WEAK-COUPLING THEORY OF CHANNELING:
THE ENERGY DISSIPATION TO PHONONS

Advisor: Prof. Nicola Manini
Co-advisor: Prof. Giuseppe Santoro

Tesi di Laurea di:
Nicolas Trojani
Matricola n°884894
Codice PACS: 68.35.-p

A.A. 2017-2018
WEAK-COUPLING THEORY OF CHANNELING:
THE ENERGY DISSIPATION TO PHONONS

Abstract

We address the problem of weak phononic and dissipation friction by means of analytic many-body techniques. Our model consists of a particle (the "slider") moving inside a three-dimensional crystal and therefore exciting its phonons. With ad-hoc application the linear-response theory we obtain a formula for the friction force slowing down the slider, as a function of its speed and of the details of the crystal phonons and of the slider-crystal interaction.

Advisor: Prof. Nicola Manini
Co-advisor: Prof. Giuseppe Santoro

Tesi di Laurea di:
Nicolas Trojani
Matricola n°884894
Codice PACS: 68.35.-p
## Contents

1 Introduction ................................................. 7

2 Linear Response Theory ................................. 8
   2.1 Linear Response Functions ......................... 8
       2.1.1 Fluctuation-Dissipation Theorem ........ 11
   2.2 Spectral Representation .......................... 12

3 Application to a particle sliding on a linear chain .... 13

4 Particle channeling through a crystal .................. 15
   4.1 The model ........................................... 15
   4.2 Dissipated power from a crystal lattice .......... 20
       4.2.1 Symmetries ................................... 21
       4.2.2 Response of the harmonic crystal .......... 23
       4.2.3 Dynamic structure factor for the harmonic crystal ........ 25
       4.2.4 Evaluation of the dissipated power .... 28
   4.3 Numerical calculation of Eq. (101) ................. 33

5 Conclusions and future developments ..................... 33
1 Introduction

When we refer to friction we talk about all the conditions in which we witness the transformation of mechanical energy into thermal energy. Friction phenomena affect the dynamics of moving objects over many different scales, from the macroscopic to the atomic ones, and, for this reason it is very important to have reliable models to control and predict the features of frictional interactions.

The first scientist who has recorded phenomenological but quantitative investigations of this topic was Leonardo da Vinci, in the 15th century. According to da Vinci, frictional resistance was the same for two different objects of the same weight but making contact over different widths and lengths. In 1699 Guillaume Amontons formalized these results in the two fundamental laws of frictions, that can be summarized as follows: frictional force is independent of the apparent area of contact and the friction acting between two sliding surfaces is proportional to the load pressing the surfaces together. These laws were later developed by Charles-Augustin de Coulomb (in 1785), who noticed that sliding friction is approximately independent of the sliding velocity.

Thanks to the huge amount of empirical data, serious attempts were made in the first half of the 20th century in order to have a microscopic understanding of these laws. In the last decades the study of friction was extended to the nanometric scales of the atoms individually involved in this process, giving rise to a new branch of research called nanotribology [1],[2]. This branch of physics is important for many reasons, mainly because: (i) in the last years the miniaturization of electro-mechanic devices led to the increase of the ratio surface/volume and the consequent increase to the relative importance of friction, (ii) recent development of experimental and computational techniques, such as the atomic force microscope (AFM) and molecular-dynamics (MD), are producing a mass of fresh data and information on well-defined systems, surfaces, and materials which are not yet fully explained theoretically.

