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A Noncommutative Glass Model and the Boson Peak

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<p>Työssä esitellään uusi teoreettinen malli lasien rakenteelle, ja sitä hyödynnetään lasien niin sanotun bosonipiikin tutkinnassa. Malli perustuu yksinkertaiseen kiteistä tuttuun hilaan, joka muutetaan epäjärjestyneeksi epäkommutoivista fluidimalleista tutuilla menetelmillä.</p> <p>Aluksi tutkielmassa käydään läpi kiteiden rakenteen kannalta tärkeitä käsitteitä, keskittyen erityisesti akustisiin ja optisiin aaltoihin, hilavärähtelyjen tilatiheyteen, lämpökapasiteettiin sekä Debyen värähtelymalliin. Sen jälkeen perehdytään lyhyesti epäkommutoiviin fluidimalleihin sekä epäkommutoivaan geometriaan, jotta lasimallia esitellessä nähtäisiin sen yhteys fluideihin. Lopuksi esitellään itse malli lasien rakenteelle, ja siitä lasketaan lasien dispersiorelaatiot, tilatiheys sekä lämpökapasiteetti.</p> <p>Tilatiheydessä havaitaan Van Hoven singulariteetti matalilla taajuuksilla, joka vastaa lasien kokeissa löydettyä bosonipiikkiä. Lasilla on sekä akustisia että optisia aaltoja, joista akustiset aallot sijaitsevat hyvin lähellä Van Hoven singulariteetin taajuutta. Löydön perusteella lasien bosonipiikki johtuu akustisista aalloista.</p> <p>A new theoretical model for the structure of glasses is presented and used to study the boson peak found in glasses. The model is based on a simple lattice model familiar from crystals, which is disordered using techniques from noncommutative fluid models.</p> <p>First classical crystal models and concepts of lattice vibrations are reviewed, focusing on acoustic and optical waves, the density of vibrational states, heat capacity and the Debye model. Then noncommutative fluid theory and noncommutative geometry are shortly introduced to show the connection to fluids in our model. After these introductions, the glass model is formulated and used to calculate the dispersion relations, the density of vibrational states and the heat capacity.</p> <p>The density of states has a Van Hove singularity at low frequencies, which generates the boson peak seen in experiments. The glass is found to have both acoustic and optical waves, and the acoustic waves are located very close to the frequency of the Van Hove singularity, which hints that the boson peak should be related to acoustic waves.</p>			
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1 Glasses and the boson peak

When a liquid is cooled down cold enough to make it solid and fast enough to prevent it from attaining a crystalline structure, it can reach a variety of states in which it still looks like a liquid but flows too slowly for an experiment to even consider it to be flowing. These states are called amorphous, and the lowest-potential-energy amorphous state is called a glass. The transition temperature can be given different definitions depending on how viscous a material is viscous enough to be called a glass for the experiment, and also how fast the material was cooled down [1]. Several materials can be considered glasses, ranging from the silicate glasses used in windows to foams and proteins. Most liquids [2] can be turned to glass by rapid cooling.

Glasses are familiar from everyday life and widely used in industry, but their microscopic study is still lacking [2, 3]. The rigidity of glasses resembles that of crystals, but the disordered microscopic structure is closer to liquids, and a good theoretical model for the structure of glasses has yet to be developed. The theory of crystals and liquids has already been well studied [4–7] [8], so all the tools for researching glasses should be available.

Several techniques of statistical physics have been used for researching glasses. Field theory, renormalization groups, far-from-equilibrium systems, mode-coupling theory and kinetic glass models [9–12] have been tried in the last decades, to name a few, but a derivation for a complete and well-accepted theory of glasses is still missing [13].

In this thesis, we will introduce a model for glasses starting from a crystal model for solids, which will then be disordered using a technique from noncommutative fluid mechanics. The phenomenon we are interested in is the so-called boson peak, which is an increase in the density of states of amorphous materials at specific vibrational frequencies in low temperatures compared to the density of states of crystals. Our system is a static glass, so we shall not try to answer questions in some major glass topics like fragility and what is the transition time or temperature between liquids and glasses. We are interested in the density of states and the heat capacity of glasses. The model was first published in [14].

The boson peak is a feature found in all glasses in measurements of specific heat and heat capacity and light, x-ray, and neutron scattering. The thermal conductivity of glasses is significantly smaller than that of crystals, and it increases monotonically as temperature rises, opposed to the thermal conductivity of crystals which starts to decrease after a certain point. Another difference compared to crystals is that the thermal conductivity of glasses does not depend on the chemical composition. Many glasses consisting of completely different molecules have very similar thermal conductivities. [15]

The standard model for the heat capacity of crystals is the Debye model, which predicts a T^3 dependence for the heat capacity at low temperatures. In very low temperatures the specific heat of glasses, on the other hand, rises linearly with temperature, and C/T^3 as a function of T has a peak at low frequencies, as shown in figure (1.1), taken from [16]. All these anomalous behaviours hint that there is an excess of vibrational states in glasses in low temperatures.

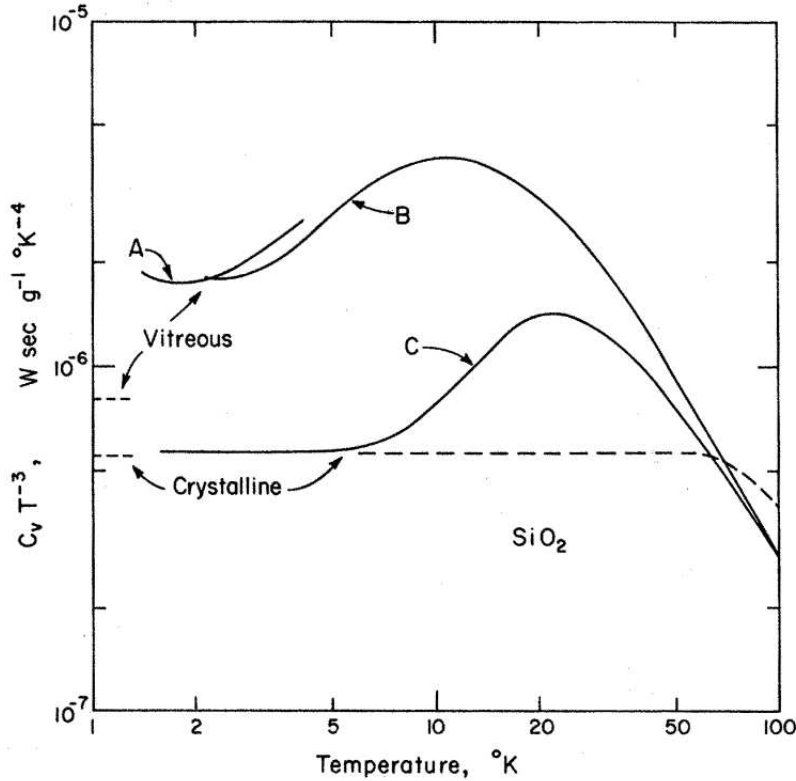


Figure 1.1: The heat capacity C scaled as C/T^3 , taken from [16]. The continuous lines are experimental values for vitreous SiO_2 and crystal quartz, whereas the long dashed line is what the Debye model predicts for quartz. Graph A is I. R. Vitreosil, B is vitreous silica and C is α -quartz.

Indeed plotting $g_{\text{glass}}(\omega)/g_{\text{Debye}}(\omega)$ as a function of the frequency ω , where $g_{\text{glass}}(\omega)$ is the density of states of a glass and $g_{\text{Debye}}(\omega)$ is the frequency dependence given by the Debye model, gives a peak at low frequencies. This is the boson peak. [17]

There are several different explanations for the boson peak, but none of them have been generally accepted and most of the experimental results fit many models. For example localization of vibrations [18] mode-coupling [19] and locally favoured structures [20] have been tried. One thing that is generally agreed on is that the peak is related to the disordered structure of glasses. [17, 21]

A general model used often to explain low temperature glass behaviour is the tunneling two-level system published separately by Phillips [22] and Anderson, Halperin and Varma [23]. The model suggests that there are atoms or groups of atoms in glasses that have two nearly degenerate states that they can tunnel

in between, and this tunneling is responsible for the anomalous behaviour of glasses in low temperatures. Mathematically this means defining a Hamiltonian with some distributions for the tunneling coefficients and the differences between the energy levels of the two states. The idea is not very restricting, so many variations of the model can be formulated and the model has evolved since it was published in 1972.

The tunneling two-level system has been thought to be a unique explanation for the low temperature behaviour of glasses, but recently this uniqueness has been questioned by Leggett and Vural [24]. Also the microscopic origin for the tunneling has yet to be properly explained. Our noncommutative model aims to explain glass behaviour at intermediate temperatures (1-40 K), where the boson peak occurs, but it might potentially shed light on low temperatures too.

Another approach to glasses and condensed matter is the interstitialcy theory. The theory is based on interstitialcies, which are atoms that occupy normally unoccupied sites in a crystal lattice. According to the theory liquids are crystals with enough interstitialcies, while glasses are frozen liquids, but there is still theoretical work to be done in developing the theory [25, 26]. Unlike interstitialcy theory, our model does not depend on how atoms are dislocated from their usual lattice sites, but instead only on how much on average they are dislocated.

2 Some main features of crystals

In 1912 a paper by Laue, Friedrich and Knipping was presented. In “Interference effects with Röntgen rays” it was first shown that x-rays should diffract when entering matter with a periodic structure, and then reported that crystalline solids cause a diffraction just like this. Thus it was shown that crystals consist of a periodic lattice structure and solid state physics was born. [27]

Crystals vary from metals consisting of a single chemical element to compound metals or even snowflakes and can thus be of microscopic or macroscopic size. The lattice structure of macroscopic crystals can often be macroscopically visible, resulting in beautiful objects. The study of crystals is called crystallography, but it is not the focus of this thesis. [6]

Later the study of solids started covering also solids without a crystal structure and afterwards even liquids. Solid state physics became condensed matter physics, the biggest field of physics today. [6] In this thesis we will first develop mathematical techniques used in crystal calculations, and then use these techniques to study amorphous materials, or glasses as they are often called, which lie somewhere between solids and liquids.

2.1 Lattice structure

[6, chapter 1] Since the defining property of a crystal is the lattice structure, the mathematical study of crystals is basically the study of lattices. Therefore we shall first review the concept of a lattice.

The simplest model of a crystal is a lattice structure that repeats a finite formation of atoms or molecules. In for example copper, gold, iron and alkali metals, the structure is formed by similar single atoms at every point of a lattice, and in table salt NaCl the lattice sites consist of 2x2 blocks of sodium and chloride. The repeating formation of lattice points that forms the whole crystal is called the primitive cell of the lattice. The primitive cell can also be very large, consisting of thousands of atoms in for example protein crystals [6]. However for macroscopic crystals, the primitive cell is still very small compared to the whole crystal, so the crystal lattice is usually assumed to be infinite.

Mathematically lattices are described through vectors. For parallelepiped lattices, the distance between each neighbouring lattice point is described with three orthogonal primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 , which each tell the length of the primitive cells in one direction. Since the lattice is periodic, the primitive translation vectors have the same value for each lattice point.

Using the primitive translation vectors, the separation between every lattice point can be written as $\mathbf{L} = l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$, where l , m and n are integers telling how many lattice sites separate the two points. Since the infinite crystal looks the same at point \mathbf{r} and at point $\mathbf{r} + \mathbf{L}$, translation by \mathbf{L} is a symmetry operation. Other symmetry operations for crystals are reflections and rotations around certain points or axes in the lattice. Compound operations consisting of translations, rotations and reflections that are symmetry operations are also

of course symmetries. Translations like \mathbf{L} that consist of primitive translation vectors are called just translation vectors.

Using symmetries it can be seen that only certain types of lattice shapes are possible. For example shapes symmetric under rotations of $\frac{2\pi}{5}$ radians, like pentagons in two-dimensional cases, cannot form infinite lattices. There are only 14 different possible shapes of three-dimensional lattices. The shapes are however not important here, since the aim of this thesis is to study solids with irregular structure.

2.2 Reciprocal space

[6, chapter 2] Crystals can be given different kinds of lattices. The lattices constructed by the primitive translation vectors are called Bravais lattices or direct lattices, but for each direct lattice there is also a lattice called the reciprocal lattice, which is the Fourier transformation of the direct lattice.

Let $U(\mathbf{r})$ describe a physical property of a lattice. Since the lattice is symmetric under translations of the form $\mathbf{r} \rightarrow \mathbf{r} + l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$, $U(\mathbf{r})$ has to remain unchanged under these transformations, so

$$U(\mathbf{r}) = U(\mathbf{r} + l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3). \quad (2.1)$$

Thus the Fourier series of $U(\mathbf{r})$

$$\sum_{\mathbf{b}} U_{\mathbf{b}} e^{i\mathbf{r} \cdot \mathbf{b}}, \quad (2.2)$$

where \mathbf{b} is a vector, is also left unchanged under the transformation, so

$$\sum_{\mathbf{b}} U_{\mathbf{b}} e^{i\mathbf{r} \cdot \mathbf{b}} = \sum_{\mathbf{b}} U_{\mathbf{b}} e^{i(\mathbf{r} + l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3) \cdot \mathbf{b}}. \quad (2.3)$$

l , m and n are arbitrary integers, so this means that for all the components of \mathbf{b}

$$\mathbf{b}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}. \quad (2.4)$$

The solutions to the these equation are

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \mathbf{a}_j \times \mathbf{a}_k}. \quad (2.5)$$

The vectors \mathbf{b}_i are called reciprocal primitive translations, and they form the reciprocal lattice. Sums of reciprocal primitive translations are called reciprocal translations or reciprocal vectors. The reciprocal space might seem like a very abstract construction, but diffraction patterns of crystals map the reciprocal space of the crystal.

As is seen from the form of \mathbf{b}_i , the reciprocal vectors are orthogonal if and only if the translation vectors \mathbf{a}_i are. The definition also shows that the primitive translations are inverse to the reciprocal primitive translations, and thus the direct lattice can be called reciprocal to the reciprocal lattice. Other things worth noting are that the lengths of the reciprocal primitive translations are $b_i = 2\pi/a_i$ and their dimension is $[length]^{-1}$.

2.2.1 Brillouin zones

[6, chapter 2] There are several different geometries to choose from when forming a cell or a primitive cell for a lattice. For a primitive cell, the simplest choice is to choose a lattice point and then draw the translation vectors from it. The parallelepiped formed by the vectors is the primitive cell. If other lattice points are on the boundaries of the cell, they are excluded from the cell and included in the neighbouring cells.

Another choice is the Wigner-Seitz cell. It consists of a chosen lattice point and all the points between lattice points that are closer to the chosen point than to other lattice points. The easiest way to visualize it is to draw the lattice, then draw straight lines from a site to the nearest neighbouring sites and to the middle points of these lines draw straight lines normal to the first lines. The area inside the normal lines is the Wigner-Seitz cell. Drawing a cell like this to each lattice point fills the whole lattice with no gaps nor overlapping, just like with the simpler cell choice. What makes the cell different from just drawing the translation vectors is that this cell is preserved under rotation and reflection symmetries of the lattice.

Drawing differently shaped cells is not particularly important for applications. The importance of the Wigner-Seitz cell is unveiled by drawing it in the reciprocal space, forming what is called the Brillouin zones. Drawing the Wigner-Seitz cell in the reciprocal space using nearest neighbours of a lattice site gives the first Brillouin zone of the site, using the second nearest neighbouring sites gives the second Brillouin zone and so on. Different Brillouin zones are important in diffraction, but as shall be shown, only the first Brillouin zone is needed when studying vibrations of the lattice, which is what we are interested in here.

3 Vibrating lattices

The movement of atoms in matter is a major part of condensed matter physics. Considering the atomic movement of crystals, i.e. the effects of external forces and the thermal movement of the atoms, leads to different kinds of effects in the crystal. Thermal properties and the transport of heat and sound inside a crystal are based on the atomic vibrations of the crystal, and vibrations affect also electric and magnetic properties of materials. Large movement inside a solid object leads to the breaking of the object. [6]

We will consider low-temperature vibrations, which means vibrations that do not break the solid and where the atoms can always be assumed to be near their equilibrium lattice sites. Vibrations are usually studied using generalized coordinates, because there are many atoms to consider. Here it means using Hamiltonian mechanics.

3.1 One dimensional lattice

[5, chapter 4.2] A good way to start is to consider a one-dimensional chain of identical atoms. After this, we will consider a three-dimensional system. We will assume that the chain is infinitely long to simplify the system. The assumption will not have much of an effect on the result, since real crystals have an astronomical amount of atoms.

Since we are considering small vibrations around the equilibrium points of the atoms, each atom in the chain is a Harmonic oscillator. Let the distance between the atoms in the chain be a , so that the position of the n th atom is $x_n = na + u_n$, where u_n is the displacement of the atom from its equilibrium point. Now the potential energy of each atom is $\frac{\zeta}{2}(u_n - u_{n+1})^2 + \frac{\zeta}{2}(u_n - u_{n-1})^2$, where ζ is called the elastic constant and describes “spring tension” between each atom. We get the whole Hamiltonian H_n for one atom by adding kinetic energy to this, so

$$H_n = \frac{p_n^2}{2m} + \frac{\zeta}{2}(u_n - u_{n+1})^2 + \frac{\zeta}{2}(u_n - u_{n-1})^2, \quad (3.1)$$

where p_n is the momentum of the n :th atom and m is its mass.

