Motivating Exercise for Taylor Series: Vibrations in a Crystal

Consider a nucleus in a one dimensional crystal, held in place by the repulsive forces from its neighbors. This force obeys Coulomb's Law, $\left|\vec{F}\right| = (1/4\pi\varepsilon_0)(q_1 q_2/r^2)$, where r is the distance between two nuclei. We'll assume for simplicity that all the nuclei have the same charge so we can combine $q_1 q_2/(4\pi\varepsilon_0)$ into one constant κ and write $\left|\vec{F}\right| = \kappa/r^2$.

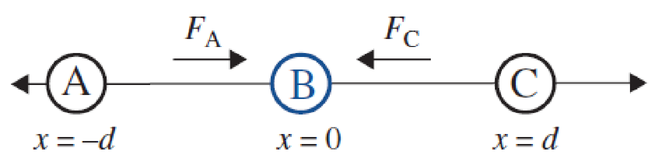

Figure 1: Nucleus B at $x = 0$ is pushed to the right by nucleus A at $x = -d$, and pushed to the left with equal force by nucleus C at $x = d$.

1. Explain what will happen to nucleus B, assuming the surrounding nuclei are perfectly fixed in position.

Now suppose nucleus B is displaced slightly to a new position x.

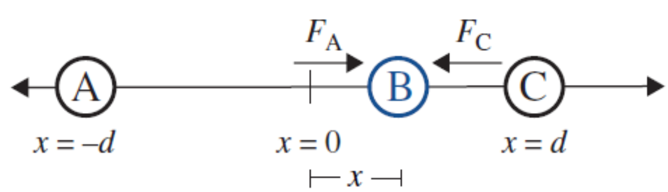

Figure 2: When Nucleus B is displaced to the right a distance x, the two forces on it no longer balance.

2. Write the formula for F_A, the force that nucleus A exerts on nucleus B.

3. Write the formula for F_C, the force that nucleus C exerts on nucleus B.

4. Write the formula for the net force on nucleus B. (Be careful about signs!)

5. Recalling that $F_{net} = ma$ where $a = d^2x/dt^2$, write a second-order differential equation to model the motion of nucleus B.

6. Based on your understanding of the physical situation, describe in words the motion that this differential equation should describe for nucleus B.

If you rearrange your answer to Part 5, you should be able to write it as:

$$\frac{d^2x}{dt^2} = \frac{\kappa}{m}\left(\frac{1}{(d+x)^2} - \frac{1}{(d-x)^2}\right)$$

The good news is, you should now have the correct equation to describe the motion of a vibrating nucleus in a crystal. The bad news is, the equation is difficult to solve. (Try it on a computer if you don't believe us!)

Now comes the key step. If we assume that the displacement x is small compared to the distance between nuclei d, we can make the following approximation:

$$\frac{\kappa}{m}\left(\frac{1}{(d+x)^2} - \frac{1}{(d-x)^2}\right) \approx -\frac{4\kappa}{md^3}x \tag{1}$$

We are not asking you to prove this approximation—we are waving our hands magically and pulling it out of a hat—although we will ask you, in Part 7, to confirm that it works pretty well.

7. Using the values $\kappa/m = 0.1$ N·m^2/kg, $d = 3 \times 10^{-10}$m, and $x = d/20$, compute both the original function (on the left side of Equation 1) and the approximation (right side).

8. The new differential equation $d^2x/dt^2 = -(4\kappa/md^3)x$ is much easier. Solve it by inspection. How does the resulting motion compare to your answer to Part 6?

The moral of the story should be clear: some equations are difficult or impossible to solve as given, but can be made reasonable by approximating difficult functions with simpler ones. But where did that particular approximation, $-(4\kappa/md^3)x$, come from? The technique of "linear approximations" allows you to generate very simple functions that approximate more complicated ones close to a certain value. More generally, "Taylor series" can give more accurate approximations when required.