This thesis addresses the problem of weak phononic friction: this problem was investigated and essentially solved in the recent work which addressed the atomic friction for a one-dimensional system in [3]. That work studied a point slider moving at velocity $v_{SL}$ interacting with a harmonic chain underneath, through Van-der-Waals forces. In the present work we address the real-life three-dimensional crystals. We study the energy loss by a particle channeling through a simple-cubic crystal and gently losing energy to the crystal phonons. We obtain a formula for the frictional force as a function of the slider velocity. These results can be extended and adapted to study microscopic friction by considering the slider moving on a surface.
2 Linear Response Theory

In this chapter we summarize the Linear Response Theory, following the notes written by Michele Fabrizio \[5\]. Linear Response Theory (LRT) studies how a system in thermal equilibrium is modified by the introduction of a weak external perturbation. In order to study the physical properties of the perturbed system we have to add to the unperturbed Hamiltonian \( \hat{H}_0 \) a time-dependent term of the general form:

\[
\hat{V}(t) = \int d^3 x \hat{A}(x)V(x, t),
\]

where \( V(x, t) \) is the external perturbation which couples with the Hermitian operator \( \hat{A}(x) \).

We want to study the effects of \( \hat{V}(t) \) on some measurable quantity described for example by some operator \( \hat{B}(x) \). In other words we want to calculate

\[
\hat{B}(x, t) = \text{Tr}[\hat{\rho}(t) \hat{B}(x)]
\]

where \( \hat{\rho}(t) \) is the time-dependent density matrix of the perturbed system.

2.1 Linear Response Functions

If we assume that the perturbation is switched on a time \( t \to -\infty \), and that system is initially in equilibrium we can write:

\[
\lim_{t \to -\infty} \hat{\rho}(t) = \hat{\rho}_0
\]

with the density operator at equilibrium given by

\[
\hat{\rho}_0 = \frac{1}{Z_0} \sum_n e^{-\beta \hat{H}_0} = \frac{1}{Z_0} \sum_n e^{-\beta E_n} |\phi_n(t) \rangle \langle \phi_n(t)|.
\]

Here \( \hat{H}_0 |\phi_n) = E_n |\phi_n) \) and \( Z_0 = \sum_n e^{-\beta E_n} \). The equation of motion for the density matrix is:

\[
i\hbar \frac{\partial}{\partial t} \hat{\rho}(t) = [\hat{H}_0 + \hat{V}(t), \hat{\rho}(t)]
\]

We can introduce the so called interaction representation of the density matrix as

\[
\hat{\rho}_I(t) = e^{i\hat{H}_0 t/\hbar} \hat{\rho}(t) e^{-i\hat{H}_0 t/\hbar}
\]

which satisfies

\[
i\hbar \frac{\partial}{\partial t} \hat{\rho}_I(t) = -[\hat{H}_0, \hat{\rho}_I(t)] + e^{i\hat{H}_0 t/\hbar} [\hat{H}_0 + \hat{V}(t), \hat{\rho}_I(t)] e^{-i\hat{H}_0 t/\hbar}
\]

\[
= [\hat{V}_I(t), \hat{\rho}_I(t)],
\]

\[8\]
where

\[
\hat{V}_I(t) = \int d^3 x \, e^{i\hat{H}_0 t/\hbar} \hat{A}(x) e^{-i\hat{H}_0 t/\hbar} \hat{V}(x, t) = \int d^3 x \hat{A}(x, t) \hat{V}(x, t).
\] (8)

\(\hat{A}(x, t)\) is the Heisenberg time evolution of \(\hat{A}(x)\) with the unperturbed Hamiltonian.

We solve perturbatively equation (7) in \(\hat{V}_I\), i.e. \(\hat{\rho}_I(t) = \hat{\rho}_I(0) + \hat{\rho}_I^{(1)}(t) + \ldots\) where \(\hat{\rho}^n(t)\) contains the \(n\)-powers of the perturbation. Obviously

\[
\lim_{t \to -\infty} \hat{\rho}_I(t) = \hat{\rho}_0 = \hat{\rho}_I^{(0)}(t)
\] (9)