The equations of motion are derived simply by using Hamilton’s equations

$$\dot{q} = \frac{\partial H_n}{\partial p} \quad (3.2)$$

$$\text{and } \dot{p} = -\frac{\partial H_n}{\partial q} \quad (3.3)$$

where p describes the generalized momenta and q describes the generalized coordinates. Now $p = p_n$ and $q = u_n$. Using the first equation we get

$$\dot{u}_n = \frac{\partial}{\partial p_n} \left(\frac{p_n^2}{2m} + \frac{\zeta}{2}(u_n - u_{n+1})^2 + \frac{\zeta}{2}(u_n - u_{n-1})^2 \right) = \frac{p_n}{m}. \quad (3.4)$$

The second equation gives

$$\dot{p}_n = -\frac{\partial}{\partial u_n} \left(\frac{p_n^2}{2m} + \frac{\zeta}{2} (u_n - u_{n+1})^2 + \frac{\zeta}{2} (u_n - u_{n-1})^2 \right) = -\zeta (2u_n - u_{n+1} - u_{n-1}). \quad (3.5)$$

The former of Hamilton's equations gives the expression $p_n = m\dot{u}_n$, which when inserted into the latter one yields the equation of motion

$$m\ddot{u}_n = -\zeta (2u_n - u_{n+1} - u_{n-1}) \quad (3.6)$$

Since n varies from $-\infty$ to ∞ , we got an infinite set of equations. Second order ordinary differential equations with constant coefficients are solved with exponentials, so $u_n = A_n e^{-i\omega t}$, where A_n and ω are constants, should be a good trial solution. Plugging it in yields

$$-\omega^2 A_n e^{-i\omega t} = \frac{\zeta}{m} (-2A_n + A_{n+1} + A_{n-1}) e^{-i\omega t} \quad (3.7)$$

Next we want an ansatz for the constants A_n . Again we want an exponential, so let us use $A_n = A e^{ikan}$, where A is a constant describing the amplitude of the wave and k is the amplitude of a wave vector. Now we get the equation

$$-\omega^2 A e^{ikan} e^{-i\omega t} = \frac{\zeta}{m} (-2A e^{ikan} + A e^{ika(n+1)} + A e^{ika(n-1)}) e^{-i\omega t} \quad (3.8)$$

Dividing by $A e^{ikan} e^{-i\omega t}$ leads to

$$-\omega^2 = \frac{\zeta}{m} (-2 + e^{ika} + e^{-ika}) = \frac{2\zeta}{m} (-1 + \cos(ka)) = -\frac{4\zeta}{m} \sin^2 \left(\frac{ka}{2} \right) \quad (3.9)$$

Hence the frequency ω depends on k as

$$\omega = 2\sqrt{\frac{\zeta}{m}} \left| \sin \left(\frac{ka}{2} \right) \right| \quad (3.10)$$

and the solutions of the equation are the waves

$$u_n(k) = A e^{ikan} e^{-i\omega(k)t}. \quad (3.11)$$

The solution of course only describes a single wave. Waves can be in superposition, so the full solution to the equations of motion is a linear combination of the waves we got.

Exponents must be dimensionless, so the dimension of ω must be $[time]^{-1}$. Thus ω describes the frequency of the wave. a is the distance between the equilibrium points of atoms in the lattice, so its dimension is $[length]$. Thus the dimension of k is $[length]^{-1}$, so it is a wavevector in the reciprocal space of the lattice. The very important equation (3.10) telling the relation between the frequency and the wavevector is called the dispersion relation. It also tells that the frequency of atomic vibrations is proportional to $m^{-1/2}$, and since atoms are very light, atoms must vibrate with huge frequencies.

The waves we derived are called elastic waves. Writing the wave as

$$u_n(k) = Ae^{-i\omega(t-kan/\omega)} \quad (3.12)$$

and noting that an tells the position of each lattice site shows that the velocity of the waves is $v = \omega/k$ and the wavelength is $\lambda = 2\pi/k$. When k is small, elastic waves describe sound propagation. For small k

$$\omega = 2\sqrt{\frac{\zeta}{m}} \left| \sin\left(\frac{ka}{2}\right) \right| \approx 2\sqrt{\frac{\zeta}{m}} \frac{ka}{2} = ka\sqrt{\frac{\zeta}{m}}, \quad (3.13)$$

so the velocity of the wave is

$$v = a\sqrt{\frac{\zeta}{m}}, \quad (3.14)$$

which is in fact the velocity of sound in a crystal.

3.1.1 Brillouin zones of the 1D model

[5, chapter 4.2] Analyzing the dispersion relation (3.10) shows the importance of Brillouin zones in lattice dynamics. The vibrational frequency ω is a function of $\left| \sin\left(\frac{ka}{2}\right) \right|$, so it is periodic in k . More precisely all the values of ω are found inside

$$-\frac{\pi}{a} < k \leq \frac{\pi}{a}. \quad (3.15)$$

Since the distance between sites in the reciprocal lattice is $\frac{2\pi}{a}$ and the first Brillouin zone of a lattice site is defined as the set of points in the reciprocal space that are closer to the lattice site than to its neighbouring sites, we see that the values of k in (3.15) form the first Brillouin zone of the lattice site.

It is important to notice that all the values of the wave

$$u_n(k) = Ae^{ikan} e^{-i\omega(k)t} \quad (3.16)$$

are contained within the first Brillouin zone. If for example $k > \frac{\pi}{a}$ or $k < -\frac{\pi}{a}$, then $k - \frac{2m\pi}{a}$ lies within the first Brillouin zone for some integer m , and

$$e^{i(k-2m\pi/a)an} = e^{ikan} e^{-i2m\pi n} = e^{ikan} \quad (3.17)$$

and thus the wave $u_n(k)$ gets the same values as a wave defined within the first Brillouin zone. Therefore only values of k within the first Brillouin zone need to be considered.

3.1.2 Optical and acoustic branches

[5, chapter 4.2] Next we shall take a look at a one dimensional lattice with two different mass atoms in the unit cell, in order to introduce some concepts and techniques that will be useful later. Let the masses of the atoms be m_1 and m_2 and let u_n and v_n be the displacements of the atoms respectively. The Hamiltonian describing the n th unit cell is

$$H_n = \frac{p_{u;n}^2}{m_1} + \frac{p_{v;n}^2}{2m_2} + \frac{\zeta}{2}(u_n - v_{n-1})^2 + \frac{\zeta}{2}(v_n - u_n)^2 + \frac{\zeta}{2}(u_{n+1} - v_n)^2. \quad (3.18)$$

Using Hamilton's equations results in the differential equations

$$\dot{u}_n = \frac{p_{u;n}}{m_1} \quad (3.19)$$

$$\dot{v}_n = \frac{p_{v;n}}{m_2} \quad (3.20)$$

$$\dot{p}_{u;n} = -\zeta(2u_n - v_n - v_{n-1}) \quad (3.21)$$

$$\dot{p}_{v;n} = -\zeta(2v_n - u_n - u_{n+1}), \quad (3.22)$$

which yield the equations of motion

$$m_1 \ddot{u}_n = -\zeta(2u_n - v_n - v_{n-1}) \quad (3.23)$$

and

$$m_2 \ddot{v}_n = -\zeta(2v_n - u_n - u_{n+1}). \quad (3.24)$$

To get a wave like solution, we will use the trial functions

$$u_n = U e^{-i\omega t} e^{ikan} \quad (3.25)$$

$$v_n = V e^{-i\omega t} e^{ikan}, \quad (3.26)$$

where $a/2$ is the distance between the two atoms of the cell. This results in the equations

$$m_1 \omega^2 U = \zeta(2U - V - V e^{-ika}) \quad (3.27)$$

and

$$m_2 \omega^2 V = \zeta(2V - U - U e^{ika}). \quad (3.28)$$

It is useful to write the equation in the matrix form

$$\begin{pmatrix} m_1 \omega^2 - \zeta & \zeta(1 + e^{-ika}) \\ \zeta(1 + e^{ika}) & m_2 \omega^2 - \zeta \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = 0. \quad (3.29)$$

Now we do not have to actually solve the equations in order to get the dispersion relation. The matrix equation has nontrivial solutions only if its determinant is equal to zero, so

$$(m_1 \omega^2 - \zeta)(m_2 \omega^2 - \zeta) - \zeta^2(1 + e^{-ika})(1 + e^{ika}) = 0. \quad (3.30)$$

The equation is quadratic in ω^2 , so it results in two different dispersion relations, which are

$$\begin{aligned}\omega_{\pm}^2 &= \frac{\zeta(m_1 + m_2) \pm \sqrt{\zeta^2(m_1 + m_2)^2 - 4m_1m_2\zeta^2(1 + e^{-ika})(1 + e^{ika})}}{m_1m_2} \\ &= \frac{\zeta}{m_1m_2} \left(m_1 + m_2 \pm \sqrt{(m_1 + m_2)^2 - 4m_1m_2 \sin^2\left(\frac{ka}{2}\right)} \right).\end{aligned}\quad (3.31)$$

The relation with a plus sign is called the optical branch, and the relation with a minus sign is called the acoustic branch. The reason for these names is seen by calculating the amplitudes U and V of the waves. It is important to distinguish different branches, because different dispersion relations lead to different properties for the system. Plugging in the dispersion relation to for example the first of the equations (3.27) yields

$$m_1\omega_{\pm}^2 U = \zeta(2U - V - Ve^{-ika}), \quad (3.32)$$

which results in

$$U_{\pm} = \frac{\zeta(1 + e^{-ika})}{2\zeta - \omega_{\pm}^2 m_1} V_{\pm}. \quad (3.33)$$

This tells how the amplitudes of the atoms with different mass depend on each other.

Using the very long wavelength limit $k = 0$ in (3.31) leads to

$$\omega_+^2 = \frac{2\zeta}{m_1m_2} (m_1 + m_2) \quad (3.34)$$

and

$$\omega_-^2 = 0, \quad (3.35)$$

and thus

$$U_+ = -\frac{m_2}{m_1} V_+ \quad (3.36)$$

and

$$U_- = V_-. \quad (3.37)$$

As is seen, in the acoustic branch all the atoms vibrate in the same phase. This is the reason the branch is called acoustic, since when sound passes through a medium, all the atoms in the medium vibrate in phase. For the optical branch the atoms vibrate in opposite phases instead, and the center of mass of each unit cell remains still, since the amplitude for the center of mass of a unit cell where the first atom is at location x is

$$\frac{m_1 U_- x + m_2 V_- (x + a/2)}{m_1 + m_2} = \frac{a}{2(m_1 + m_2)} V_- = \text{constant}. \quad (3.38)$$

Thus the optical branch describes, for example, the passing of electromagnetic waves, and the name optical branch is sensible.

When k is increased from zero, the expression inside the square root in (3.31) starts to decrease, making the optical branch ω_- smaller and the acoustic branch ω_+ larger. This is an essential property separating the two kinds of branches from each other. Optical branches start at a constant in the centre of the Brillouin zone where $k = 0$ and decrease towards the edges of the zone, whereas acoustic branches start at zero and increase towards the boundaries of the Brillouin zone. Another important difference is that optical branches have always a higher frequency than acoustic branches, as can be seen from the dispersion relations.

The rest of the calculations in the thesis shall only consider lattices with particles that have equal mass, but the concepts of optical and acoustic branches will remain relevant.

3.2 Three dimensional lattices

[5, chapter 4.3] Next we want to introduce the concepts of the density of states and specific heat capacity. In this thesis we are interested in three-dimensional solids, so we will continue with a three-dimensional lattice from now on to get just the tools that we need.

In the model that will later be introduced to describe the boson peak, we will only consider nearest neighbour interactions, so that is what we will do here. The boson peak is also studied only in very small temperatures, so we need to consider only small oscillations of atoms.

Consider a lattice that is symmetric under the change of any two axes and has only one atom in each unit cell. Let the primitive translation vectors of the lattice be \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 . The Hamiltonian describing the system is

$$\begin{aligned}
H_{l,m,n} = & \frac{p_{u;l,m,n}^2 + p_{v;l,m,n}^2 + p_{w;l,m,n}^2}{2m} \\
& + \frac{\zeta}{2} (u_{l,m,n} - u_{l+1,m,n})^2 + \frac{\zeta}{2} (u_{l,m,n} - u_{l-1,m,n})^2 \\
& + \frac{\zeta}{2} (v_{l,m,n} - v_{l,m+1,n})^2 + \frac{\zeta}{2} (v_{l,m,n} - v_{l,m-1,n})^2 \\
& + \frac{\zeta}{2} (w_{l,m,n} - w_{l,m,n+1})^2 + \frac{\zeta}{2} (w_{l,m,n} - w_{l,m,n-1})^2, \quad (3.39)
\end{aligned}$$

where $u_{l,m,n}$, $v_{l,m,n}$, and $w_{l,m,n}$ are the displacements of the atom at the lattice site l, m, n and $p_{u;l,m,n}$, $p_{v;l,m,n}$ and $p_{w;l,m,n}$ are the momenta in the three directions. This is a sum of three independent one dimensional chains considered in the previous subsection. Thus the result should also be three instances of the dispersion relation in (3.10).

Let us consider one of the directions. Using Hamilton's equations

$$\dot{q} = \frac{\partial H_n}{\partial p} \quad (3.40)$$

$$\text{and } \dot{p} = -\frac{\partial H_n}{\partial q} \quad (3.41)$$

for $q = u_{l,m,n}$ and $p = p_{u;l,m,n}$ yields the equations

$$\dot{u}_{l,m,n} = \frac{p_{u;l,m,n}}{m} \quad (3.42)$$

and

$$\dot{p}_{u;l,m,n} = -\zeta (2u_{l,m,n} - u_{l+1,m,n} - u_{l-1,m,n}), \quad (3.43)$$

which when combined yield the familiar equation of motion

$$m\ddot{u}_{l,m,n} = -\zeta (2u_{l,m,n} - u_{l+1,m,n} - u_{l-1,m,n}). \quad (3.44)$$

We got the same equation as in the one dimensional case, except that now our variables have three indices instead of one. For the other two directions we get similarly the equations

$$m\ddot{v}_{l,m,n} = -\zeta (2v_{l,m,n} - v_{l,m+1,n} - v_{l,m-1,n}) \quad (3.45)$$

and

$$m\ddot{w}_{l,m,n} = -\zeta (2w_{l,m,n} - w_{l,m,n+1} - w_{l,m,n-1}). \quad (3.46)$$

Lets now try the solutions

$$u_{l,m,n}(\mathbf{k}) = U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}}, \quad (3.47)$$

$$v_{l,m,n}(\mathbf{k}) = V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}} \text{ and} \quad (3.48)$$

$$w_{l,m,n}(\mathbf{k}) = W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}}, \quad (3.49)$$

where U , V and W are the amplitudes of the wave in the three directions, $\mathbf{k} = (k_1, k_2, k_3)$ is the wave vector, $\mathbf{L}_{l,m,n} = l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$ is the translation vector telling the location of the lattice site and ω is the frequency of the wave.

Plugging in the functions yields

$$-\omega^2 U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}} m = -\zeta (2 - e^{ik_1 a_1} - e^{-ik_1 a_1}) U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}}, \quad (3.50)$$

$$-\omega^2 V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}} m = -\zeta (2 - e^{ik_2 a_2} - e^{-ik_2 a_2}) V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}} \text{ and} \quad (3.51)$$

$$-\omega^2 W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}} m = -\zeta (2 - e^{ik_3 a_3} - e^{-ik_3 a_3}) W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}_{l,m,n}}. \quad (3.52)$$

Solving ω from each of these equations gives three of the dispersion relations familiar from the one dimensional case:

$$\begin{aligned} \omega &= 2\sqrt{\frac{\zeta}{m}} \sin\left|\left(\frac{a_1 k_1}{2}\right)\right|, \\ \omega &= 2\sqrt{\frac{\zeta}{m}} \sin\left|\left(\frac{a_2 k_2}{2}\right)\right| \text{ and} \\ \omega &= 2\sqrt{\frac{\zeta}{m}} \sin\left|\left(\frac{a_3 k_3}{2}\right)\right|. \end{aligned} \quad (3.53)$$

The three dispersion relations represent three different branches of vibrations going in different directions. If a wave is passing through the lattice in the direction of one of the primitive translation vectors, then the branch associated with that direction is called the longitudinal branch, while the two other branches are called transverse.

3.2.1 Boundary conditions

[5, chapter 4.2] Next we want to calculate a quantity called the density of states, but in order to do that we need to set boundary conditions for our system. There is a variety of different possible boundary conditions, but we are looking for conditions that restrict the system only a little. This is reasonable since systems with an enormous amount of atoms should not depend too much on the conditions we set for specific atoms.

We make the popular choice of the Born and von Karman boundary conditions, which make the system periodically symmetric. This is mathematically very convenient. Assume that the lattice repeats a formation of $N = N_1 \times N_2 \times N_3$ atoms. This means that for the waves at the site l, m, n

$$u_{l,m,n} = u_{l+N_1,m,n} = u_{l,m+N_2,n} = u_{l,m,n+N_3}. \quad (3.54)$$

The larger N_1, N_2 and N_3 are, the less the conditions restrict the system. If we have three solutions $u_{l,m,n}, v_{l,m,n}$ and $w_{l,m,n}$ for the three directions, we set the same conditions also for $v_{l,m,n}$ and $w_{l,m,n}$.

The condition sets a restriction on \mathbf{k} . If

$$u_{l,m,n}(\mathbf{k}) = U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \quad (3.55)$$

as it was earlier, then

$$u_{l+N_1,m,n}(\mathbf{k}) = U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L} + ia_1 k_1 N_1} = u_{l,m,n}(\mathbf{k}) = U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \quad (3.56)$$

and thus

$$e^{ia_1 k_1 N} = 1. \quad (3.57)$$

This means that

$$k_1 = \frac{2\pi}{a_1 N} g_1, \quad (3.58)$$

where $g_1 = 1, \dots, N_1$. Therefore k_1 has only N_1 possible values. Similarly

$$k_2 = \frac{2\pi}{a_2 N} g_2, \quad g = 1, \dots, N_2 \quad (3.59)$$

and

$$k_3 = \frac{2\pi}{a_3 N} g_3, \quad g_3 = 1, \dots, N_3, \quad (3.60)$$

and k_2 and k_3 have only N_2 and N_3 possible values.

Thus the whole wavevector \mathbf{k} has $N_1 N_2 N_3$ possible values. $\frac{2\pi}{a_1}, \frac{2\pi}{a_2}$ and $\frac{2\pi}{a_3}$ are the lengths of the reciprocal primitive translation vectors. Let us call these vectors again $\mathbf{b}_1, \mathbf{b}_2$ and \mathbf{b}_3 , so

$$\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 = \frac{g_1}{N_1} \mathbf{b}_1 + \frac{g_2}{N_2} \mathbf{b}_2 + \frac{g_3}{N_3} \mathbf{b}_3. \quad (3.61)$$

Since g_1, g_2 and g_3 take discrete values, we see that the expression for \mathbf{k} forms the reciprocal lattice, and the lattice points must be distributed evenly.

Thus using the fact that there are $N_1 N_2 N_3$ different values for \mathbf{k} we see that each value takes the space

$$\Delta k = \frac{V_B}{N_1 N_2 N_3} \quad (3.62)$$

in the Brillouin zone, where V_B is the volume of the zone. Let us express this using volumes in the direct lattice. Comparing to the one dimensional case shows that the volume is $V_B = (2\pi)^3 / V_C$, where V_C is the volume of the physical unit cell, because the lattice consists of three one dimensional chains. Since we started by assuming that the whole crystal repeats a formation of $N_1 \times N_2 \times N_3$ atoms, $V_C N_1 N_2 N_3 = V$ must give the volume of the whole crystal and

$$\Delta k = \frac{(2\pi)^3}{V}. \quad (3.63)$$

This volume is needed to solve the density of states.

3.2.2 Density of state

[5, chapter 4.3.5] After deriving the dispersion relation, i.e. after showing how the frequency of atomic oscillations depends on the wave vector of the oscillations, a natural question is to ask what is the amount of oscillations in a specific frequency. This is called the phonon density states.

