The atoms in a solid are in constant thermally induced motion. In “born” we study the dynamics of a linear chain of atoms. We assume that the atomic arrangement that has minimum energy is the periodic array discussed in “bravais”. We then expand the potential energy of the system in powers of the displacement of the atoms from these equilibrium positions, stopping at the quadratic terms. In this harmonic approximation the equations of motion reduce to a set of independent harmonic oscillator equations. The solutions, called the normal modes, correspond to traveling plane waves.

Let’s consider an infinite chain of atoms of mass M coupled by springs with force constant K. Note that “born” works in dimensionless units for all the parameters. The packet width is expressed in units of the lattice constant a, the wave vector in units of $\pi/a$, and the time in unit timesteps.

Preset 1 shows a short segment of an infinite chain. The static display gives the initial atomic displacements. Click on RUN to start the motion. It is a traveling wave

$$u_n(t) = A \cos(qna - \omega t),$$

with $u_n$ the displacement from equilibrium of the $n$th atom. The frequency $\omega$ and the wave vector $q=2\pi/\lambda$ are related by the dispersion relation

$$\omega(q) = \sqrt{2K/M} \sin\left(\frac{qa}{2}\right)$$

Ex.1. RUN to have the graph display the time dependence of the displacement of the center atom of the chain. From this graph determine the angular frequency $\omega$ of the wave. Take the unit of time to be $10^{-14}$ s. Let $q$ vary over the range 0 - $\pi/a$ (entered as a number in the range 0 – 1 since $q$ is expressed in units of $\pi/a$). Make a plot of the dispersion relation $\omega(q)$ versus $q$. Does it agree with the above formula?
Ex. 2. Taking the atomic mass to be M=50 amu (atomic mass units), determine from data in “born” the spring constant of the interatomic forces. Express that spring constant in units of eV/Å². Why do you not need information about the amplitude of the wave or the lattice constant? Read page 64 in the SSS book. Do your results agree with the estimate given there?

Choose TRIPLE from the DISPLAY menu and RUN again briefly. This graph gives the displacement versus time for three successive atoms in the chain.

Ex. 3. One of the colored traces is for the central atom in the chain. The other two are for the two atoms to its right. Which color trace goes with which atom?

Ex. 4. Determine from “born” the value of $\omega$ for some choice of $q>2\pi/a$. What are the two q values in the range $-\pi/a<q<\pi/a$ for which $\omega(q)$ has this same value? Verify that one of these q values differs from the chosen $q>2\pi/a$ by the subtraction of $2n\pi/a$ where n is an integer.

Ex. 5. Use the dispersion relation to show that $\omega(q) = \omega(q+2\pi/a)$. 
Ex. 6. The “born” display shows both the initial displacements of the atoms, described by the discrete function \( u_n(t) = A \sin(qna) \), and the continuous function \( u(x) = A \sin(qx) \). Set the WAVE VECTOR to 0.3; you see a clear sinusoidal displacement function for the atoms which follows the continuous sine function very well. Now type into the slider \( q = 2.3 \). Watch the screen as you hit ENTER. Why does the continuous curve change while the atomic displacements remain fixed?

Hint: read page 65 of the SSS book.

Ex. 7. Verify by calculation that all wave vectors of the set \( q_n = q + 2\pi n/a \) give identical sets of atomic displacements.

Ex. 8. The traveling waves are moving from left to right with a phase velocity \( v_\phi = \omega / q \). Start with a WAVE VECTOR of 0.3 or less. Find a peak or valley of the wave for the initial configuration. RUN the simulation until the peak has traveled some distance and then stop. The TIME counter gives the elapsed time. Calculate the phase velocity. Repeat for a couple of values of \( q \) in the first Brillouin zone and compare with the given formula.
Select PRESET 2. The initial displacements you see are nearly identical to those of PRESET 1. Click on RUN and you see not a traveling wave but a standing wave.

Ex. 9. What is different about the initial conditions that give rise to these two very different types of motion?

Ex. 10. RUN and use the graph to compare the relative amplitudes and phases of the motion of the successive atoms in the chain. How does this differ from the behavior for the traveling wave?

Read pages 68-69 in the SSS book.
Ex. 11. Derive a relation for the values of wave vector q for which standing wave solutions will satisfy the fixed boundary conditions for a chain of length N, where the N atoms include the two fixed atoms at either end. Now select PRESET 2. Drag the wave vector slider and watch the readings that “born” is willing to accept. Do they correspond to the values you just calculated? Each of these q values yields a standing wave motion with is a normal mode of motion of the chain with fixed boundary conditions.
Ex. 12. What are the q values in the range $-\pi/a < q < \pi/a$ for which traveling wave solutions satisfy the periodic boundary conditions? Check that these are the wave vectors allowed by “born” in PRESET 1.

We often prefer to consider the thermal excitation of solids in terms of wave packets that are localized linear combinations of plane waves of nearly the same frequency. PRESET 4 constructs a TRAVELING PACKET with initial displacements

$$u_n = A \cos[q(n - n_0) a] \exp\left(-\frac{(n - n_0)^2 a^2}{2\sigma_0^2}\right),$$

where $\sigma_0$ is the packet width, $n_0$ the number of the atom on which it is centered (peak position) and $A$ the packet’s amplitude.

Ex. 13. PRESET 4 sets the boundary conditions to periodic. Run and you will see that the meaning of periodic boundary conditions is much more evident for the packet than for the infinite wave if you let the packet propagate to the end of the chain. Switch the boundary conditions to FIXED. What do you observe?
Ex. 14. Continue using fixed boundary conditions. Explain why during reflection from the end of the chain the displacement amplitude a few atoms from the end of the chain is roughly twice the maximum displacement at the center of the original packet.

Select PRESET 4 but with the initial condition changed to STANDING PACKET. The initial displacements are the same as for the traveling packet. Run with this initial condition and see what happens.

Ex.15. Explain qualitatively what must be different about the two initial conditions.

Ex. 16. Make sure that the boundary conditions are periodic. Let the program run until the two packets wrap around the ends and meet again. What feature of the equations of motion, in the harmonic approximation, insures that the packets can pass through each other without interaction?

Hint: read page 62 and 71 in the SSS book.
Ex. 17. Select PRESET 4 again, run, and follow one of the individual peaks of the cosine function as the packet propagates to the right. With a little attention you can pick up the same peak as the packet wraps around and comes back in at the left hand end. Does the peak stay in the same relative position within the envelope?

The velocity of the point you were following is the **phase velocity**, while the velocity of the overall packet is the **group velocity**. To measure the group velocity, RUN the program long enough that the packet passes the center atom a second time (increase the SPEED to save time).

Ex. 18. Choose a number of q values, determine the phase and group velocities and plot them as a function of q. You will want to vary both the packet width and the wave vector. Use q values above 0.2. What happens with the group velocity at $q = \pm \pi / a$?

Ex. 19. Use the data you have taken for $\omega(q)$ in Ex. 1 and for $v_g(q)$ to verify qualitatively the expression $v_g = \frac{d\omega(q)}{dq}$. What does this expression say about the group velocity at $q = \pm \pi / a$?
Ex. 20. Reselect PRESET 4, change the wave vector to $q=\pi/a$ and RUN. What happens?