We limit our analysis to the linear response, so we need only the first order term which satisfies:

\[
i\hbar \frac{\partial}{\partial t} \hat{\rho}_I^{(1)}(t) = [\hat{V}_I(t), \hat{\rho}_I^{(0)}(t)]
\] (10)

with solution:

\[
\hat{\rho}_I^{(1)}(t) = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' [\hat{V}_I(t'), \hat{\rho}_0].
\] (11)

Thus, at linear order we can write:

\[
\langle \hat{B}(x, t) \rangle = Tr[\hat{\rho}(t) \hat{B}(x)] = Tr[\hat{\rho}_I(t) e^{i\hat{H}_0 t/\hbar} \hat{B}(x) e^{-i\hat{H}_0 t/\hbar}] = Tr[\hat{\rho}_I(t) \hat{B}(x, t)] \\
\simeq Tr[\hat{\rho}_0(t) \hat{B}(x)] + Tr[\hat{\rho}_I(t)^{(1)} \hat{B}(x, t)] = \langle \hat{B}(x) \rangle_0 + Tr[\hat{\rho}_I(t)^{(1)} \hat{B}(x, t)],
\] (12)

where we use the fact that the unperturbed average value is given by

\[
Tr[\hat{\rho}_0(t) \hat{B}(x, t)] = Tr[\hat{\rho}_0 \hat{B}(x)] = \langle \hat{B}(x) \rangle_0.
\] (13)
We are interested in the deviation of the average value, namely:

\[
\langle \hat{B}(x, t) \rangle - \langle \hat{B}(x) \rangle_0 = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' Tr\left( [\hat{V}_t(t'), \hat{\rho}_0] \hat{B}(x, t) \right)
\]

\[
= -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3 x' Tr\left( [\hat{A}(x', t'), \hat{\rho}_0] \hat{B}(x, t) \right) V(x', t')
\]

\[
= -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3 x' Tr\left( [\hat{\rho}_0 \hat{A}(x', t'), \hat{B}(x, t)] \right) V(x', t')
\]

\[
= -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3 x' \theta(t - t') Tr\left( [\hat{\rho}_0 [\hat{B}(x, t), \hat{A}(x', t')]] \right) V(x', t') = -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \int d^3 x' \chi_{BA}^{R}(x, x', t - t') V(x', t'),
\]

where in the fourth line we used the linearity and the cyclic property of the trace and in the last line we defined the retarded linear response function as:

\[
\chi_{BA}^{R}(x, x', t - t') = -\frac{i}{\hbar} \theta(t - t') \langle [\hat{B}(x, t), \hat{A}(x', t')] \rangle
\]

where \( \langle \ldots \rangle \) indicates the thermal and quantum average with the unperturbed density matrix.

We now show that any average of pairs of time-evolved operators in the Heisenberg representation only depends on the time difference, since the Schrödinger equation is time-translationally invariant:

\[
\langle \hat{B}(t) \hat{A}(t') \rangle = \frac{1}{Z} Tr\left[ e^{\beta \hat{H}} e^{i\hat{H}t'/\hbar} \hat{B}(x) e^{-i\hat{H}t'/\hbar} e^{i\hat{H}t/\hbar} \hat{A}(x) e^{-i\hat{H}t/\hbar} \right] = \frac{1}{Z} Tr\left[ e^{\beta \hat{H}} e^{i\hat{H}(t-t')/\hbar} \hat{B} e^{-i\hat{H}(t-t')/\hbar} \hat{A} \right] = \langle \hat{B}(t - t') \hat{A}(0) \rangle = \frac{1}{Z} Tr\left[ e^{\beta \hat{H}} \hat{B} e^{i\hat{H}(t-t')/\hbar} e^{i\hat{H}(t-t')/\hbar} \hat{A} \right] = \langle \hat{B}(0) \hat{A}(t' - t) \rangle.
\]