The name phonon comes from the normal modes of the oscillations. The name is in analogy to photons, which are the quanta of vibrations of the electromagnetic field, because phonons are the quanta of atomic vibrations. Thus the question is how many phonons are there of a specific frequency. The derivation of the normal modes or phonons is an interesting calculation, but it does not bring any relevant techniques to the main calculation of this thesis, so it will not be shown here.

If $g(\omega)$ is the density of states telling the frequency distribution of the oscillations, then $g(\omega) d\omega$ tells the number of phonons whose frequencies are between ω and $\omega + d\omega$. We will derive $g(\omega)$ by first calculating $g(\omega) d\omega$.

Consider the surface S_ω in the reciprocal space defined by $\omega = \omega_{\mathbf{k}} = \text{constant}$ for a specific branch of the vibrations. Different branches give different surfaces, since they have a different dispersion relation. $dS_\omega dk_\perp$ gives the infinitesimal of the volume containing the vibrations with a frequency between ω and $\omega + d\omega$, where dk_\perp is the part of $d\mathbf{k}$ that is perpendicular to S_ω .

Since each value of \mathbf{k} and thus each value of ω takes the space $\Delta k = (2\pi)^3 / V$ in the reciprocal space, there must be

$$\frac{dS_\omega dk_\perp}{\Delta k} = \frac{V}{(2\pi)^3} dS_\omega dk_\perp \quad (3.64)$$

phonons in the volume $dS_\omega dk_\perp$. Integrating over the surface gives the number of phonons in the frequency range $[\omega, \omega + d\omega]$

$$g(\omega) d\omega = \frac{V}{(2\pi)^3} \iint_{\omega=\omega_{\mathbf{k}}} dS_\omega dk_\perp \quad (3.65)$$

This is not yet the result we want. ω is a function of \mathbf{k} and grows in the direction perpendicular to S_ω , so $d\omega = |\nabla_{\mathbf{k}}\omega_{\mathbf{k}}| dk_\perp$, and

$$g(\omega) d\omega = \frac{V}{(2\pi)^3} \iint_{\omega=\omega_{\mathbf{k}}} \frac{d\omega}{|\nabla_{\mathbf{k}}\omega_{\mathbf{k}}|} dS_\omega, \quad (3.66)$$

so the density of states is

$$g(\omega) = \frac{V}{(2\pi)^3} \iint_{\omega=\omega_{\mathbf{k}}} \frac{dS_\omega}{|\nabla_{\mathbf{k}}\omega_{\mathbf{k}}|}. \quad (3.67)$$

For the special case when the dispersion relation is isotropic there is a simpler way to calculate $g(\omega)$. Isotropy means that the surface defined by $\omega = \omega_{\mathbf{k}} = \text{constant}$ is a sphere. If V_ω is the volume of the sphere, there are

$$\frac{V V_\omega}{(2\pi)^3} \quad (3.68)$$

phonons with frequency $\omega_{\mathbf{k}}$ or less. Thus when the radius of the sphere is increased by $d\omega$, the amount of phonons inside the sphere grows by

$$\frac{V}{(2\pi)^3} \frac{dV_\omega}{d\omega} d\omega, \quad (3.69)$$

which means that the frequency distribution, or density of states, at $\omega_{\mathbf{k}}$ is

$$g(\omega) = \frac{V}{(2\pi)^3} \frac{dV_\omega}{d\omega}. \quad (3.70)$$

If the dispersion relation was not isotropic, its dependence on direction would have to be considered when the volume inside the $\omega = \text{constant}$ surface was increased, so the density of states would need to depend on the gradient $\nabla_{\mathbf{k}}\omega_{\mathbf{k}}$.

3.2.3 Van Hove singularities

[7, chapter 6] Since the integral in the formula for the density of states has a denominator, it also could have singularities at $\nabla_{\mathbf{k}}\omega_{\mathbf{k}} = 0$. The singularity points can be minima, maxima or saddle points of the frequency. Let \mathbf{k}_0 be such a point. Expanding ω up to the second order around \mathbf{k}_0 gives

$$\omega = \omega_0 + \sum_{i,j} \frac{1}{2} C_{ij} (k_i - k_{0,i}) (k_j - k_{0,j}), \quad (3.71)$$

where $\omega_0 = \omega(\mathbf{k}_0)$. The coefficients C_{ij} form a matrix, so we can choose the axes of the \mathbf{k} space along the principal axes of the matrix, so that the matrix becomes diagonal and

$$\omega = \omega_0 + \frac{1}{2} \sum_{\lambda} C_{\lambda} (k_{\lambda} - k_{0,\lambda})^2. \quad (3.72)$$

The last change we will do to this expression for ω is the change of variables $\chi_\lambda = \sqrt{|C_\lambda|} (k_\lambda - k_{0,\lambda})$, so

$$\omega = \omega_0 + \frac{1}{2} \sum_{\lambda} \text{sgn}(C_\lambda) \chi_\lambda^2, \quad (3.73)$$

where $\text{sgn}(C_\lambda)$ is the sign of C_λ .

Now the form is easier to analyze. There are three possible signs $\text{sgn}(C_\lambda)$ and different choices of them give different types of critical points for ω . If all the signs are positive, ω has a minimum at \mathbf{k}_0 and the isofrequency surfaces in χ space are spheres. The surface element of the sphere is $dS_\omega = dS_{\omega,\chi}/\sqrt{C} = \chi^2 d\Omega/\sqrt{C}$, where $d\Omega$ is the differential of the solid angle and $1/\sqrt{C}$ is the Jacobian from the change of variables. The gradient $\nabla_\chi \omega_\chi = \chi$, so the density of states is

$$g(\omega) = \frac{V}{(2\pi)^3 \sqrt{C}} \iint_{\omega=\omega_\mathbf{k}} \frac{\chi^2 d\Omega}{|\chi|} = g(\omega_0) + \frac{V}{2\pi^2 \sqrt{C}} |\chi| = g(\omega_0) + \frac{V}{\pi^2 \sqrt{2C}} \sqrt{\omega - \omega_0}. \quad (3.74)$$

for $\omega \geq \omega_0$ and $g(\omega) = g(\omega_0)$ for $\omega \leq \omega_0$. After the change of variables to χ -space we could also have used the rule (3.70) for isotropic dispersion relations yielding the same result.

The case where all the signs $\text{sgn}(C_\lambda)$ are negative is similar, but it describes a maximum of ω , and the density of states is

$$g(\omega_0) + \frac{V}{4\pi^2 \sqrt{C}} \sqrt{\omega_0 - \omega} \quad (3.75)$$

for $\omega \leq \omega_0$ and $g(\omega) = g(\omega_0)$ for $\omega \geq \omega_0$.

If one of the signs $\text{sgn}(C_\lambda)$ is different from the other two, there is a saddle point at \mathbf{k}_0 . Take as an example the case

$$\omega = \omega_0 + \frac{1}{2} (\chi_1^2 + \chi_2^2 - \chi_3^2). \quad (3.76)$$

The constant frequency surfaces are now hyperboloids. In the case $\omega < \omega_0$ the hyperboloid has two sheets and in the case $\omega > \omega_0$ the hyperboloid has one sheet. The integral is most easily done in cylindrical coordinates $(\chi_\perp, \phi, \chi_3)$, where $\chi_\perp = \sqrt{\chi_1^2 + \chi_2^2}$ and ϕ is the polar angle in the $\chi_1\chi_2$ plane. When $\omega < \omega_0$

$$dS_\omega = \frac{2\pi\chi_\perp\chi_3}{|\chi_3|} d\chi_\perp \quad (3.77)$$

and again $|\nabla_\chi \omega_\chi| = 2\chi$, and

$$\begin{aligned} g(\omega) &= \frac{2}{(2\pi)^3 \sqrt{C}} \int_0^K \frac{2\pi\chi_\perp d\chi_\perp}{\sqrt{\chi_\perp^2 + 2(\omega_0 - \omega)}} = \frac{1}{2\pi^2 \sqrt{C}} \left(K - \sqrt{2(\omega_0 - \omega)} \right) \\ &= g(\omega_0) - \frac{1}{\pi^2 \sqrt{2C}} \sqrt{\omega_0 - \omega}, \end{aligned} \quad (3.78)$$

where K is some constant. The case $\omega > \omega_0$ yields

$$g(\omega) = \frac{2}{(2\pi)^3 \sqrt{C}} \int_{2(\omega-\omega_0)}^K \frac{2\pi\chi_{\perp} d\chi_{\perp}}{\sqrt{\chi_{\perp}^2 - 2(\omega_0 - \omega)}} = \frac{K}{2\pi^2 \sqrt{C}} = g(\omega_0). \quad (3.79)$$

The case where two of the signs are negative and one positive gives a similar result, except that

$$g(\omega) = g(\omega_0) - \frac{1}{\pi^2 \sqrt{2C}} \sqrt{\omega_0 - \omega} \quad (3.80)$$

for $\omega > \omega_0$ and

$$g(\omega) = g(\omega_0) \quad (3.81)$$

for $\omega < \omega_0$.

3.3 Heat capacity

[5, chapter 4.5.3] Heat capacity is one of the properties which separate amorphous solids from crystals. There are several models for the heat capacity of crystals, which apply to different situations, and we will introduce two of them, so that we can compare the results for amorphous materials to them.

The heat capacity C of an object tells how much the internal energy U of the object changes when the temperature T of the object changes, or in other words how much energy is needed to change the temperature of the object a specific amount. We will use the definition

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V \quad (3.82)$$

for the heat capacity C_V , in which we calculate the change $\partial U/\partial T$ when the volume of the system V is kept constant. Another way to define the heat capacity is to keep the pressure of the system constant, and this is the definition used usually in experiments. [6]

The energy levels of a harmonic oscillator vibrating at frequency ω are

$$\left(\frac{1}{2} + n \right) \omega, \quad n \in \mathbb{N}. \quad (3.83)$$

The vibrations of a crystal are a sum of harmonic oscillators, or phonons, in different frequencies, so the internal energy in the crystal caused by the vibrations is

$$U = \sum_{\mathbf{k}j} \left(\frac{1}{2} + n_{\mathbf{k}j} \right) \omega_{\mathbf{k}j}, \quad (3.84)$$

where $n_{\mathbf{k}j}$ is the number of phonons with wave number \mathbf{k} in branch j . There is no Pauli exclusion principle for bosons, so $n_{\mathbf{k}j}$ is given by the Bose-Einstein distribution

$$n_{\mathbf{k}j} = \frac{1}{e^{\omega_{\mathbf{k}j}/T} - 1}. \quad (3.85)$$

The sum over different wave numbers and branches can be replaced by an integral, if we know the total density of states $g(\omega)$ of the system, that includes different branches:

$$U = \int d\omega g(\omega) \left(\frac{1}{2} + \frac{1}{e^{\omega/T} - 1} \right) \omega \quad (3.86)$$

Now taking the derivative with respect to T we get

$$C_V = \int d\omega g(\omega) \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T}. \quad (3.87)$$

The high temperature limit is easy to calculate. Using L'Hôpital's rule twice we see that

$$\begin{aligned} C_V &= \int d\omega g(\omega) \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T} \rightarrow \int d\omega g(\omega) \frac{-\omega^2/T^2 - 2\omega/T}{-e^{\omega/T} 2 + 2} \\ &\rightarrow \int d\omega g(\omega) = 3Nn, \end{aligned} \quad (3.88)$$

which is the number of possible oscillations in a three-dimensional crystal of N primitive cells with n atoms. An important remark is that acoustic vibrations have nothing to do with the number of atoms in a unit cell, so the number of acoustic branches depends only on N . Indeed there are $3N$ acoustic branches in a three-dimensional crystal, so the remaining $3N(n - 3)$ vibrations are optical. Next, we shall consider two models that describe the contributions of acoustic and optical waves to the heat capacity.

3.3.1 Debye model

[5, chapter 4.5.3] In low temperatures there are only low energy excitations, so the wave numbers of oscillations must be small. As was shown in subsection (3.1.2) there are only acoustic waves in the $k = 0$ limit in one-dimensional systems, but simple three dimensional systems are no different since they consist of one dimensional chains. Thus we expect to find only long wavelength acoustic waves at very low temperatures.

Consider the three dimensional dispersion relations in (3.53). Taking now the long wavelength limit $|\mathbf{k}| \ll 1$ gives

$$\omega_j = \sqrt{\frac{\zeta}{m}} a_j |\mathbf{k}| = v_j |\mathbf{k}|, \quad (3.89)$$

for each of the three branches j , where v_j is the velocity of sound in each of the branches, as in (3.14) in the one dimensional case. Now that the three branches correspond to three orthogonal directions in the lattice, each v_j tells the velocity of sound in a different direction.

The isofrequency surfaces in the reciprocal space of each of the branches are spheres with radius $k_j = \omega/v_j$, and the gradients $\nabla_{\mathbf{k}} \omega_{\mathbf{k},j} = v_j \hat{\mathbf{k}}$, so using the

formula for the density of states (3.67) we get for each branch

$$g_j(\omega) = \frac{V}{(2\pi)^3} \iint_{\omega=\omega_{\mathbf{k}}} \frac{dS_{\omega}}{v_j} = \frac{V\omega^2}{2\pi^2 v_j^3}. \quad (3.90)$$

Adding together the branches we get

$$g(\omega) = \frac{V\omega^2}{2\pi^2} \left(\frac{2}{v_{\perp}^3} + \frac{1}{v_{\parallel}^3} \right) = \frac{3V\omega^2}{2\pi^2 v_{eff}^3} \quad (3.91)$$

where $2/v_{\perp}$ stands for the two transverse branches, $1/v_{\parallel}$ comes from the longitudinal branch, and v_{eff} is the effective sound velocity that comes from combining the branches.

Before inserting the above expression of $g(\omega)$ to the formula for the heat capacity, we need to add something to our model. Now the density of states only grows with the frequency, resulting in an infinite amount of states if integrated to infinity. We however want the maximum amount of states from acoustic oscillations to be $3N$, so we will introduce a cut off frequency ω_D for which

$$\int_0^{\omega_D} g(\omega) d\omega = 3N. \quad (3.92)$$

ω_D is called the Debye frequency. Inserting the density of states (3.91) to the above integral shows that

$$\frac{V\omega_D^3}{2\pi^2 v_{eff}^3} = 3N, \quad (3.93)$$

so that

$$\omega_D = v_{eff} \left(\frac{6N\pi^2}{V} \right)^{1/3} = v_{eff} \left(\frac{6\pi^2}{V_C} \right)^{1/3}, \quad (3.94)$$

where V_C is again the volume of a unit cell. The Debye frequency also defines a temperature called the Debye temperature, which is $T_D = \hbar\omega_D/k_B$, but now that we have set $\hbar = k_B = 1$ it is equivalent to the frequency.

Using the cut off the heat capacity is

$$C_V = \int_0^{\omega_D} d\omega \frac{3V\omega^2}{2\pi^2 v_{eff}^3} \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T} \quad (3.95)$$

Opening the square and writing the constant using the Debye frequency leads to

$$\begin{aligned} C_V &= \frac{9N}{T^2 \omega_D^3} \int_0^{\omega_D} d\omega \frac{\omega^4}{e^{\omega/T} - 2 + e^{-\omega/T}} \\ &= \frac{9N}{4T^2 \omega_D^3} \int_0^{\omega_D} d\omega \frac{\omega^4}{\sinh^2(\omega/2T)} \\ &= \frac{72NT^3}{\omega_D^3} \int_0^{\omega_D/2T} dx \frac{x^4}{\sinh^2 x}, \end{aligned} \quad (3.96)$$

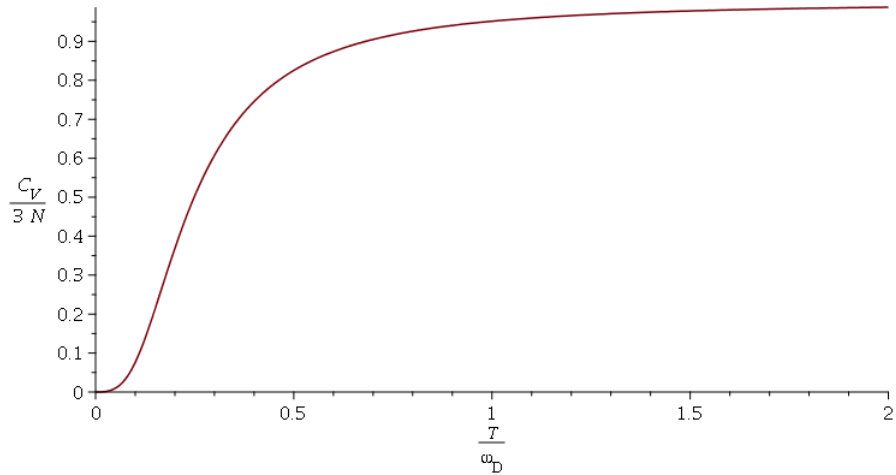


Figure 3.1: The Debye model heat capacity scaled as $\frac{C_V}{3N}$ as a function of $\frac{T}{\omega_D}$

where $x = \omega/2T$. This is the Debye model for the heat capacity of a crystal.

In the low temperature limit $\omega_D/2T \rightarrow \infty$. Taking the upper bound of the integral to infinity results in

$$C_V = \frac{72NT^3}{\omega_D^3} \frac{\pi^4}{30} = \frac{12\pi^4 NT^3}{5\omega_D^3}. \quad (3.97)$$

The T^3 proportionality is indeed in good agreement with experiments for several crystals [5].

An interesting thing is that the Debye model is also correct in the high temperature limit. In high temperatures $\omega/T \ll 1$, so $\sinh(\omega/T) \approx \omega/T$ and

$$\begin{aligned} C_V &= \frac{72NT^3}{\omega_D^3} \int_0^{\omega_D/2T} dx x^2 \\ &= 3N, \end{aligned} \quad (3.98)$$

which is exactly the maximum amount of acoustic states.

The plot of the whole function C_V is in figure (3.1).

3.3.2 Einstein model

[5, chapter 4.5.3] A simple model describing the contribution of optical waves to the heat capacity is the Einstein model. Assume that there are $3N(n-3)$ optical branches and they all have the same frequency ω_E , so $g(\omega) = 3N(n-3)\delta(\omega - \omega_E)$. Now the heat capacity

$$C_V = \int d\omega g(\omega) \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T} = 3N(n-3) \left(\frac{\omega_E/T}{e^{\omega_E/T} - 1} \right)^2 e^{\omega_E/T}. \quad (3.99)$$

In the high temperature limit $e^{\omega_E/T} \approx 1 + \omega_E/T$, so

$$C_V \approx 3N(n-3) \left(\frac{\omega_E}{T} + 1 \right) \rightarrow 3N(n-3) \quad \text{as } T \rightarrow \infty, \quad (3.100)$$

which is indeed the contribution optical waves should have so that the maximum amount of vibrational modes is $3Nn$. In low temperatures

$$C_V \approx 3N(n-3) \frac{\omega_E^2/T^2}{e^{\omega_E/T}} \rightarrow 0 \quad \text{as } T \rightarrow 0, \quad (3.101)$$

so according to this model optical waves should not contribute to the heat capacity in low temperatures. Thus when we discuss our model for the boson peak we should compare it to the Debye model and expect the peak to be created by acoustic modes.

