] \pm \sqrt{\kappa^2\left(\frac{1}{m_x^2} + \frac{1}{m_y^2} - \frac{6\kappa^2}{m_x m_y}\right) - \frac{4\kappa\cos(ka)}{m_x m_y}}}
$$

As ω can take values of both ω_+ and ω_-, there are two branches.

At $k = 0$ this has values

$$
\omega_\pm = \sqrt{\kappa\left[\frac{1}{m_x} + \frac{1}{m_y}\right] \pm \sqrt{\kappa^2\left(\frac{1}{m_x^2} + \frac{1}{m_y^2} - \frac{6\kappa^2}{m_x m_y}\right) - \frac{4}{m_x m_y}}}
$$

Below is a sketch of the real(orange) and imaginary (blue) parts of the postivie part (ω_+) dispersion from $k \in [-6, 6]a$. κ is set to 1, m_x is set to 1, and $m_y = 1.5$.