This fact implies that:

\[
\chi_{BA}^{R}(x, x', t - t') = -\frac{i}{\hbar} \theta(t - t') \langle [\hat{B}(x, t - t'), \hat{A}(x')] \rangle
\]
and as \( \hat{A} \) and \( \hat{B} \) are Hermitian operators we obtain the following symmetry property:

\[
\chi_{AB}^R(x, x', t - t')^* = \frac{i}{\hbar}\theta(t - t')\langle[\hat{B}(x', t'), \hat{A}(x, t)]\rangle = \chi_{AB}^R(x, x', t - t')
\] (18)

### 2.1.1 Fluctuation-Dissipation Theorem

We now introduce two other types of correlation functions. The first is the dynamic structure factor, defined by

\[
S_{AB}(x, x', t) = \frac{1}{2\hbar}\langle[\hat{A}(x, t), \hat{B}(x')]\rangle = \frac{1}{2}[S_{AB}(x, x', t) - S_{BA}(x', x, -t)].
\] (19)

The second is the so-called dissipation response function, defined through

\[
\chi_{AB}'(x, x', t) = \frac{1}{2\hbar}\langle[\hat{A}(x, t), \hat{B}(x')]\rangle = \frac{1}{2}\langle[\hat{A}(x, t), \hat{B}(x')]\rangle.
\] (20)

One can verify that \( \chi_{AB}' \) is related to the response function through:

\[
\chi_{AB}'(x, x', t) = \frac{i}{2}[\chi_{AB}^R(x, x', t) - \chi_{BA}^R(x', x, -t)].
\] (21)

If we define the Fourier transform

\[
\chi_{AB}^R(x, x', \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}\chi_{AB}^R(x, x', t)
\] (22)

and

\[
\chi_{AB}'(x, x', \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}\chi_{AB}'(x, x', t)
\] (23)

we obtain

\[
\chi_{AB}'(x, x', \omega) = \frac{i}{2}[\chi_{AB}^R(x, x', \omega) - \chi_{AB}^R(x', x, -\omega)].
\] (24)

In particular if \( \hat{A} = \hat{B} \) we have

\[
\chi_{AA}'(x, x, \omega) = -Im\chi_{AA}'(x, x, \omega).
\] (25)

Likewise, we can Fourier transform relative to time as well:

\[
\chi_{AB}^R(Q, Q', \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}\int d^3xd^3x'e^{-iQ\cdot x}\chi_{AB}^R(x, x', \omega)e^{iQ'\cdot x'}
\] (26)

and similarly for \( \chi_{AB}'(Q, Q', \omega) \). For equal \( Q = Q' \) one can show that:

\[
\chi_{AA}'(Q, Q, \omega) = -Im\chi_{AA}'(Q, Q, \omega).
\] (27)
By applying the definition of the dynamical structure factor we find the following symmetry property:

\[ S_{BA}(x', x, -t) = \frac{1}{Z_0} \text{Tr} \left[ e^{-\beta H_0} e^{-iH_0 t/\hbar} \hat{B}(x') e^{-iH_0 t/\hbar} \hat{A}(x) \right] = \]
\[ = \frac{1}{Z_0} \text{Tr} \left[ e^{-\beta H_0} e^{-iH_0 (t-i\hbar \beta)/\hbar} \hat{A}(x') e^{-iH_0 (t-i\hbar \beta)/\hbar} \hat{B}(x') \right] = \]
\[ = S_{AB}(x, x', t - i\hbar \beta). \quad (28) \]

In the frequency domain Eq.(28) implies that

\[ S_{BA}(x', x, -\omega) = \int_{-\infty}^{\infty} dt e^{-i\omega t} S_{BA}(x', x, t) = \int_{-\infty}^{\infty} dt e^{i\omega t} S_{BA}(x, x', -t) = \]
\[ = \int_{-\infty}^{\infty} dt e^{-i\omega t} S_{AB}(x, x', t - i\hbar \beta) = e^{-\beta \hbar \omega} S_{AB}(x, x', \omega) \quad (29) \]

which leads us to write:

\[ \chi''_{AB}(x, x', \omega) = \frac{1}{2} S_{AB}(x, x', \omega)(1 - e^{-\beta \hbar \omega}). \quad (30) \]