4 Noncommutative fluid theory

The aim of this thesis is to introduce a disordered lattice-like model for glasses, even though glasses do not resemble a lattice. The trick is to make parts of the lattice noncommutative, which will result in an uncertainty for location, similar to the uncertainty of canonical variables in quantum mechanics, thus making the lattice less fixed. Our model is based on the works of Polychronakos, Jackiw, Pi, Susskind and others [28–31] on noncommutative fluids. We will cover some of the noncommutative fluid theory shortly after introducing the formalism.

The noncommutativity in fluid theory means using the noncommutative geometry greatly developed by Alain Connes. In physics, noncommutative geometry has mostly been tied to the study of space-time, but the language has found its way to condensed matter theory too. Noncommutative spaces have been used for quantizing spacetime since Snyder’s Quantized Space-Time [32] and such geometries arise from certain limits in string theory [33]. In condensed matter noncommutativity has been used for studying, for example, the quantum Hall effect [31] and insulators [34].

4.1 Noncommutative geometry

Fairly little noncommutative geometry is needed in this thesis, but it is reasonable to give a short introduction to the subject. A good introduction would need to be rather lengthy, so we will not prove results and the introduction will be left a bit abstract.

The background of noncommutative geometry is in C*-algebras. A C*-algebra is a unital Banach algebra on \mathbb{C} defined with an involution $x \rightarrow x^*$ s.t. $\|x\|^2 = \|x^*x\|$. The square of the norm $\|x\|^2$ is the spectral radius i.e. the largest absolute value of the eigenvalues of x , so it is a spectral property. As usual, an element x is self-adjoint if $x^* = x$ and unitary if $x^{-1} = x^*$. C* algebras are important both in classical and quantum mechanics.

In physics the space of the elements x is the phase space. The Gelfand-Naimark theorem gives an equivalence between C*-algebras and the geometry of the phase space and thus gives a geometric approach to the algebra [35]. The theorem is an important starting point in noncommutative geometry.

The basic elements in noncommutative geometry are observables as in quantum mechanics. The observables obey a noncommutative C*-algebra, and the irreducible representations of the algebra form a noncommutative space, so in the physics context we are talking of noncommutative C*-algebras operating on Hilbert spaces.

Noncommutative geometry gives a common language and unifies various topics in physics. In addition to being useful in space-time and the condensed matter subjects just mentioned, the formalism unifies for example gauge fields, membranes, matrix models and many-body systems [28].

4.1.1 Noncommuting coordinates

A good starting point for noncommutative spaces in physics is turning coordinates into operators that have a small commutator similarly to the canonical variables in quantum mechanics:

$$[x_\mu, x_\nu] = i\theta_{\mu\nu}. \quad (4.1)$$

The product of coordinates is still associative. In flat noncommutative spaces the antisymmetric tensor θ is taken to commute with the coordinates, as will be done here, so it will consist of constant c-numbers of dimension $[length]^2$. In some cases with even dimensions [30] θ has an inverse $\omega_{\mu\nu} = (\theta^{-1})_{\mu\nu}$.

Changing the coordinate system changes of course θ and the commutation rules. This way the space can be divided into two-dimensional noncommutative subspaces that commute with each other, plus into possible additional commuting coordinates [28]. Thus there will be $2n$ noncommuting coordinates and $d - 2n$ commuting ones, where d is the dimension of the whole space. Then the inverse $\omega_{\mu\nu} = (\theta^{-1})_{\mu\nu}$ if μ and ν are noncommuting coordinates, and for other indices $\omega_{\mu\nu}$ will be set zero.

Take as an example a three dimensional noncommuting space with

$$\theta = \begin{pmatrix} 0 & \theta_{12} & \theta_{31} \\ -\theta_{12} & 0 & \theta_{23} \\ -\theta_{31} & -\theta_{23} & 0 \end{pmatrix}. \quad (4.2)$$

The coordinates can be changed so that there is an even amount of noncommuting coordinates, and now the only possible nonzero even amount is two, so with a change of coordinates θ should be able to be written in the form

$$\theta' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \theta_\alpha \\ 0 & -\theta_\alpha & 0 \end{pmatrix}, \quad (4.3)$$

where θ_α is a new noncommutativity parameter. Indeed if the old coordinates are x_1, x_2 and x_3 , and we define the coordinates $y_1 = \theta_{23}x_1 + \theta_{31}x_2 + \theta_{12}x_3$, $y_2 = \theta_{23}x_1 - \theta_{31}x_2$ and $y_3 = \theta_{23}x_1 - \theta_{12}x_3$, then y_2 and y_3 do not commute with each other, but they both commute with y_1 , and the commutation relations are described by

$$\theta' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \theta_{12}\theta_{23}\theta_{31} \\ 0 & -\theta_{12}\theta_{23}\theta_{31} & 0 \end{pmatrix}. \quad (4.4)$$

The noncommutative space is a representation of the operator algebra defined by (4.1). For real spaces the operators x_μ are Hermitian, and the imaginary unit serves to make the commutator anti-Hermitian. The eigenvalues of the operators are possible values of the coordinates in the representation. However, all of the coordinate operators cannot be diagonalized simultaneously [28], so all of

the coordinates in the representation space cannot be given a value simultaneously. Therefore points cannot be defined in the representation space, and the space gets a similar blurring as the canonical variables in quantum mechanics.

It is important to notice that taking the limit $\theta \rightarrow 0$ gives a commutative limit of the theory. This shall be useful later on after constructing our glass model, where taking the commutative limit yields a normal crystal lattice. We shall discuss later the meaning of θ in our system.

4.2 Fluid mechanics

[31] There are two main formulations for fluid mechanics called the Euler and Lagrange formulations. The difference between the two approaches is that in the Euler description the fluid is studied from a fixed frame of reference and the variables are written as functions of just space and time, whereas in the Lagrange formulation variables are written for specific particles of the fluid with the help of comoving coordinates. We are interested in the Lagrange formulation.

Let the Lagrangian for a fluid with n particles of mass m be

$$L = \sum_{i=1}^n \frac{m\dot{\mathbf{X}}_i^2}{2} - U(\mathbf{X}), \quad (4.5)$$

where $\dot{\mathbf{X}}_i$ tells the velocity of each particle and U is the potential governing the motion at point \mathbf{X} . In order to get to the proper Lagrange formulation we will pass to the continuum limit, where the index i of particles is replaced by continuous coordinates \mathbf{x} that act as labels for the particles. The coordinates \mathbf{X} become vector fields $\mathbf{X}(t, \mathbf{x})$. The initial value of the coordinates is usually chosen to be $\mathbf{X}(0, \mathbf{x}) = \mathbf{x}$, as will be done here, so that the comoving coordinates \mathbf{x} tell the initial position of each particle. Thus summing over particles can be done by integration over the x space. An easy way to think of the coordinates is with the parametrization

$$\mathbf{X}(t, \mathbf{x}) = \mathbf{x} + \mathbf{a}(t, \mathbf{x}), \quad (4.6)$$

where the deviation \mathbf{a} tells how far the particle has moved from its initial location \mathbf{x} .

Let us choose the coordinates so that the number of particles per unit area of x space is given by the constant ρ_0 . Now the density of particles in the physical X space is

$$\rho = \rho_0 \left| \det \frac{\partial x_i}{\partial X_j} \right|. \quad (4.7)$$

Assuming that the system reaches equilibrium and the potential vanishes when $\rho = \rho_0$, and that the temperature of the system is zero so that the potential cannot depend on temperature [31, page 3 footnote], the Lagrangian can be written as

$$L = \int d\mathbf{x} \rho_0 \left[\frac{m\dot{\mathbf{X}}^2(t, \mathbf{x})}{2} - V \left(\rho_0 \left| \det \frac{\partial x_i}{\partial X_j} \right| \right) \right]. \quad (4.8)$$

The zero temperature assumption is fine for our use, since the boson peak for which we shall need the techniques of fluid mechanics is a very low-temperature phenomenon.

The Lagrangian must obviously be invariant under relabeling of the particles by choosing the coordinates \mathbf{x} differently, as long as the density is left unchanged, so it has a symmetry. More precisely this means invariance under unit Jacobian diffeomorphisms of the x space, i.e. changes of variables from \mathbf{x} to \mathbf{x}' for which

$$\det \frac{\partial x'_i}{\partial x_j} = 1. \quad (4.9)$$

Let the transformation

$$\mathbf{x} \rightarrow \mathbf{x} + \delta\mathbf{x}, \quad (4.10)$$

where $\delta\mathbf{x}$ is infinitesimal, be such a diffeomorphism. This means that

$$\nabla \cdot \delta\mathbf{x} = 0, \quad (4.11)$$

so the transformation $\delta\mathbf{x}$ must be transverse. In other words it can be written as the derivative of some gauge function f as

$$\delta\mathbf{x} = \nabla \times f. \quad (4.12)$$

Now we will make a step towards noncommutativity. Let us define the Poisson bracket

$$\{g, h\} = \theta_{ij} \frac{\partial g}{\partial x^i} \frac{\partial h}{\partial x^j}, \quad (4.13)$$

where θ is an antisymmetric tensor whose diagonal values are zero. For the coordinates \mathbf{x} the bracket is

$$\{x_i, x_j\} = \theta_{ij}. \quad (4.14)$$

Assuming that θ is not singular we can now parametrize the fields \mathbf{X} as

$$X_i(t, \mathbf{x}) = x_i + \theta_{ij} A^j(t, \mathbf{x}), \quad (4.15)$$

so their bracket will be

$$\{X_i, X_j\} = \theta_{ij} + \theta_{ik} \theta_{jl} \left(\frac{\partial A_l}{\partial x_k} - \frac{\partial A_k}{\partial x_l} + \{A_k, A_l\} \right) \equiv \theta_{ij} + \theta_{ik} \theta_{jl} F^{jl}, \quad (4.16)$$

where F is a gauge field. F resembles a conventional Abelian gauge field when the deviation \mathbf{A} is small.

The Poisson brackets can be used to rewrite for example the diffeomorphisms (4.12) and the fluid density [28–30]. Using this formulation provides an easy way to transition to noncommutative fluids. To make the fluid noncommutative we will replace the Poisson brackets by i times a commutator, similarly to the transition from classical mechanics to quantum mechanics. This will result in a quantification of the x space, so the new noncommutative theory will describe

systems with “fuzzy” coordinates. The Poisson bracket of the comoving coordinates in (4.14) will be replaced by the commutator in (4.1), so our system will be described by a noncommutative geometry.

Note that the values of the noncommutativity parameter θ are still arbitrary. The standard choice is to make all of its off-diagonal values equal and to relate them to the inverse of the two-dimensional fluid density as

$$\theta_{12} = \theta_{23} = \theta_{31} \equiv \theta = \frac{1}{2\pi\rho_0}. \quad (4.17)$$

The choice can be justified by thinking of the quantization of coordinate space brought by the noncommutativity. In quantum mechanics the canonical commutator $[x, p] = i\hbar$ makes the phase space quantized in cells of area $2\pi\hbar$. Similarly the commutator $[x_i, x_j] = i\theta$ makes the coordinate space quantized in cells of area $2\pi\theta$. If we want each particle of the fluid to occupy one cell of the x space, the density ρ_0 will be exactly the density in (4.17).

This was our aim when introducing the fluid formalism. We want our glass model to be a disordered version of a crystal lattice, so a “fuzzy” coordinate space where points cannot be defined is desirable. This kind of fluid formalism has already been used for describing, for example, the quantum Hall effect [31].

5 The glass model

[14] Now we have gathered the tools needed for our glass model. The idea is to describe the glass using the three dimensional lattice in subsection (3.2), and to treat some of the particles as if they were particles of a nonmoving noncommutative fluid. This is physically very sound, since the disorder in a glass is a remnant of the liquid form the matter was in before its quick cooling.

If the fluid particles do not move, then in the parametrization of the Lagrange fluid

$$\mathbf{X}(t, \mathbf{x}) = \mathbf{x} + \mathbf{a}(t, \mathbf{x}) \quad (5.1)$$

we can set the deviation $\mathbf{a}(t, \mathbf{x})$ to zero, so the coordinates will be described by their initial values \mathbf{x} . Thus in the noncommutative setting the coordinates \mathbf{X} will inherit the commutator (4.1) so that

$$[X_i, X_j] = i\theta_{ij}. \quad (5.2)$$

In addition we will use the quantum mechanical canonical commutators

$$[X_i, p_j] = i\hbar\delta_{ij}, \quad (5.3)$$

although \hbar will be set to 1.

Since there is no actual lattice structure in glasses, we can choose some of the parameters in the system quite simply. The idea is to place a lattice *on* the glass, instead of finding a lattice structure, so our system should not depend too much on how we orient the lattice. In other words, we should try to make the system as isotropic as possible. This means that the distance between lattice sites should be the same in all directions, so the absolute values of the primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 will be equal. Similarly the noncommutativity parameter should be the same for all directions, i.e. $\theta_{12} = \theta_{23} = \theta_{31} \equiv \theta$. Isotropy will be discussed more when we calculate the dispersion relations in the glass.

We shall not make every lattice site noncommutative. Equations of motion in the lattice will be calculated using only nearest neighbour interactions, so the lattice will already get disordered by treating every other particle in the glass with noncommutative coordinates. This means that for each particle with commuting coordinates the nearest neighbours will have noncommuting coordinates, so the distance between all of the particles in the system will be disordered. The whole system will have two kinds of Hamiltonians, ones for the particles with commuting coordinates and ones for the particles with noncommuting coordinates. The whole system will be described by a sum of all of the Hamiltonians, so we will have to consider both kinds of Hamiltonians when deriving quantities for the whole glass. We shall call the Hamiltonians for particles with commutative coordinates ordered, and the Hamiltonians for particles with noncommutative coordinates disordered. Similarly we shall call the particles and lattice sites ordered and disordered. Note that by a particle having noncommutative coordinates we mean that the particles coordinates will not commute with *each other*, but they will commute with the coordinates of other particles. All of this will become clear in the calculation.

Because of the noncommutativity, the system cannot be solved completely similarly to usual crystals. Hamilton's equations will not give correct results in noncommutative spaces, so time derivatives of coordinates and momenta will have to be calculated differently. In noncommutative quantum mechanics, differentials are defined by commutators, and derivatives are given similarly to the Heisenberg picture in quantum mechanics as

$$\frac{df}{dt} = i [H, f], \quad (5.4)$$

where H is the Hamiltonian of the system. [35] Calculating the time derivatives this way will prove to be effective in our calculations.

Calculating the commutators will be significantly easier after doing the transformation

$$x_i \rightarrow x_i - \epsilon_{ij} \frac{\theta}{2} p_j \quad (5.5)$$

called the Bopp shift for the noncommutative coordinates, where ϵ_{ij} is the Levi-Civita symbol and p_j is the momentum in the direction j . This is a mapping to a corresponding commutative coordinate system, so now the transformed coordinates will commute with each other [36]. In noncommutative quantum mechanics, where the commutator (4.1) applies, the Bopp shift appears for example in the Schrödinger equation [37]. This technique has been used in for example calculating the correction to the Lamb shift in noncommutative quantum electrodynamics [38].

After doing the transformation we could also calculate the equations of motion using Hamilton's equations, but we will use the Heisenberg version anyway. The only thing left to consider in the Heisenberg commutator is now the commutator of x and p , as will be seen.

5.1 Equations of motion

5.1.1 Ordered lattice sites

[14] The Hamiltonian for the point l, m, n in a three dimensional vibrating lattice is

$$\begin{aligned} H_{l,m,n} &= \frac{p_{u;l,m,n}^2 + p_{v;l,m,n}^2 + p_{w;l,m,n}^2}{2m} \\ &+ \frac{\zeta}{2} (u_{l,m,n} - u_{l+1,m,n})^2 + \frac{\zeta}{2} (u_{l,m,n} - u_{l-1,m,n})^2 \\ &+ \frac{\zeta}{2} (v_{l,m,n} - v_{l,m+1,n})^2 + \frac{\zeta}{2} (v_{l,m,n} - v_{l,m-1,n})^2 \\ &+ \frac{\zeta}{2} (w_{l,m,n} - w_{l,m,n+1})^2 + \frac{\zeta}{2} (w_{l,m,n} - w_{l,m,n-1})^2, \quad (5.6) \end{aligned}$$

where p describes the momenta to the directions of the displacements u, v and w and the indices l, m and n tell the lattice site whose momentum and displacement we are considering.

Now every other particle in the lattice is treated using noncommutative coordinates, so that the displacements with indices l, m, n commute with each other and the displacements where one of the indices l, m and n has been shifted by ± 1 do not commute with each other. Had one of the indices of a displacement been changed by ± 2 , or had two of the indices been changed by ± 1 , the displacement would again commute with other displacements.

We will start by doing the Bopp shift on the noncommutative displacements, that is, do the changes of variables

$$u_{l\pm 1,m,n} \rightarrow u_{l\pm 1,m,n} - \frac{\theta}{2} p_{v;l\pm 1,m,n} + \frac{\theta}{2} p_{w;l\pm 1,m,n} \quad (5.7)$$

$$v_{l,m\pm 1,n} \rightarrow v_{l,m\pm 1,n} - \frac{\theta}{2} p_{w;l,m\pm 1,n} + \frac{\theta}{2} p_{u;l,m\pm 1,n} \quad (5.8)$$

$$w_{l,m,n} \rightarrow w_{l,m,n\pm 1} - \frac{\theta}{2} p_{u;l,m,n\pm 1} + \frac{\theta}{2} p_{v;l,m,n\pm 1}. \quad (5.9)$$

Now the Hamiltonian is

$$\begin{aligned} H_{l,m,n} &= \frac{p_{u;l,m,n}^2 + p_{v;l,m,n}^2 + p_{w;l,m,n}^2}{2m} \\ &+ \frac{\zeta}{2} \left(u_{l,m,n} - u_{l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - \frac{\theta}{2} p_{w;l+1,m,n} \right)^2 \\ &+ \frac{\zeta}{2} \left(u_{l,m,n} - u_{l-1,m,n} + \frac{\theta}{2} p_{v;l-1,m,n} - \frac{\theta}{2} p_{w;l-1,m,n} \right)^2 \\ &+ \frac{\zeta}{2} \left(v_{l,m,n} - v_{l,m+1,n} + \frac{\theta}{2} p_{w;l,m+1,n} - \frac{\theta}{2} p_{u;l,m+1,n} \right)^2 \\ &+ \frac{\zeta}{2} \left(v_{l,m,n} - v_{l,m-1,n} + \frac{\theta}{2} p_{w;l,m-1,n} - \frac{\theta}{2} p_{u;l,m-1,n} \right)^2 \\ &+ \frac{\zeta}{2} \left(w_{l,m,n} - w_{l,m,n+1} + \frac{\theta}{2} p_{u;l,m,n+1} - \frac{\theta}{2} p_{v;l,m,n+1} \right)^2 \\ &+ \frac{\zeta}{2} \left(w_{l,m,n} - w_{l,m,n-1} + \frac{\theta}{2} p_{u;l,m,n-1} - \frac{\theta}{2} p_{v;l,m,n-1} \right)^2. \end{aligned} \quad (5.10)$$

The equations of motion for the particles in ordered lattice sites are calculated using the ordered Hamiltonian above, so that

$$\dot{u}_{l,m,n} = i[H_{l,m,n}, u_{l,m,n}]. \quad (5.11)$$

We will soon introduce also the disordered Hamiltonian.