### 2.2 Spectral Representation

The spectral representation of the response functions gives instructive information about their physical meaning. We start from the structure factor which can be written in the following way:

\[ S_{AB}(t) = \frac{1}{\hbar Z} \sum_n e^{-\beta E_n} \langle n | e^{i\hat{H} t/\hbar} \hat{A} e^{-i\hat{H} t/\hbar} \hat{B} | n \rangle = \frac{1}{\hbar Z} \sum_{m,n} e^{-\beta E_n} e^{i(E_n - E_m)t/\hbar} \]
\[ \times \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle. \quad (31) \]

where we do not explicitly indicate the space dependence because the operator \( \hat{A} \) will always refer to \( x \) and \( \hat{B} \) to \( x' \). By its Fourier transformation

\[ S_{AB}(\omega) = \frac{2\pi}{Z} \sum_{m,n} e^{-\beta E_n} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\hbar \omega + E_n - E_m), \quad (32) \]

we identify the physical meaning for \( S_{AB} \): the matrix element \( \langle m | \hat{B} | n \rangle \) is the transition amplitude for the excitation of the initial state \( |n \rangle \) to the final one \( |m \rangle \) induced by the operator \( \hat{B} \). Meanwhile \( \langle n | \hat{A} | m \rangle \) describes the reverse process, now induced by \( \hat{A} \). The excitation followed by relaxation process is weighted by the Boltzmann factor for the initial state and contributes to the spectral function \( S_{AB}(\omega) \) only under the condition that the energy difference \( E_m - E_n \) is \( \hbar \omega \).
Now we write the spectral representation of the dissipation response function, finding that:

\[ \chi''_{AB}(\omega) = \frac{\pi}{Z} \sum_{m,n} e^{-\beta E_n} (1 - e^{\beta \bar{h} \omega}) \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\bar{h} \omega + E_n - E_m) = \]

\[ \frac{\pi}{Z} \sum_{m,n} (e^{-\beta E_n} - e^{-\beta E_m}) \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \delta(\bar{h} \omega + E_n - E_m) \]  

(33)

which means that \( \chi''_{AB}(\omega) \) is the transition amplitude from \(|n\rangle\) to \(|m\rangle\) induced by \(\hat{B}\) and from \(|m\rangle\) to \(|n\rangle\) induced by \(\hat{A}\) weighted by the occupation probability \(p_n = e^{-\beta E_n} / Z\) of the state \(|n\rangle\) minus \(p_m = e^{-\beta E_m} / Z\) of the state \(|m\rangle\).

We can also notice that the difference

\[ p_n - p_m = p_n(1 - p_m) - p_m(1 - p_n) \]  

(34)

represents the probability of \(|n\rangle\) being occupied with empty \(|m\rangle\) minus the opposite, so the \(\chi''_{AB}(\omega)\) measures the absorption minus the emission probability of an energy \(\bar{h} \omega\), so the net absorption probability.

Finally one can analogously derive the spectral representation of the retarded response function \(\chi^R_{AB}(t)\):

\[ \chi^R_{AB}(t) = -\frac{i}{\hbar} \theta(t) \frac{1}{Z} \sum_{m,n} e^{-\beta E_n} \left[ e^{i(E_n - E_m)t/\hbar} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle - e^{-i(E_n - E_m)t/\hbar} \langle n | \hat{B} | m \rangle \langle m | \hat{A} | n \rangle \right] \]

(35)

One can calculate the Fourier transform of this function, which is:

\[ \chi^R_{AB}(\omega) = \frac{1}{Z} \sum_{m,n} \langle n | \hat{A} | m \rangle \langle m | \hat{B} | n \rangle \frac{e^{-\beta E_n} - e^{-\beta E_m}}{\bar{h} \omega - (E_m - E_n) + i\eta} \]

(36)

where \(\eta/\hbar\) is the rate at which the perturbation is switched on, and is taken to be an infinitesimal positive number.