After doing the Bopp shift, the only part of the Hamiltonian that does not commute with $u_{l,m,n}$ is $p_{u;l,m,n}^2$, so the commutator yields the usual result

$$\dot{u}_{l,m,n} = i \left[\frac{p_{u;l,m,n}^2}{2m}, u_{l,m,n} \right] = -\frac{i}{2m} [u_{l,m,n}, p_{u;l,m,n}^2] = \frac{p_{u;l,m,n}}{m}. \quad (5.12)$$

For the second time derivative we get

$$\begin{aligned}
\ddot{u}_{l,m,n} &= i [H_{l,m,n}, \dot{u}_{l,m,n}] = \frac{i}{m} [H_{l,m,n}, p_{u;l,m,n}] \\
&= \frac{\zeta}{2m} \left[\left(u_{l,m,n} - u_{l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - \frac{\theta}{2} p_{w;l+1,m,n} \right)^2 \right. \\
&\quad \left. + \left(u_{l,m,n} - u_{l-1,m,n} + \frac{\theta}{2} p_{v;l-1,m,n} - \frac{\theta}{2} p_{w;l-1,m,n} \right)^2, p_{u;l,m,n} \right] \\
&= -\frac{\zeta}{m} (2u_{l,m,n} - u_{l+1,m,n} - u_{l-1,m,n}) \\
&\quad - \frac{\zeta\theta}{2m} (p_{v;l+1,m,n} - p_{w;l+1,m,n} + p_{v;l-1,m,n} - p_{w;l-1,m,n}). \quad (5.13)
\end{aligned}$$

To solve this equation we need an expression for the momenta of the lattice points for which the first index is $l \pm 1$. To get that we need the Hamiltonian of those lattice points. Consider the point $l + 1, m, n$, for which the Hamiltonian is

$$\begin{aligned}
H_{l+1,m,n} &= \frac{p_{u;l+1,m,n}^2 + p_{v;l+1,m,n}^2 + p_{w;l+1,m,n}^2}{2m} \\
&\quad + \frac{\zeta}{2} (u_{l+1,m,n} - u_{l+2,m,n})^2 + \frac{\zeta}{2} (u_{l+1,m,n} - u_{l,m,n})^2 \\
&\quad + \frac{\zeta}{2} (v_{l+1,m,n} - v_{l+1,m+1,n})^2 + \frac{\zeta}{2} (v_{l+1,m,n} - v_{l+1,m-1,n})^2 \\
&\quad + \frac{\zeta}{2} (w_{l+1,m,n} - w_{l+1,m,n+1})^2 + \frac{\zeta}{2} (w_{l+1,m,n} - w_{l+1,m,n-1})^2. \quad (5.14)
\end{aligned}$$

Again we want to do a Bopp shift for the lattice points where only one of the indices has been shifted by ± 1 . The shift is the same as it was for the previous

Hamiltonian, so we get

$$\begin{aligned}
H_{l+1,m,n} &= \frac{p_{u;l+1,m,n}^2 + p_{v;l+1,m,n}^2 + p_{w;l+1,m,n}^2}{2m} \\
&+ \frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l+2,m,n} \right)^2 \\
&+ \frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l,m,n} \right)^2 \\
&+ \frac{\zeta}{2} \left(v_{l+1,m,n} - \frac{\theta}{2} p_{w;l+1,m,n} + \frac{\theta}{2} p_{u;l+1,m,n} - v_{l+1,m+1,n} \right)^2 \\
&+ \frac{\zeta}{2} \left(v_{l+1,m,n} - \frac{\theta}{2} p_{w;l+1,m,n} + \frac{\theta}{2} p_{u;l+1,m,n} - v_{l+1,m-1,n} \right)^2 \\
&+ \frac{\zeta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n+1} \right)^2 \\
&+ \frac{\zeta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n-1} \right)^2.
\end{aligned} \tag{5.15}$$

As stated earlier, the displacements where the indices have been shifted by an even amount describe ordered particles.

Lets first calculate the time derivative of $v_{l+1,m,n}$.

$$\begin{aligned}
\dot{v}_{l+1,m,n} &= i [H, v_{l+1,m,n}] \\
&= i \left[\frac{p_{v;l+1,m,n}^2}{2m} + \frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l+2,m,n} \right)^2 \right. \\
&\quad + \frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l,m,n} \right)^2 \\
&\quad + \frac{\zeta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n+1} \right)^2 \\
&\quad \left. + \frac{\zeta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n-1} \right)^2, v_{l+1,m,n} \right],
\end{aligned} \tag{5.16}$$

which equals

$$\begin{aligned}
\dot{v}_{l+1,m,n} &= \frac{p_{v;l+1,m,n}}{m} - \frac{\zeta\theta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l+2,m,n} \right) \\
&\quad - \frac{\zeta\theta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l,m,n} \right) \\
&\quad + \frac{\zeta\theta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n+1} \right) \\
&\quad + \frac{\zeta\theta}{2} \left(w_{l+1,m,n} - \frac{\theta}{2} p_{u;l+1,m,n} + \frac{\theta}{2} p_{v;l+1,m,n} - w_{l+1,m,n-1} \right) \\
&= \frac{p_{v;l+1,m,n}}{m} + \frac{\zeta\theta}{2} (u_{l,m,n} - 2u_{l+1,m,n} + u_{l+2,m,n}) \\
&\quad + \frac{\zeta\theta}{2} (+2w_{l+1,m,n} - w_{l+1,m,n+1} - w_{l+1,m,n-1}) \\
&\quad + \frac{\zeta\theta^2}{4} (4p_{v;l+1,m,n} - p_{w;l+1,m,n} - p_{u;l+1,m,n}). \tag{5.17}
\end{aligned}$$

This gives us the following equation for $p_{v;l+1,m,n}$

$$\begin{aligned}
p_{v;l+1,m,n} &= m\dot{v}_{l+1,m,n} - \frac{m\zeta\theta}{2} (u_{l,m,n} - 2u_{l+1,m,n} + u_{l+2,m,n}) \\
&\quad - \frac{m\zeta\theta}{2} (2w_{l+1,m,n} - w_{l+1,m,n+1} - w_{l+1,m,n-1}) + \mathcal{O}(\theta^2). \tag{5.18}
\end{aligned}$$

Doing the same calculation for $\dot{w}_{l+1,m,n}$ gives us the equation for $p_{w;l+1,m,n}$.

$$\begin{aligned}
p_{w;l+1,m,n} &= m\dot{w}_{l+1,m,n} - \frac{m\zeta\theta}{2} (-u_{l,m,n} + 2u_{l+1,m,n} - u_{l+2,m,n}) \\
&\quad - \frac{m\zeta\theta}{2} (-2v_{l+1,m,n} + v_{l+1,m+1,n} + v_{l+1,m-1,n}) + \mathcal{O}(\theta^2). \tag{5.19}
\end{aligned}$$

The equations for $p_{v;l-1,m,n}$ and $p_{w;l-1,m,n}$ are derived similarly using $H_{l-1,m,n}$. $H_{l-1,m,n}$ is completely similar to $H_{l+1,m,n}$ except that all the l indices will be shifted by -2 . Thus we get

$$\begin{aligned}
p_{v;l-1,m,n} &= m\dot{v}_{l-1,m,n} - \frac{m\zeta\theta}{2} (u_{l,m,n} - 2u_{l-1,m,n} + u_{l-2,m,n}) \\
&\quad - \frac{m\zeta\theta}{2} (2w_{l-1,m,n} - w_{l-1,m,n+1} - w_{l-1,m,n-1}) + \mathcal{O}(\theta^2) \tag{5.20}
\end{aligned}$$

and

$$\begin{aligned}
p_{w;l-1,m,n} &= m\dot{w}_{l-1,m,n} - \frac{m\zeta\theta}{2} (-u_{l,m,n} + 2u_{l-1,m,n} - u_{l-2,m,n}) \\
&\quad - \frac{m\zeta\theta}{2} (-2v_{l-1,m,n} + v_{l-1,m+1,n} + v_{l-1,m-1,n}) + \mathcal{O}(\theta^2). \tag{5.21}
\end{aligned}$$

Now we can solve $\ddot{u}_{l,m,n}$. Inserting the expressions for $p_{v;l+1,m,n}$, $p_{w;l+1,m,n}$, $p_{v;l-1,m,n}$ and $p_{w;l-1,m,n}$ into the expression for $\ddot{u}_{l,m,n}$ yields

$$\begin{aligned}
\ddot{u}_{l,m,n} = & -\frac{\zeta}{m} (2u_{l,m,n} - u_{l+1,m,n} - u_{l-1,m,n}) \\
& -\frac{\zeta\theta}{2} \dot{v}_{l+1,m,n} + \frac{\zeta^2\theta^2}{4} (u_{l,m,n} - 2u_{l+1,m,n} + u_{l+2,m,n}) \\
& + \frac{\zeta^2\theta^2}{4} (2w_{l+1,m,n} - w_{l+1,m,n+1} - w_{l+1,m,n-1}) \\
& + \frac{\zeta\theta}{2} \dot{w}_{l+1,m,n} - \frac{\zeta^2\theta^2}{4} (-u_{l,m,n} + 2u_{l+1,m,n} - u_{l+2,m,n}) \\
& - \frac{\zeta^2\theta^2}{4} (-2v_{l+1,m,n} + v_{l+1,m+1,n} + v_{l+1,m-1,n}) \\
& - \frac{\zeta\theta}{2} \dot{v}_{l-1,m,n} + \frac{\zeta^2\theta^2}{4} (u_{l,m,n} - 2u_{l-1,m,n} + u_{l-2,m,n}) \\
& + \frac{\zeta^2\theta^2}{4} (2w_{l-1,m,n} - w_{l-1,m,n+1} - w_{l-1,m,n-1}) \\
& + \frac{\zeta\theta}{2} \dot{w}_{l-1,m,n} - \frac{\zeta^2\theta^2}{4} (-u_{l,m,n} + 2u_{l-1,m,n} - u_{l-2,m,n}) \\
& - \frac{\zeta^2\theta^2}{4} (-2v_{l-1,m,n} + v_{l-1,m+1,n} + v_{l-1,m-1,n}) + \mathcal{O}(\theta^3). \quad (5.22)
\end{aligned}$$

Arranging the terms a bit leads to the equation of motion we were looking for

$$\begin{aligned}
\ddot{u}_{l,m,n} = & -\frac{\zeta}{m} (2u_{l,m,n} - u_{l+1,m,n} - u_{l-1,m,n}) \\
& -\frac{\zeta\theta}{2} (\dot{v}_{l+1,m,n} + \dot{v}_{l-1,m,n} - \dot{w}_{l+1,m,n} - \dot{w}_{l-1,m,n}) \\
& + \frac{\zeta^2\theta^2}{4} (4u_{l,m,n} - 4u_{l+1,m,n} - 4u_{l-1,m,n} + 2u_{l+2,m,n} + 2u_{l-2,m,n}) \\
& + \frac{\zeta^2\theta^2}{4} (2v_{l+1,m,n} - v_{l+1,m+1,n} - v_{l+1,m-1,n}) \\
& + \frac{\zeta^2\theta^2}{4} (2v_{l-1,m,n} - v_{l-1,m+1,n} - v_{l-1,m-1,n}) \\
& + \frac{\zeta^2\theta^2}{4} (2w_{l+1,m,n} - w_{l+1,m,n+1} - w_{l+1,m,n-1}) \\
& + \frac{\zeta^2\theta^2}{4} (2w_{l-1,m,n} - w_{l-1,m,n+1} - w_{l-1,m,n-1}) + \mathcal{O}(\theta^3). \quad (5.23)
\end{aligned}$$

5.1.2 Disordered lattice sites

[14] Next we want to solve the equation of motion for the disordered lattice sites. Similarly to the equation of $\dot{v}_{l+1,m,n}$ in (5.17), we get an equation for $\dot{u}_{l+1,m,n}$

as

$$\begin{aligned}
\dot{u}_{l+1,m,n} &= \frac{p_{u;l+1,m,n}}{m} + \frac{\zeta\theta}{2} (2v_{l+1,m,n} - v_{l+1,m+1,n} - v_{l+1,m-1,n}) \\
&\quad + \frac{\zeta\theta}{2} (-2w_{l+1,m,n} + w_{l+1,m,n+1} + w_{l+1,m,n-1}) \\
&= + \frac{\zeta\theta^2}{2} (2p_{u;l+1,m,n} - p_{v;l+1,m,n} - p_{w;l+1,m,n}). \tag{5.24}
\end{aligned}$$

With the help of this we get an equation for the momentum

$$\begin{aligned}
p_{u;l+1,m,n} &= \frac{1}{1/m + \zeta\theta^2} \left(\dot{u}_{l+1,m,n} - \frac{\zeta\theta}{2} (2v_{l+1,m,n} - v_{l+1,m+1,n} - v_{l+1,m-1,n} \right. \\
&\quad \left. - 2w_{l+1,m,n} + w_{l+1,m,n+1} + w_{l+1,m,n-1}) \right. \\
&\quad \left. + \frac{\zeta\theta^2}{2} (p_{v;l+1,m,n} + p_{w;l+1,m,n}) \right). \tag{5.25}
\end{aligned}$$

Next we want to derive the time derivatives of the momenta. Using the disordered Hamiltonian $\dot{p}_{u+1;l,m,n}$ is

$$\begin{aligned}
\dot{p}_{u+1;l,m,n} &= i \left[\frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l+2,m,n} \right)^2 \right. \\
&\quad \left. + \frac{\zeta}{2} \left(u_{l+1,m,n} - \frac{\theta}{2} p_{v;l+1,m,n} + \frac{\theta}{2} p_{w;l+1,m,n} - u_{l,m,n} \right)^2, p_{u;l,m,n} \right] \\
&= -\zeta (2u_{l+1,m,n} - u_{l+2,m,n} - u_{l,m,n} - \theta p_{v;l+1,m,n} + \theta p_{w;l+1,m,n}). \tag{5.26}
\end{aligned}$$

Similarly

$$\dot{p}_{v+1;l,m,n} = -\zeta (2v_{l+1,m,n} - v_{l+1,m+1,n} - v_{l+1,m-1,n} - \theta p_{w;l+1,m,n} + \theta p_{u;l+1,m,n}) \tag{5.27}$$

and

$$\dot{p}_{w+1;l,m,n} = -\zeta (2w_{l+1,m,n} - w_{l+1,m+1,n} - w_{l+1,m-1,n} - \theta p_{u;l+1,m,n} + \theta p_{v;l+1,m,n}). \tag{5.28}$$

Inserting the expression for $p_{u;l+1,m,n}$ to the expression for $\dot{p}_{u+1;l,m,n}$ gives us the equation

$$\begin{aligned}
&\frac{1}{1/m + \zeta\theta^2} \left(\ddot{u}_{l+1,m,n} - \frac{\zeta\theta}{2} (2\dot{v}_{l+1,m,n} - \dot{v}_{l+1,m+1,n} - \dot{v}_{l+1,m-1,n} \right. \\
&\quad \left. - 2\dot{w}_{l+1,m,n} + \dot{w}_{l+1,m,n+1} + \dot{w}_{l+1,m,n-1}) + \frac{\zeta\theta^2}{2} (\dot{p}_{v;l+1,m,n} + \dot{p}_{w;l+1,m,n}) \right) \\
&= -\zeta (2u_{l+1,m,n} - u_{l+2,m,n} - u_{l,m,n} - \theta p_{v;l+1,m,n} + \theta p_{w;l+1,m,n}). \tag{5.29}
\end{aligned}$$

From here we can solve $\ddot{u}_{l+1,m,n}$.

$$\begin{aligned}
\ddot{u}_{l+1,m,n} &= -\left(\frac{\zeta}{m} + \zeta^2\theta^2\right) (2u_{l+1,m,n} - u_{l+2,m,n} - u_{l,m,n}) \\
&\quad + \frac{\zeta\theta}{m} (p_{v;l+1,m,n} - p_{w;l+1,m,n}) \\
&\quad + \frac{\zeta\theta}{2} (2\dot{v}_{l+1,m,n} - \dot{v}_{l+1,m+1,n} - \dot{v}_{l+1,m-1,n}) \\
&\quad + \frac{\zeta\theta}{2} (-2\dot{w}_{l+1,m,n} + \dot{w}_{l+1,m,n+1} + \dot{w}_{l+1,m,n-1}) \\
&\quad - \frac{\zeta\theta^2}{2} (\dot{p}_{v;l+1,m,n} + \dot{p}_{w;l+1,m,n}) + \mathcal{O}(\theta^3). \tag{5.30}
\end{aligned}$$

Now we just have to insert the expressions for the momenta and their time derivatives to get the equation of motion

$$\begin{aligned}
\ddot{u}_{l+1,m,n} &= -\left(\frac{\zeta}{m} + \zeta^2\theta^2\right) (2u_{l+1,m,n} - u_{l+2,m,n} - u_{l,m,n}) \\
&\quad + \zeta\theta (\dot{v}_{l+1,m,n} - \dot{w}_{l+1,m,n}) \\
&\quad - \frac{\zeta^2\theta^2}{2} (u_{l,m,n} - 2u_{l+1,m,n} + u_{l+2,m,n}) \\
&\quad - \frac{\zeta^2\theta^2}{2} (2w_{l+1,m,n} - w_{l+1,m,n+1} - w_{l+1,m,n-1}) \\
&\quad + \frac{\zeta^2\theta^2}{2} (-u_{l,m,n} + 2u_{l+1,m,n} - u_{l+2,m,n}) \\
&\quad + \frac{\zeta^2\theta^2}{2} (-2v_{l+1,m,n} + v_{l+1,m+1,n} + v_{l+1,m-1,n}) \\
&\quad + \frac{\zeta\theta}{2} (2\dot{v}_{l+1,m,n} - \dot{v}_{l+1,m+1,n} - \dot{v}_{l+1,m-1,n}) \\
&\quad + \frac{\zeta\theta}{2} (-2\dot{w}_{l+1,m,n} + \dot{w}_{l+1,m,n+1} + \dot{w}_{l+1,m,n-1}) \\
&\quad + \frac{\zeta^2\theta^2}{2} (2v_{l+1,m,n} - v_{l+1,m+1,n} - v_{l+1,m-1,n}) \\
&\quad + \frac{\zeta^2\theta^2}{2} (2w_{l+1,m,n} - w_{l+1,m+1,n} - w_{l+1,m-1,n}) + \mathcal{O}(\theta^3). \tag{5.31}
\end{aligned}$$

Again with a bit of rearranging and cancelling of terms we get the simple expression

$$\begin{aligned}
\ddot{u}_{l+1,m,n} &= -\frac{\zeta}{m} (2u_{l+1,m,n} - u_{l+2,m,n} - u_{l,m,n}) \\
&\quad + \frac{\zeta\theta}{2} (4\dot{v}_{l+1,m,n} - \dot{v}_{l+1,m+1,n} - \dot{v}_{l+1,m-1,n}) \tag{5.32}
\end{aligned}$$

$$\begin{aligned}
&\quad + \frac{\zeta\theta}{2} (-4\dot{w}_{l+1,m,n} + \dot{w}_{l+1,m,n+1} + \dot{w}_{l+1,m,n-1}) + \mathcal{O}(\theta^3). \tag{5.33}
\end{aligned}$$

5.2 Density of states

Next we want to solve the density of states from the equations of motion we derived. The main interest is to look for Van Hove singularities and to see if they are related to the frequencies of the boson peak.

5.2.1 Ordered lattice site

[14] Now we want to solve the equation of motion given in (5.23). The situation is very similar to the usual three dimensional lattice discussed in subsection (3.2), so we will try the same ansatz

$$\begin{aligned} u_{l,m,n} &= U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}}, \\ v_{l,m,n} &= V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \text{ and} \\ w_{l,m,n} &= W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}}, \end{aligned} \quad (5.34)$$

where again U , V and W are constants telling the amplitude of the wave in different directions, $\mathbf{k} = (k_1, k_2, k_3)$ is the wave vector, $\mathbf{L}_{l,m,n} = l\mathbf{a}_1 + m\mathbf{a}_2 + n\mathbf{a}_3$ is the translation vector telling the location of the lattice site and ω is the frequency of the wave. Note that the absolute values of the primitive translation vectors \mathbf{a}_1 , \mathbf{a}_2 and \mathbf{a}_3 are equal, as explained in the beginning of this chapter, so $\mathbf{k}\cdot\mathbf{L} = a(lk_1 + mk_2 + nk_3)$, where a is the absolute value discussed.

The ansatz results in the equation

$$\begin{aligned} & -\omega^2 U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ = & -\omega_0^2 (2 - e^{iak_1} - e^{-iak_1}) U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} - i \frac{K\omega}{2} (e^{iak_1} + e^{-iak_1}) V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ & + i \frac{K\omega}{2} (e^{iak_1} + e^{-iak_1}) W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ & + \frac{K^2}{4} (4 - 4e^{iak_1} - 4e^{-iak_1} + 2e^{2iak_1} + 2e^{-2iak_1}) U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ & + \frac{K^2}{4} (2e^{iak_1} - e^{i(ak_1+ak_2)} - e^{i(ak_1-ak_2)}) V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ & + \frac{K^2}{4} (2e^{-iak_1} - e^{i(-ak_1+ak_2)} - e^{-i(ak_1+ak_2)}) V e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} \\ & + \frac{K^2}{4} (2e^{iak_1} - e^{i(ak_1+ak_3)} - e^{i(ak_1-ak_3)}) W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}}, \\ & + \frac{K^2}{4} (2e^{-iak_1} - e^{i(-ak_1+ak_3)} - e^{-i(ak_1+ak_3)}) W e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} + \mathcal{O}(\theta^3), \end{aligned} \quad (5.35)$$

where we have defined the constants $\omega_0 = \sqrt{\frac{\zeta}{m}}$ and $K = \zeta\theta$ to shorten the notation.

Dividing with $e^{i\omega t}e^{i\mathbf{k}\cdot\mathbf{L}}$ and recognizing the cosines yields

$$\begin{aligned}
-\omega^2 U &= -2\omega_0^2 (1 - \cos(ak_1))U + iK\omega \cos(ak_1) (-V + W) \\
&\quad + \frac{K^2}{2} (2 - 4\cos(ak_1) + 2\cos(2ak_1))U \\
&\quad + K^2 (\cos(ak_1) - \cos(ak_1)\cos(ak_2))V \\
&\quad + K^2 (\cos(ak_1) - \cos(ak_1)\cos(ak_3))W + \mathcal{O}(\theta^3), \quad (5.36)
\end{aligned}$$

which after collecting terms with the same constant becomes

$$\begin{aligned}
0 &= \left\{ \omega^2 - 2\omega_0^2 (1 - \cos(ak_1)) + \frac{K^2}{2} (2 - 4\cos(ak_1) + 2\cos(2ak_1)) \right\} U \\
&\quad + \left\{ -iK\omega \cos(ak_1) + K^2 (\cos(ak_1) - \cos(ak_1)\cos(ak_2)) \right\} V \\
&\quad + \left\{ iK\omega \cos(ak_1) + K^2 (\cos(ak_1) - \cos(ak_1)\cos(ak_3)) \right\} W + \mathcal{O}(\theta^3). \quad (5.37)
\end{aligned}$$

We can yet simplify the equation by using the identity $\cos x = 1 - 2\sin^2 \frac{x}{2}$:

$$\begin{aligned}
0 &= \left\{ \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_1}{2} \right) + 2K^2 \left(2\sin^2 \left(\frac{ak_1}{2} \right) - \sin^2(ak_1) \right) \right\} U \\
&\quad + \left\{ -iK\omega \cos(ak_1) + 2K^2 \cos(ak_1) \sin^2 \left(\frac{ak_2}{2} \right) \right\} V \\
&\quad + \left\{ iK\omega \cos(ak_1) + 2K^2 \cos(ak_1) \sin^2 \left(\frac{ak_3}{2} \right) \right\} W + \mathcal{O}(\theta^3). \quad (5.38)
\end{aligned}$$

To get rid of the three constants U , V and W we need more equations. Thus we shall consider the equations for $\ddot{v}_{l,m,n}$ and $\ddot{w}_{l,m,n}$. Looking at our Hamiltonians we see that they are symmetric under the change $u \rightarrow v$, $v \rightarrow w$ and $w \rightarrow u$. Therefore the equations of motion for $\ddot{v}_{l,m,n}$ and $\ddot{w}_{l,m,n}$ are derived and solved completely similarly to $\ddot{u}_{l,m,n}$, so they must yield the same solution, except for changing U , V and W as well as k_1 , k_2 and k_3 in the same manner as u , v and w can be changed. Thus starting with $\ddot{v}_{l,m,n}$ we should get the equation

$$\begin{aligned}
0 &= \left\{ \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_2}{2} \right) + 2K^2 \left(2\sin^2 \left(\frac{ak_2}{2} \right) - \sin^2(ak_2) \right) \right\} V \\
&\quad + \left\{ -iK\omega \cos(ak_2) + 2K^2 \cos(ak_2) \sin^2 \left(\frac{ak_3}{2} \right) \right\} W \\
&\quad + \left\{ iK\omega \cos(ak_2) + 2K^2 \cos(ak_2) \sin^2 \left(\frac{ak_1}{2} \right) \right\} U + \mathcal{O}(\theta^3). \quad (5.39)
\end{aligned}$$

and from the equation for $\ddot{w}_{l,m,n}$ we get

$$\begin{aligned}
0 &= \left\{ \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_3}{2} \right) + 2K^2 \left(2 \sin^2 \left(\frac{ak_3}{2} \right) - \sin^2 (ak_3) \right) \right\} W \\
&+ \left\{ -iK\omega \cos (ak_3) + 2K^2 \cos (ak_3) \sin^2 \left(\frac{ak_1}{2} \right) \right\} U \\
&+ \left\{ iK\omega \cos (ak_3) + 2K^2 \cos (ak_3) \sin^2 \left(\frac{k_2}{2} \right) \right\} V + \mathcal{O}(\theta^3). \quad (5.40)
\end{aligned}$$

Since all three of these equations have the same constants U , V and W , we can combine the equations to matrix form. The matrix will be quite large, so we will write all of the equations as

$$AU + BV + CW = 0, \quad (5.41)$$

$$DU + EV + FW = 0 \text{ and} \quad (5.42)$$

$$GU + HV + IW = 0, \quad (5.43)$$

where

$$A = \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_1}{2} \right) + 2K^2 \left(2 \sin^2 \left(\frac{ak_1}{2} \right) - \sin^2 (ak_1) \right), \quad (5.44)$$

$$B = -iK\omega \cos (ak_1) + 2K^2 \cos (ak_1) \sin^2 \left(\frac{ak_2}{2} \right), \quad (5.45)$$

$$C = iK\omega \cos (ak_1) + 2K^2 \cos (ak_1) \sin^2 \left(\frac{ak_3}{2} \right), \quad (5.46)$$

$$D = iK\omega \cos (ak_2) + 2K^2 \cos (ak_2) \sin^2 \left(\frac{ak_1}{2} \right), \quad (5.47)$$

$$E = \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_2}{2} \right) + 2K^2 \left(2 \sin^2 \left(\frac{ak_2}{2} \right) - \sin^2 (ak_2) \right), \quad (5.48)$$

$$F = -iK\omega \cos (ak_2) + 2K^2 \cos (ak_2) \sin^2 \left(\frac{ak_3}{2} \right), \quad (5.49)$$

$$G = -iK\omega \cos (ak_3) + 2K^2 \cos (ak_3) \sin^2 \left(\frac{ak_1}{2} \right), \quad (5.50)$$

$$H = iK\omega \cos (ak_3) + 2K^2 \cos (ak_3) \sin^2 \left(\frac{ak_2}{2} \right) \text{ and} \quad (5.51)$$

$$J = \omega^2 - 4\omega_0^2 \sin^2 \left(\frac{ak_3}{2} \right) + 2K^2 \left(2 \sin^2 \left(\frac{ak_3}{2} \right) - \sin^2 (ak_3) \right). \quad (5.52)$$

Now we can write the equations as

$$\begin{pmatrix} A & B & C \\ D & E & F \\ G & H & J \end{pmatrix} \begin{pmatrix} U \\ V \\ W \end{pmatrix} = 0. \quad (5.53)$$

Since we are interested in the density of states of the system, we do not need to solve the eigenvalues and eigenvectors of the matrix. Just as in the calculation for optical and acoustic waves in (3.1.2), there are nontrivial solutions to this matrix equation only if the determinant

$$\det \begin{pmatrix} A & B & C \\ D & E & F \\ G & H & J \end{pmatrix} = 0. \quad (5.54)$$

This gives us another equation for the system. Solving ω from this equation gives us the spectrum of vibrations and subsequently the density of states.

Since the entries of the matrix are quite large, the determinant is enormous. Therefore we will expand the sines to second order in k_1 , k_2 and k_3 , so that for example $\sin^2(ak_1)$ becomes $a^2k_1^2$ and the determinant equation becomes

$$-\omega^4 (3K^2 - \omega^2) + a^2\omega_0^2\omega^2 (K^2 - \omega^2) (k_1^2 + k_2^2 + k_3^2) = 0. \quad (5.55)$$

This is a reasonable approximation, since in low temperatures the wavevectors \mathbf{k} should be small.

The isofrequency surfaces in this equation are spheres with radius

$$r = \sqrt{k_1^2 + k_2^2 + k_3^2}, \quad (5.56)$$

so this is one of the isotropic situations discussed in the end of the subsection (3.2.2). This is natural since we assumed the system to be isotropic in the beginning of this chapter. Therefore the density of states can be calculated with the volume inside the isofrequency surfaces.

Since the determinant equals zero we get

$$r = \sqrt{\frac{\omega^2 (3K^2 - \omega^2)}{a^2\omega_0^2 (K^2 - \omega^2)}}. \quad (5.57)$$

Thus the volumes of the spheres are

$$\frac{4\pi r^3}{3} = \frac{4\pi}{3\omega_0^3 a^3} \left(\frac{\omega^2 (3K^2 - \omega^2)}{(K^2 - \omega^2)} \right)^{3/2}. \quad (5.58)$$

Here we can recognize the velocity of sound $v_c = \sqrt{\frac{\zeta}{m}}a = \omega_0 a$ for a crystal corresponding to our system shown in (3.89).

If we proceeded similarly to the calculations in subsection (3.2.2), the density of states g would be $V/(2\pi)^3$ times the derivative of this volume with respect to ω , where V is the volume of the whole glass. However now we have split the lattice into two kinds of particles, ordered and disordered, and both of the two

kinds take only half of the lattice sites in the whole glass. Thus the density of states has to be divided by two, so that for the ordered particles

$$\begin{aligned}
g_0(\omega) &= \frac{1}{2} \frac{V}{(2\pi)^3} \left| \frac{\partial}{\partial \omega} \frac{4\pi}{3\omega_0^3 a^3} \left(\frac{\omega^2 (3K^2 - \omega^2)}{(K^2 - \omega^2)} \right)^{3/2} \right| \\
&= \frac{V}{8\pi^2 v_c^3} \left| \sqrt{\frac{\omega^2 (3K^2 - \omega^2)}{(K^2 - \omega^2)}} \left| \frac{\omega (6K^2 - 4\omega^2)}{(K^2 - \omega^2)} + \frac{2\omega^3 (3K^2 - \omega^2)}{(K^2 - \omega^2)^2} \right| \right| \\
&= \frac{V\omega^2}{4\pi^2 v_c^3} \left| \frac{\sqrt{3K^2 - \omega^2} (3K^4 - 2K^2\omega^2 + \omega^4)}{(K^2 - \omega^2)^{5/2}} \right|. \tag{5.59}
\end{aligned}$$

The purpose of the absolute value is to keep g_o positive. Expanding the denominator and omitting the K^4 terms, since K is proportional to the small θ , simplifies the expression into

$$\begin{aligned}
g_o(\omega) &= \frac{V\omega^2}{4\pi^2 v_c^3} \left| \frac{\sqrt{3K^2 - \omega^2} (3K^4 - 2K^2\omega^2 + \omega^4)}{\sqrt{K^2 - \omega^2} (K^4 - 2K^2\omega^2 + \omega^4)} \right| \\
&\approx \frac{V\omega^2}{4\pi^2 v_c^3} \left| \sqrt{\frac{3K^2 - \omega^2}{K^2 - \omega^2}} \right|. \tag{5.60}
\end{aligned}$$

The density of states has a divergence at

$$\omega_{o,div} = K. \tag{5.61}$$

Thus the glass really has behaviour similar to van Hove singularities. Recalling that $K = \zeta\theta$ we see that the singularity is related to the noncommutativity of our model. The more disordered the system is, the larger the noncommutativity parameter θ should be, and therefore the higher the frequency of the singularity should be.

5.2.2 Disordered lattice sites

[14] Now we want to solve the equation of motion (5.32), which describes the particles in the disordered lattice sites. The procedure is the same as for the ordered sites. Plugging in the same ansatz (5.34) as for the ordered particles and dropping the $\mathcal{O}(\theta^3)$ terms yields

$$\begin{aligned}
& -\omega^2 U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} e^{iak_1} \\
&= -\omega_0^2 U e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} (2e^{iak_1} - e^{2iak_1} - 1) \\
& \quad + i\omega \frac{K}{2} e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} e^{iak_1} (4V - V e^{iak_2} - V e^{-iak_2}) \\
& \quad + i\omega \frac{K}{2} e^{i\omega t} e^{i\mathbf{k}\cdot\mathbf{L}} e^{iak_1} (-4W + W e^{iak_3} + W e^{-iak_3}). \tag{5.62}
\end{aligned}$$

Dividing with $e^{i\mathbf{k}\cdot\mathbf{L}}e^{iak_1}$ gives the equation

$$\begin{aligned} & \{\omega^2 - \omega_0^2 (2 - e^{iak_1} - e^{-iak_1})\} U \\ & + i\omega \frac{K}{2} \{4 - e^{iak_2} - e^{-iak_2}\} V \\ & - i\omega \frac{K}{2} \{4 - e^{iak_3} - e^{-iak_3}\} W = 0. \end{aligned} \quad (5.63)$$

Expressed with cosines it is

$$\begin{aligned} & \{\omega^2 - 2\omega_0^2 (1 - \cos(ak_1))\} U \\ & + i\omega K \{2 - \cos(ak_2)\} V \\ & - i\omega K \{2 - \cos(ak_3)\} W = 0. \end{aligned} \quad (5.64)$$

Again the equation of motion for $\ddot{v}_{l+1,m,n}$ should lead to the same result, except that U should be changed to V , V should be changed to W and W should be changed to U , and k_1 , k_2 and k_3 should be permuted similarly. Thus we get

$$\begin{aligned} & \{\omega^2 - 2\omega_0^2 (1 - \cos(ak_2))\} V \\ & + i\omega K \{2 - \cos(ak_3)\} W \\ & - i\omega K \{2 - \cos(ak_1)\} U = 0. \end{aligned} \quad (5.65)$$

For $\ddot{w}_{l+1,m,n}$ the permutation should be done twice, leading to

$$\begin{aligned} & \{\omega^2 - 2\omega_0^2 (1 - \cos(ak_3))\} W \\ & + i\omega K \{2 - \cos(ak_1)\} U \\ & - i\omega K \{2 - \cos(ak_2)\} V = 0. \end{aligned} \quad (5.66)$$

Collecting the three equations leads to the matrix

$$\begin{pmatrix} \omega^2 - 2\omega_0^2 (1 - \cos(ak_1)) & i\omega K (2 - \cos(ak_2)) & -i\omega K (2 - \cos(ak_3)) \\ -i\omega K (2 - \cos(ak_1)) & \omega^2 - 2\omega_0^2 (1 - \cos(ak_2)) & i\omega K (2 - \cos(ak_3)) \\ i\omega K (2 - \cos(ak_1)) & -i\omega K (2 - \cos(ak_2)) & \omega^2 - 2\omega_0^2 (1 - \cos(ak_3)) \end{pmatrix}, \quad (5.67)$$

which has non-trivial solutions only if its determinant equals 0. Expanding in \mathbf{k} yields

$$-\omega^4 (3K^2 - \omega^2) + a^2 (-K^2\omega^4 + K^2\omega^2\omega_0^2 - \omega^4\omega_0^2) (k_1^2 + k_2^2 + k_3^2) + \mathcal{O}(\mathbf{k}^3). \quad (5.68)$$

Omitting the $\mathcal{O}(\mathbf{k}^3)$ terms and setting the determinant to zero gives

$$k_1^2 + k_2^2 + k_3^2 = \frac{\omega^2 (3K^2 - \omega^2)}{a^2 (K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)}. \quad (5.69)$$

The density of states can again be calculated with the volume of the isofrequency spheres. Using $\sqrt{k_1^2 + k_2^2 + k_3^2}$ as the radius r of the sphere leads to the volume

$$\frac{4\pi}{3} r^3 = \frac{4\pi\omega^3 (3K^2 - \omega^2)^{3/2}}{3a^3 (K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)^{3/2}}. \quad (5.70)$$

Recalling the discussion about the ordered and disordered particles both taking up half of the lattice, we see that the density of states

$$\begin{aligned}
g_d(\omega) &= \frac{1}{2} \frac{V}{(2\pi)^3} \left| \frac{\partial V}{\partial \omega} \frac{4\pi\omega^3 (3K^2 - \omega^2)^{3/2}}{3a^3 (K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)^{3/2}} \right| \\
&= \frac{V}{(2\pi)^3} \frac{4\pi}{6a^3} \left| \frac{3\omega^2 (3K^2 - \omega^2)^{3/2} - 3\omega^4 (3K^2 - \omega^2)^{1/2}}{(K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)^{3/2}} \right. \\
&\quad \left. - \frac{3\omega^4 (3K^2 - \omega^2)^{3/2} (-K^2 - \omega_0^2)}{(K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)^{5/2}} \right| \\
&= \frac{V\omega^2}{4\pi^2 a^3} \left| \frac{\sqrt{3K^2 - \omega^2} (3K^4\omega_0^2 + K^2\omega^4 - 2K^2\omega_0^2\omega^2 + \omega_0^2\omega^4)}{(K^2\omega_0^2 - (K^2 + \omega_0^2)\omega^2)^{5/2}} \right|
\end{aligned} \tag{5.71}$$

or

$$\frac{V\omega^4}{4\pi^2 v_c^3} \left| \frac{\sqrt{3K^2 - \omega^2} (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right| \tag{5.72}$$

after discarding the term with K^4 in the nominator and using the velocity of sound $v_c = \omega_0 a = \sqrt{\zeta/ma}$ in a corresponding crystal.