3 Application to a particle sliding on a linear chain

In this section we summarize the results obtained for a particle sliding on harmonic chain, as obtained by E. Panizon et al. [3]. They considered a point-like slider characterized by a mass \(M\), a position \(x_{SL} = v_{SL}t\), interacting via a two-body Lennard-Jones
potential $V_{\text{ext}}$ with each atom of an harmonic chain characterized by particles of mass $m$, nearest-neighbor harmonic couplings with spring constant $K$ and equilibrium spacing $a$.

Therefore the hamiltonian of the perturbed chain can be expressed as follows:

$$H_{\text{chain}} = H_{\text{harm}} + \int_{-\infty}^{\infty} dx V_{\text{ext}}(x,t)n(x).$$  \hspace{1cm} (37)

Using the LRT they calculated the dynamical friction force $F$ generated by sliding, which can be easily related to the dissipated power $P = Fv_{SL}$. This quantity can be expressed as:

$$\frac{dE(t)}{dt} = -\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dt V_{\text{ext}}(x,t) \frac{\partial \chi_{\text{R}}(x,x',t-t')}{\partial t} V_{\text{ext}}(x',t').$$  \hspace{1cm} (38)

Since this is a periodic problem they worked in the $(Q,\omega)$ Fourier domain. Through the study of the symmetries of the density-density response function one can prove that only its imaginary part contributes to the integral. Using the Fluctuation-Dissipation Theorem they related this quantity to the dynamical structure factor. The expression for the structure factor is analytic:

$$S(Q,Q,\omega) = \frac{1}{\hbar a} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{j=-\infty}^{\infty} e^{iQaj} e^{-Q^2 F_j(t,\beta)},$$  \hspace{1cm} (39)

where $j$ is the index which enumerates the atoms of the chain, and $F_j(t,\beta)$ is:

$$F_j(t,\beta) = 2a \int_0^{\pi} \frac{dk}{2\pi} \frac{\hbar}{2m\omega_k} \{(2n(k)+1)[1 - \cos(\omega_k t) \cos(kaj)] + i \sin(\omega_k t) \cos(kaj)\}.$$  \hspace{1cm} (40)

In this formula $n(k)$ is the average number of quanta of the harmonic oscillator, which is given by the Bose distribution, and $\omega_k$ is the frequency of the oscillator.

To proceed they resorted to the one phonon expansion of the exponential (see next section for details):

$$e^{-iQ^2 F_j(t,\beta)} \simeq 1 - Q^2 F_j(t,\beta).$$  \hspace{1cm} (41)

Putting all these results together, Panizon et al. obtained the formula:

$$F = \frac{1}{2mav_{\text{SL}}} \int_0^{\infty} dQ Q^2 |\tilde{v}(Q)|^2 \frac{1}{\pi} \frac{\gamma/2}{(\omega(Q) - Qv_{\text{SL}})^2 - (\gamma/2)^2},$$  \hspace{1cm} (42)

where $\omega(q)$ is the phonon dispersion relation in a extended-zone scheme, and $\tilde{v}(Q)$ is the Fourier transform of the 2-body interaction defining $V_{\text{ext}}$.  

14
4 Particle channeling through a crystal

In this section we come to the main subject of the present work: the dissipation through phonon excitations of a particle (the "slider") channeling through a crystal as sketched in Fig. 1. We apply LRT to evaluate the power that the slider transfers to the crystal vibrations.

4.1 The model

We analyze the dissipation of a particle moving along the z-axis, in a simple cubic crystal, starting from a cell center, moving with velocity $v_{SL} = \hat{e}_3 v_{SL}$. The slider is assumed to approximately follow a constant-speed trajectory $x(t) = x_0 + v_{SL}t$. The initial particle position $x_0 = \sum_{k=1}^{3} \frac{1}{2} a \hat{e}_k$ is located at the center of a lattice cell characterized by lattice spacing $a$. 
Table 1: Natural units of the model and expressions for the main derived mechanical quantities investigated in the present thesis. $a, K, M$ are the lattice spacing, the n.n. spring constant, and the mass of the crystal atoms respectively.

The Hamiltonian of the interacting system is:

$$H_{\text{crys}} = H_{\text{harm}} + \int d^3x V(x,t) \hat{n}(x) .$$

(43)

Its weak interaction with all atoms in the crystal can be modeled with a two body-interaction, depending only on the distance $r$ between the slider and position of the nuclei of the crystal.

Therefore when this interaction is evaluated at the generic distance $r = |x - x(t)|$ one obtains an energy $V(x,t) = v(|x - x_0 - v_{SL}t|)$. We can observe that if $v(r)$ is divergent at the origin as $r^{-u}$, with $u > 3$, also the integral of Eq. (43) diverges if the crystal density is nonzero along $x(t)$. This may causes no problem if we consider a classical crystal, with perfectly localized nuclei, but here we are considering a quantum crystal, whose nuclei are wave functions that spread out in all space. For this reason we adopt the following potential, inspired by the Lennard-Jones potential, but with a parameter $d$ which makes it convergent when $r$ tends to 0.

$$v(r) = 4\epsilon \left[ \left( \frac{\sigma^2}{r^2 + (d\sigma)^2} \right)^6 - \left( \frac{\sigma^2}{r^2 + (d\sigma)^2} \right)^3 \right] .$$

(44)

Figure 2 shows that $v(r)$ exhibits a similar general behaviour as the Lennard-Jones potential. Figure 3 shows that $v(r) \to 4\epsilon(d^{-12} - d^{-6}$ as $r \to 0$. We can also introduce the Fourier transform of the potential, defined by

$$V(x,t) = \int \frac{d^3q}{(2\pi)^3} e^{i\mathbf{q}(\mathbf{x} - v_{SL}t - x_0)} \tilde{v}(\mathbf{q}) .$$

(45)
Figure 2: Comparison between the adopted slider-crystal potential $v(r)$, Eq (44), evaluated for $d = 0.5$, green solid line, and LJ potential, violet dashed line.

Figure 3: Some of Fig. 2, but over a broader range, showing that $v(r)$ converges to a finite $v(0) = 4\epsilon(d^{-12} - d^{-6}) = 16336$ for $d = 0.5$.
Figure 4: Fourier transform of the adopted slider-crystal potential $v(r)$, Eq(47), evaluated for $d = 0.5$.

We can write $V(q)$ as follows:

$$\tilde{v}(q) = \int d^3x \, e^{-iq \cdot x} v(|x|) = 2\pi \int_0^\infty dr \, r^2 v(r) \int_{-1}^{1} d\cos \theta \, e^{-iqr\cos \theta} =$$

$$= \frac{4\pi}{q} \int_0^\infty dr \, r v(r) \sin(qr) \cdot \tag{46}$$

Here $\tilde{v}(q) = \tilde{v}(q)$ is a real function.

We calculate analytically this Fourier Transform, of our potential, which, for $d = 1/2$, is:

$$\tilde{v}(q) = \frac{\pi^2}{15} \epsilon \sigma^2 \left[ (q\sigma)^3 + 20(q\sigma)^2 + 780q\sigma + 1560 \right] e^{-q\sigma/2}. \tag{47}$$

Figure 4 reports this function $\tilde{v}(q)$. We notice that it has a finite value $104\pi^2 \epsilon^2 \sigma^2$ for $q = 0$, and that it decreases smoothly to 0 for large $q$. For comparison we also report the Fourier transform of the potential for other values of $d$, such as $d = 0.4$, Fig.5 and $d = 0.6$, Fig. 6. Note that the rapid decay at large $q$ remains a constant feature.
Figure 5: Same as Fig.4, but for $d = 0.4$