Now the density of states has a divergence at

$$\omega_{d,div} = \frac{K}{\sqrt{K^2/\omega_0^2 + 1}}. \tag{5.73}$$

Expanding in K lets us write the divergence as

$$\omega_{d,div} = K + \mathcal{O}(K^3), \tag{5.74}$$

which is the same result as for the ordered particles. Therefore we can conclude that making every second particle of a lattice disordered gives the density of states of all particles the same peak frequency. This is desirable for our model, since the boson peak appears only at one frequency for every glass.

5.2.3 Whole glass

[14] Since the ordered and disordered particles both take up half of the glass, the density of states for the whole glass has to be the sum of the densities of states of the two kinds of particles. For the ordered lattice sites

$$g_o = \frac{V\omega^2}{4\pi^2 v_c^3} \left| \sqrt{\frac{3K^2 - \omega^2}{K^2 - \omega^2}} \right| \tag{5.75}$$

and for the disordered lattice sites we got

$$g_d = \frac{V\omega^4}{4\pi^2 v_c^3} \left| \frac{\sqrt{3K^2 - \omega^2} (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right|. \tag{5.76}$$

Thus for the whole glass

$$\begin{aligned}
g_{glass} &= g_o + g_d \\
&= \frac{V\omega^2\sqrt{|3K^2 - \omega^2|}}{4\pi^2v_c^3} \left(\frac{1}{\sqrt{|K^2 - \omega^2|}} + \left| \frac{\omega^2 (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right| \right).
\end{aligned} \tag{5.77}$$

This is a good moment to compare our model to the Debye model for acoustic waves. If we set $K = \zeta\theta = 0$ in the above model to remove the disorder, then

$$g_{glass} = g_o + g_d = \frac{\omega^2V}{4\pi^2v_c^3} + \frac{\omega^2V}{4\pi^2v_c^3} = \frac{\omega^2V}{2\pi^2v_c^3}, \tag{5.78}$$

which is the density of states of one branch in the Debye model shown in (3.90). In order to describe the whole glass we have to add up the longitudinal and transverse waves. We want our system to be as isotropic as possible, so the sound velocities in longitudinal and transverse directions should be the same, which means that the density of states has only to be multiplied by three. Thus

$$g_{glass} = \frac{3V\omega^2\sqrt{|3K^2 - \omega^2|}}{4\pi^2v_c^3} \left(\frac{1}{\sqrt{|K^2 - \omega^2|}} + \left| \frac{\omega^2 (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right| \right). \tag{5.79}$$

Now the commutative limit gives exactly the same result as the Debye model. This means that the boson peak contribution has to be related to the noncommutativity in our model, as we saw when discussing the singularities in the density of states.

g_{glass} and the g_{Debye} derived from the Debye model are plotted in figure (5.1) and g_{glass}/g_{Debye} is plotted in figure (5.2). In the former we have set the constant $V/2\pi^2v_c^3 = 1$. The plots have a discontinuity just as stated in the introduction. In the first plot the discontinuity of g_{glass} is at the frequency of the divergences $\omega_{o,div} = \omega_{d,div} = K$, and it gives the boson peak frequency.

5.3 Dispersion relations

Next we will derive the dispersion relations. Using them we can check whether the boson peak in our system corresponds to acoustic or optical waves. Deriving the dispersion relations from the equations of motion would be cumbersome, so we will instead use the determinants (5.54) and (5.67) similarly as in the one dimensional model with two atoms.

Before calculating the dispersion relations, we shall make the system more symmetric. The model is not completely isotropic, since we have imposed a lattice structure. Also the noncommutativity parameter is set to have the value θ in the directions of the primitive translation vectors, but in other directions the noncommutativity is different. Recall that with a change of coordinates we can define axes where only two directions are noncommutative, as shown in (4.4). This means that the noncommutativity is actually completely in the plane

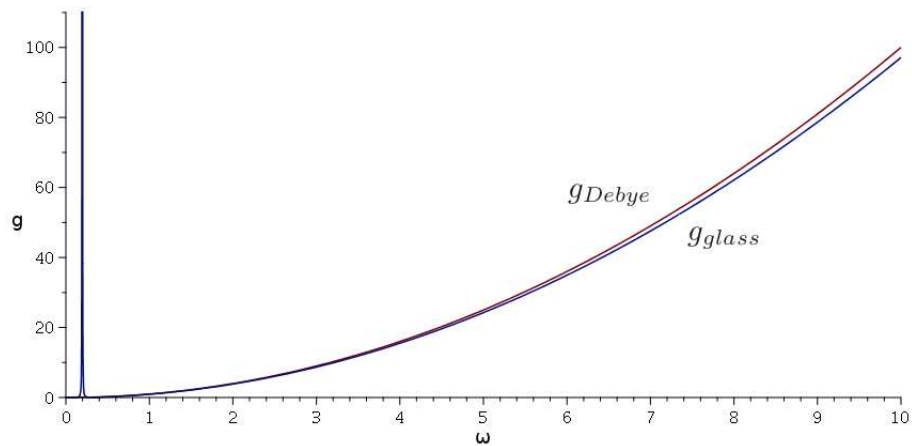


Figure 5.1: The blue line with the peak is g_{glass} with $K = 0.2$ and $\omega_0 = 1$, and the purple line that rises higher on the right is g_{Debye} . We have set $V/2\pi^2 v_c^3 = 1$, so $g_{Debye}(1) = 1$.

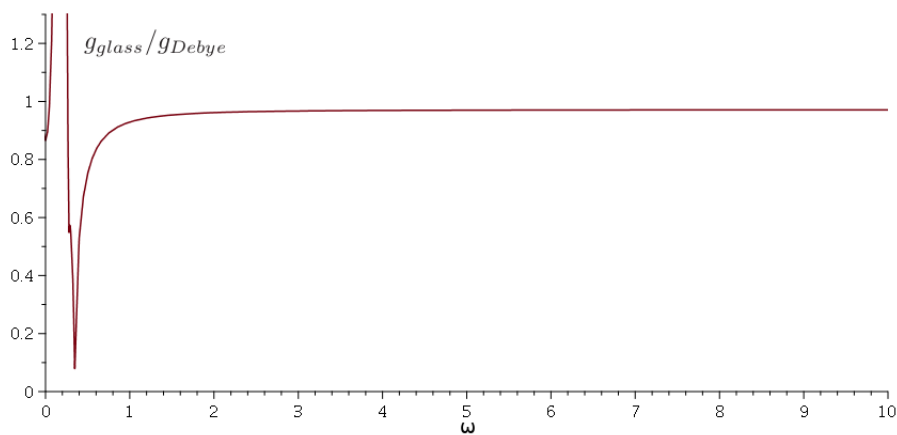


Figure 5.2: The plot of g_{glass}/g_{Debye} with $K = 0.2$ and $\omega_0 = 1$.

defined by the two noncommuting directions perpendicular to the commuting one. By choosing $\theta_{12} = \theta_{23} = \theta_{31} \equiv \theta$ we have just chosen the noncommutativity plane to have equal projections to each of the lattice axes.

To make the system more isotropic, we shall choose one of the directions of the wavevector, and use that to represent the whole wavevector. Thus we shall set $k_3 = |\mathbf{k}| \equiv k$ and $k_1 = k_2 = 0$. Now we study only waves which have proper noncommutativity, which means a proper disorder in the lattice.

Notice that had we made this simplification when calculating the density of states, we would have got the same result, since the wavevectors appeared only as the sum $k_1 + k_2 + k_3$ after doing the small angle approximation.

5.3.1 Ordered particles

[14] Let us take another look at the equation (5.54). If we set $k_3 = |\mathbf{k}| \equiv k$ and $k_1 = k_2 = 0$ the matrix becomes

$$\begin{pmatrix} \omega^2 & -iK\omega & iK\omega + 2K^2 \sin^2\left(\frac{ak}{2}\right) \\ iK\omega & \omega^2 & -iK\omega + 2K^2 \sin^2\left(\frac{ak}{2}\right) \\ -iK\omega \cos(ak) & iK\omega \cos(ak) & \omega^2 - 4\omega_0^2 \sin^2\left(\frac{ak}{2}\right) + 2K^2 \left(2 \sin^2\left(\frac{ak}{2}\right) - \sin^2(ak)\right) \end{pmatrix}. \quad (5.80)$$

Thus the determinant is

$$\begin{aligned} & \omega^2 \left(8 \cos^4\left(\frac{ak}{2}\right) K^2 \omega^2 - 16 \cos^2\left(\frac{ak}{2}\right) K^2 \omega^2 - 4\omega_0^2 K^2 \cos^2\left(\frac{ak}{2}\right) \right. \\ & \left. + 4 \cos^2\left(\frac{ak}{2}\right) \omega_0^2 \omega^2 + 5K^2 \omega^2 + 4\omega_0^2 K^2 + \omega^4 - 4\omega_0^2 \omega^2 \right). \end{aligned} \quad (5.81)$$

Setting the determinant to zero gives a quadratic equation for ω^2 :

$$\begin{aligned} & \omega^4 + \omega^2 \left(8 \cos^4\left(\frac{ak}{2}\right) K^2 + 4(\omega_0^2 - 4K^2) \cos^2\left(\frac{ak}{2}\right) + 5K^2 - 4\omega_0^2 \right) \\ & - 4\omega_0^2 K^2 \left(\cos^2\left(\frac{ak}{2}\right) - 1 \right) = 0. \end{aligned} \quad (5.82)$$

The solutions are

$$\begin{aligned} \omega_{\pm}^2 &= \frac{\omega_0^2}{2} \left\{ \left(-8 \cos^4\left(\frac{ak}{2}\right) \frac{K^2}{\omega_0^2} - 4 \left(1 - 4 \frac{K^2}{\omega_0^2} \right) \cos^2\left(\frac{ak}{2}\right) - 5 \frac{K^2}{\omega_0^2} + 4 \right. \right. \\ & \left. \pm \left[\left(8 \cos^4\left(\frac{ak}{2}\right) \frac{K^2}{\omega_0^2} + 4 \left(1 - 4 \frac{K^2}{\omega_0^2} \right) \cos^2\left(\frac{ak}{2}\right) + 5 \frac{K^2}{\omega_0^2} - 4 \right)^2 \right. \right. \\ & \left. \left. + 16 \frac{K^2}{\omega_0^2} \left(\cos^2\left(\frac{ak}{2}\right) - 1 \right) \right]^{1/2} \right\} \end{aligned} \quad (5.83)$$

or

$$\omega_{\pm}^2 = \frac{\omega_0^2}{2} \left\{ -8 \cos^4 \left(\frac{ak}{2} \right) R + 4(1 - 4R) \sin^2 \left(\frac{ak}{2} \right) + 11R \right. \\ \left. \pm \sqrt{\left(8 \cos^4 \left(\frac{ak}{2} \right) R - 4(1 - 4R) \sin^2 \left(\frac{ak}{2} \right) - 11R \right)^2 - 16R \sin^2 \left(\frac{ak}{2} \right)} \right\} \quad (5.84)$$

with the help of the Pythagorean identity and defining $R = \frac{K^2}{\omega_0^2} = m\zeta\theta^2$.

The expressions are very similar to the expressions for the acoustic and optical branches for the two atom chain discussed in chapter (3.1.2), even though we are now discussing a lattice with only identical particles. In the centre of the Brillouin zone where $k_3 = 0$ the branch $\omega_+ = \sqrt{3}K$ i.e. a constant, and the branch $\omega_- = 0$. In addition ω_+ is always greater than ω_- . Therefore ω_+ really is an optical branch and ω_- is an acoustic branch.

An interesting point is that if K is set to zero to obtain the usual commutative version, the acoustic branch gives the usual dispersion relation for a monoatomic lattice:

$$\omega_- = 2\sqrt{\omega_0^2} \sin \left(\frac{ak}{2} \right) \quad (5.85)$$

and the optical branch vanishes. This is completely expected, but it means that having both ordered and disordered particles creates optical branches for monoatomic lattices.

Next we shall solve the dispersion relations for the disordered particles and then compare the frequency ranges of the branches we have found to the frequency of the peak in the density of states. This helps us interpret which branches contribute to the boson peak.

5.3.2 Disordered particles

[14] If we set $k_3 = |\mathbf{k}| \equiv k$ and $k_1 = k_2 = 0$, the matrix in (5.67) becomes

$$\begin{pmatrix} \omega^2 & i\omega K & -i\omega K (2 - \cos(ak)) \\ -i\omega K & \omega^2 & i\omega K (2 - \cos(ak)) \\ i\omega K & -i\omega K & \omega^2 - 2\omega_0^2 (1 - \cos(ak)) \end{pmatrix}, \quad (5.86)$$

so its determinant is

$$\omega^2 \left(2K^2 \cos(ak) \omega^2 - 2K^2 \omega_0^2 \cos(ak) + 2 \cos(ak) \omega_0^2 \omega^2 \right. \\ \left. - 5K^2 \omega^2 + 2K^2 \omega_0^2 + \omega^4 - 2\omega_0^2 \omega^2 \right). \quad (5.87)$$

Equating this to zero gives again a quadratic equation in ω^2 . The solutions are

$$\begin{aligned} \omega_{\pm}^2 = & \frac{\omega_0^2}{2} \left\{ -2 \left(\frac{K^2}{\omega_0^2} + 1 \right) \cos(ak) + 5 \frac{K^2}{\omega_0^2} + 2 \right. \\ & \left. \pm \sqrt{\left(2 \left(\frac{K^2}{\omega_0^2} + 1 \right) \cos(ak) - 5 \frac{K^2}{\omega_0^2} - 2 \right)^2 - 8 \frac{K^2}{\omega_0^2} (1 - \cos(ak))} \right\} \end{aligned} \quad (5.88)$$

or

$$\begin{aligned} \omega_{\pm}^2 = & \frac{\omega_0^2}{2} \left\{ 4(R+1) \sin^2\left(\frac{ak}{2}\right) + 3R \right. \\ & \left. \pm \sqrt{\left(4(R+1) \sin^2\left(\frac{ak}{2}\right) + 3R \right)^2 + 16R \sin^2\left(\frac{ak}{2}\right)} \right\} \end{aligned} \quad (5.89)$$

using $\cos(x) = 1 - 2 \sin^2\left(\frac{x}{2}\right)$ and $R = \frac{K^2}{\omega_0^2} = m\zeta\theta^2$. Solving the above equation for ω_- would give us an imaginary frequency, so we will use the absolute value instead when discussing ω_- .

Again at the centre of the Brillouin zone ($k = 0$) the values of the branches are $\omega_+ = \sqrt{3}K$ and $\omega_- = 0$, and ω_+ is always greater than ω_- . Thus ω_+ is the optical branch and ω_- is the acoustic branch.

The branches derived from the ordered particles and the branches derived above from the disordered particles are plotted in figures (5.3) and (5.4). In addition the frequency of divergence $\omega_{div} = K = \omega_0\sqrt{R}$ found from the density of states of the ordered and disordered particles is plotted in the graphs. Since the dispersion relations are periodic in $2\pi/a$ we have plotted them on the interval $[0, 2\pi/a]$.

As is seen from the graphs, the optical branches lie above the boson peak frequency, so they cannot contribute to it, just like we anticipated when discussing the Debye and Einstein models. The acoustic modes however have a long interval where their values are very close to the peak frequency, leading to the van Hove singularity, so it is natural to assume that this interval is behind the boson peak behaviour.

Comparing the two graphs we also see that as the noncommutativity parameter $R = K^2/\omega_0^2 = m\zeta\theta^2$ is increased, the frequencies of the optical branches increase and the difference between ordered and disordered contributions increases.

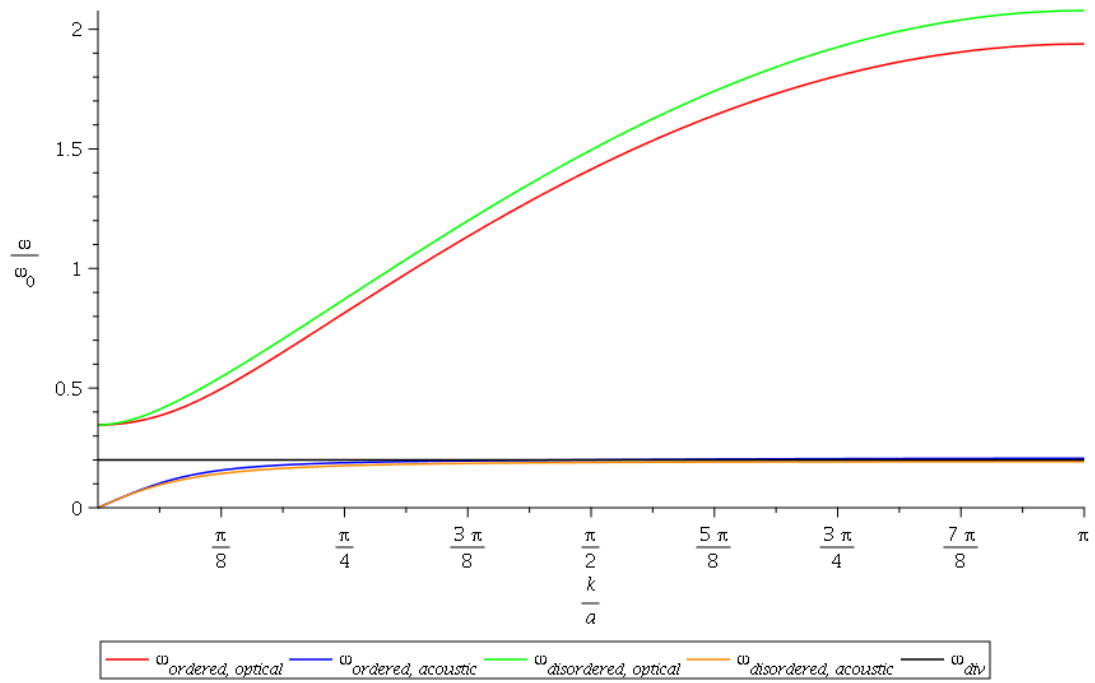


Figure 5.3: The dispersion relations with $R = 0.04$.

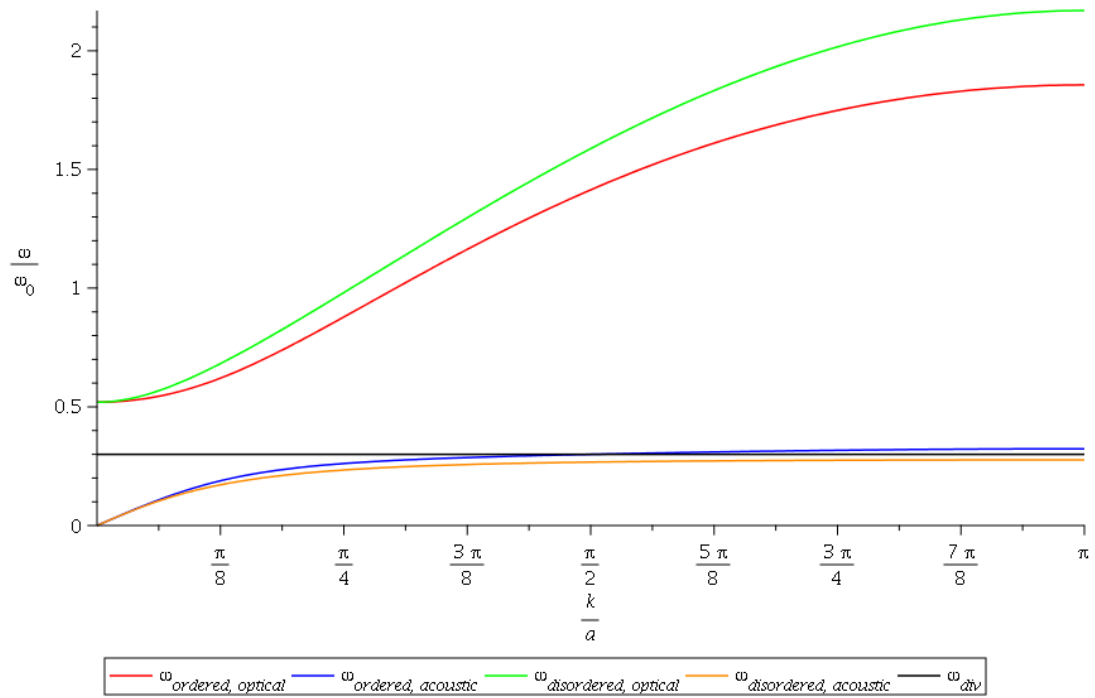


Figure 5.4: The dispersion relations with $R = 0.09$.

5.4 Heat capacity

[39] In subsection (3.3) we derived the following formula for the heat capacity of a crystal:

$$C_V = \int d\omega g(\omega) \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T}. \quad (5.90)$$

Let us see how it works for our glass model. Using the density of states we derived leads to

$$C_V = \int d\omega \left(\frac{\omega/T}{e^{\omega/T} - 1} \right)^2 e^{\omega/T} \frac{3V\omega^2 \sqrt{|3K^2 - \omega^2|}}{4\pi^2 v_c^3} \times \left(\frac{1}{\sqrt{|K^2 - \omega^2|}} + \left| \frac{\omega^2 (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right| \right). \quad (5.91)$$

C_V and the Debye model heat capacity are plotted in figure (5.5), and $C_V T^{-3}$ is plotted in figure (5.6). The latter plot shows clearly the effect of the boson peak. Finally in figure (5.7), which is taken from [14], the theoretical values are calculated for three real glasses and compared to experimental results. In the last figure the parameters ω_0 and θ are determined by first fitting the theoretical curves to the experimental results so that the heat capacity and frequency match at the peaks. The graphs show that our model produces the boson peak behaviour and especially the shape of the curves in good agreement with experimental data.

In this work we shall go further and calculate the integral, but first we shall do several changes to it. First of all we set the Debye temperature $\omega_D = v_{eff} (6N\pi^2/V)^{1/3}$ as an upper bound for the integral, and also write the coefficient in terms of ω_D as $3V/2\pi^2 v_{eff}^3 = 9N/\omega_D^3$, as we did when discussing the Debye model. Then we shall use

$$\frac{e^{\omega/T}}{(e^{\omega/T} - 1)^2} = \frac{1}{4 \sinh^2(\omega/2T)} \quad (5.92)$$

to simplify the formula. Now

$$C_V = \frac{9N}{8\omega_D^3 T^2} \int_0^{\omega_D} d\omega \frac{\omega^4 \sqrt{|3K^2 - \omega^2|}}{\sinh^2(\omega/2T)} \times \left(\frac{1}{\sqrt{|K^2 - \omega^2|}} + \left| \frac{\omega^2 (2K^2 - (K^2/\omega_0^2 + 1)\omega^2)}{(K^2 - (K^2/\omega_0^2 + 1)\omega^2)^{5/2}} \right| \right). \quad (5.93)$$

Let us next expand the integrand in K , so

$$C_V = \frac{9N}{8\omega_D^3 T^2} \int_0^{\omega_D} d\omega \frac{\omega^4}{\sinh^2(\omega/2T)} \left(\left| 1 - \frac{K^2}{\omega^2} \right| + \left| 1 - \frac{K^2}{\omega^2} - \frac{3K^2}{2\omega_0^2} \right| \right) + \mathcal{O}(K^4). \quad (5.94)$$

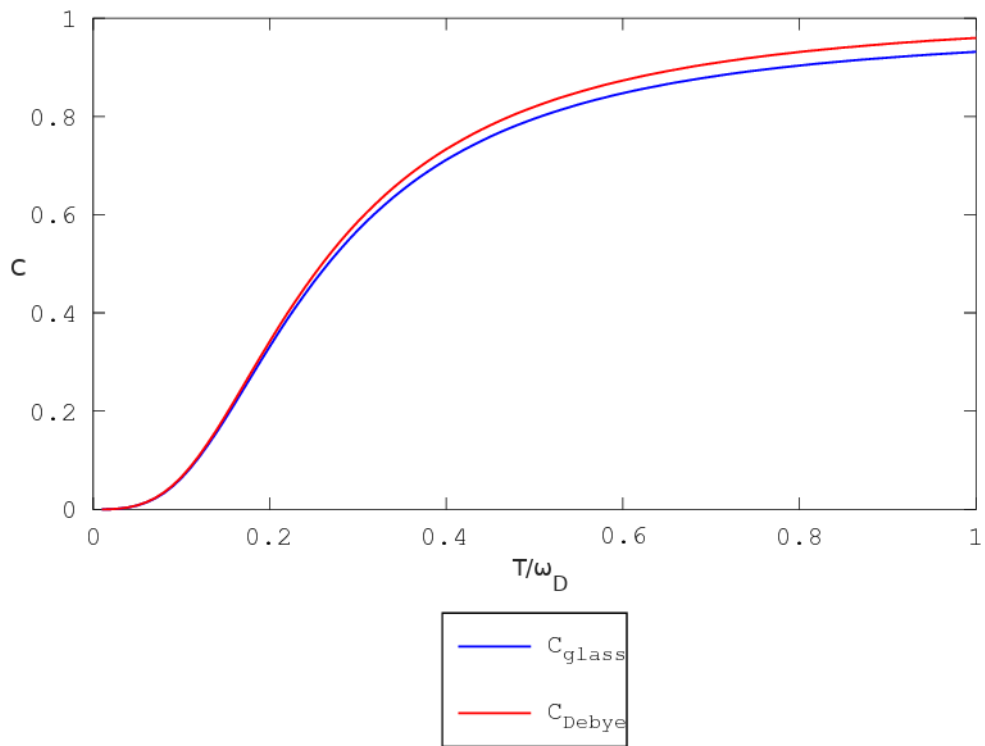


Figure 5.5: The glass heat capacity in blue and the Debye heat capacity in red, scaled as $C/3N$. We have set $\omega_D = 100$, $K = 0.2$ and $\omega_0 = 1$.

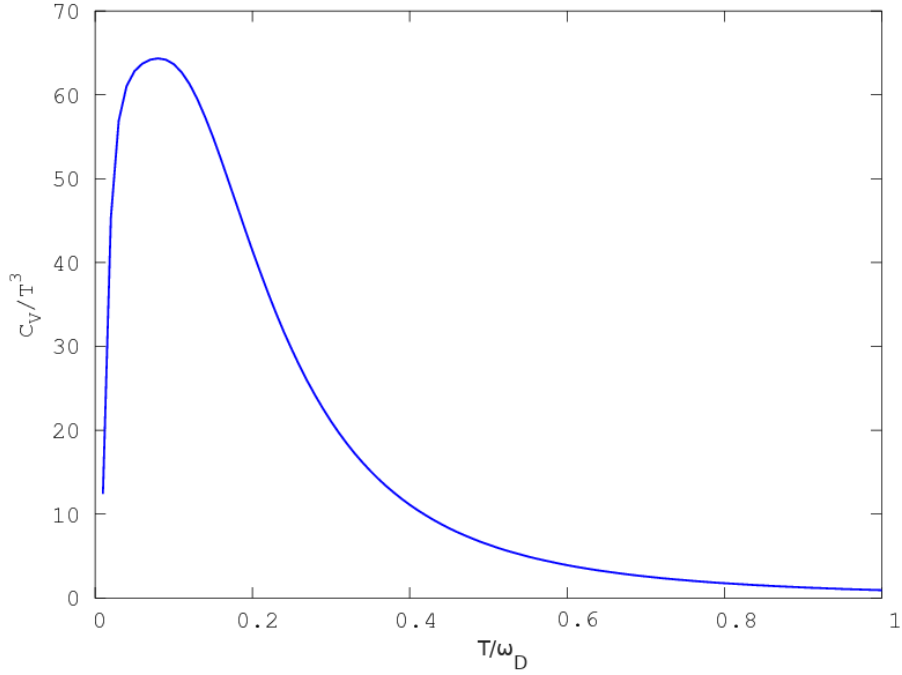


Figure 5.6: $C_V T^{-3}$ with $\omega_D = 100$, $K = 0.2$ and $\omega_0 = 1$.

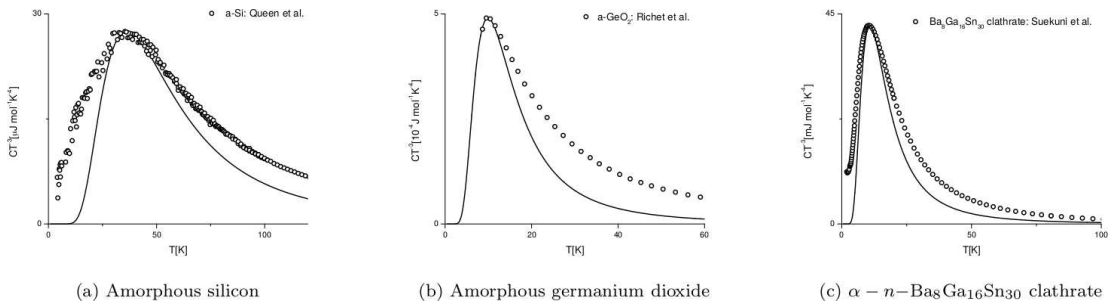


Figure 5.7: Comparison of theoretical and experimental values of the heat capacity. The graphs are taken from [14]. The circles are experimental values, while the continuous curves are theoretical values calculated using an integral similar to (5.93).

Removing the absolute values complicates the rest of the calculation. Let us first assume that the contribution to the integral below

$$\omega = K/\sqrt{1 - \frac{3K^2}{2\omega_0^2}} \approx K + \frac{3K^3}{4\omega_0^2} \quad (5.95)$$

is negligible, so we can drop the absolute values, and

$$C_V = \frac{9N}{8\omega_D^3 T^2} \int_0^{\omega_D} d\omega \frac{\omega^4}{\sinh^2(\omega/2T)} \left(2 - \frac{2K^2}{\omega^2} - \frac{3K^2}{2\omega_0^2} \right), \quad (5.96)$$

after dropping the $\mathcal{O}(K^4)$ terms.

Let us change the integration variable to $x = \omega/2T$, so

$$C_V = \frac{36NT^3}{\omega_D^3} \int_0^{\omega_D/2T} dx \frac{x^4}{\sinh^2(x)} \left(2 - \frac{K^2}{2T^2 x^2} - \frac{3K^2}{2\omega_0^2} \right), \quad (5.97)$$

and then use the low temperature limit to set the upper bound of the integral to infinity. Now the integral is simple to calculate with $\int_0^\infty x^4/\sinh^2(x) = \pi^4/30$ and $\int_0^\infty x^2/\sinh^2(x) = \pi^2/6$.

$$\begin{aligned} C_V &= \frac{36NT^3}{\omega_D^3} \int_0^\infty dx \frac{x^4}{\sinh^2(x)} \left(2 - \frac{K^2}{2T^2 x^2} - \frac{3K^2}{2\omega_0^2} \right) \\ &= \frac{12\pi^4 NT^3}{5\omega_D^3} \left(1 - \frac{3K^2}{4\omega_0^2} - \frac{5K^2}{4\pi^2 T^2} \right). \end{aligned} \quad (5.98)$$

The first term is the same result as what the Debye model gives, and the rest of the expression is a disordered addition to it.

6 Conclusions and comparison to other models

In the thesis we introduced a lattice model for glasses starting from a crystal lattice. We switched the coordinates of half of the particles in the crystal lattice to noncommutative coordinates with a small commutator θ , to give the locations of the particles an uncertainty. This resulted in a Van Hove singularity in the density of states of the particles at a frequency proportional to θ . The singularity was located at low frequencies and it resembled the boson peak found in glass experiments, which has been without a thorough theoretical model. Right after the singularity the density of states of the system reverted to the Debye crystal model.

Since the model had two kinds of particles, ones with commutative, or ordered, coordinates and ones with noncommutative disordered coordinates, both of the kinds of particles had also their own vibrational branches. Having two kinds of particles also created optical branches to the system.

Lastly we used the density of states to calculate the heat capacity of the system. The heat capacity resembled mostly the Debye crystal model, but in very low frequencies the heat capacity has a clear bump compared to the Debye T^3 law. This is exactly what has been found in experiments.

Several experiments and simulations have indicated a connection between acoustic waves and the boson peak. In [40] and [41] a connection to the acoustic Van Hove singularity is given, whilst [42] and [17] focus on acoustic waves near the pseudo-Brillouin zone. However, many of the theoretical models for the boson peak explain the phenomenon as something not related to acoustic waves [20, 43–47]

Looking at the dispersion relations we derived, we see that our model clearly relates the boson peak to acoustic waves. The frequencies of the optical waves are higher than the boson peak frequency, whereas the acoustic waves are located very close to the peak frequency for a large interval in the Brillouin zone. Also the smaller the noncommutativity parameter is, the closer the acoustic branches are to the peak frequency, which is seen easiest from the plots of the dispersion relation. However the peak still is a result of the noncommutativity, since the peak frequency is proportional to the noncommutativity parameter: $\omega_{div} = K = \zeta\theta$.

In [17] and [48] it is indicated that there are longitudinal acoustic waves well above the boson peak frequency. Another finding in the former is that the frequency of the boson peak is equal to the frequency of the Ioffe-Regel limit for transverse phonons. The Ioffe-Regel limit is the frequency where the wavelength of phonons equals their mean free path. Above the limit there are no transverse phonons. This suggests that the boson peak is linked to transverse phonons and the conclusion is drawn that the boson peak frequency might be the characteristic frequency of the transverse vibrational modes, or in other words the frequency to which the transverse waves resonate.

Our model in contrast to [17] suggests that the maximum frequency of acoustic waves is very close to the peak frequency, which means that longitudinal acoustic waves could still be related to the peak. However both models agree

that the maximum frequency of transverse acoustic waves is very close to the boson peak frequency.

There already has been introduced numerous glass models that start from a crystal and then make it slightly disordered, by for example dislocating each atom from its lattice site by a random amount [15] or by adding fluctuations to the force constants between lattice sites of the atom [40]. Our model however is vastly simpler, since the calculations can be done essentially by only pen and paper instead of with simulations. This makes our model very easy to investigate and manipulate for further developments. It should also be noted that our model has only two parameters ω_0 and θ . ω_0 is the characteristic frequency of the glass, and θ tells how disordered the glass is.

In this thesis we do not comment on the transition from a liquid to a glass. An interesting possibility for further development would be to see does this model bring anything to the transition discussion. One could for example start with a noncommutative fluid using the parametrization (4.15), and in contrast to the work here, not start with the deviation A set to zero but to see what happens when A is gradually brought to zero. Then the fluid would initially flow. This might also bring insight on whether our model can truly be compared to fluid models, or is it just a noncommutative lattice.

An easier further calculation would be to calculate the sound velocity using our dispersion relations. This should be an easy calculation, and it would allow calculating the value of θ using measured sound velocities. Another interesting calculation would be to calculate θ from the relation to the area density of particles (4.17) used in fluid models, to see whether it can be applied to the glass model.

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