Figure 6: Same as Fig.4, but for $d = 0.6$
4.2 Dissipated power from a crystal lattice

In analogy with the 1D example, Eq (38), we calculate the power dissipated by the slider through the Linear Response Theory which tells us that:

\[
P = \frac{dE(t)}{dt} = -\int d^3x V(x, t) \frac{\partial \langle \hat{n}(x) \rangle_t}{\partial t} = -\int d^3x \int d^3x' \int dt' V(x, t) \frac{\partial \chi_{nn}^R(x, x', t-t')}{\partial t} V(x', t')
\]

where \( E(t) \) is the internal energy of the crystal and the retarded density-density response function is defined by

\[
\chi_{nn}^R(x, x', t-t') = -\frac{i}{\hbar} \theta(t-t') \langle [\hat{n}(x, t), \hat{n}(x', t')] \rangle,
\]

see Eq (15). Using the translational invariance of the crystal we can write the Fourier transform of this function

\[
\chi_{nn}^R(x, x', t-t') = \sum_G \int \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} e^{iQ \cdot x} \chi_{nn}^R(Q, Q+G; \omega) e^{-i(Q+G) \cdot x'}. \tag{50}
\]

In analogy with the 1D example we expression the average power dissipated by the slider in terms of Fourier representation. In Fourier representation the power becomes:

\[
P = \frac{1}{\tau} \int_0^\tau dt \int d^3x \int d^3x' \int_{-\infty}^{+\infty} dt' \int \frac{d^3q}{(2\pi)^3} \int \frac{d^3q'}{(2\pi)^3} \sum_G \int \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \times
\]

\[
e^{-iq \cdot x_0} e^{iq' \cdot x_0} e^{i(q+Q) \cdot x} e^{-i(q'+Q+G) \cdot x'} e^{-i(t(t'+\omega+q \cdot v_{SL})} e^{it'(\omega+q' \cdot v_{SL})} (-i\omega) \times
\]

\[
\chi_{nn}^R(Q, Q+G; \omega) \tilde{v}(|q|) \tilde{v}(|q'|).
\]

where \( \tau \) is the period \( a/|v_{SL}| \), which is the time the slider takes to run across one lattice cell.
4.2.1 Symmetries

The integration over \( x \) and \( x' \) gives a delta function for \( q \) and one for \( q' \):

\[
P = \frac{i}{\tau} \int_{0}^{\tau} dt \int_{-\infty}^{+\infty} dt' \int d^{3}q \int d^{3}q' \sum_{G} \int \frac{d^{3}Q}{(2\pi)^{3}} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega \delta(q + Q)\delta(q' + Q + G) \times
\]

\[
e^{-iq_{0}e^{i\omega_{q}v_{\perp}}e^{-it(\omega+q)v_{\perp}}e^{it'(\omega+q')v_{\perp}}} \chi_{\perp}^{R}(Q, Q + G; \omega) \tilde{v}(|q|) \tilde{v}(|q'|)
\]

\[
= \frac{i}{\tau} \int_{0}^{\tau} dt \int_{-\infty}^{+\infty} dt' \sum_{G} \int \frac{d^{3}Q}{(2\pi)^{3}} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \omega \times
\]

\[
e^{-iQ_{0}e^{-i(Q + G)\cdot x_{0}}e^{-it(\omega - Q)v_{\perp}}e^{it'(\omega - (Q + G)\cdot v_{\perp})} \chi_{\perp}^{R}(Q, Q + G; \omega) \tilde{v}(|Q|) \tilde{v}(|Q + G|)
\]

\[
= \frac{i}{\tau} \int_{0}^{\tau} dt \sum_{G} \int \frac{d^{3}Q}{(2\pi)^{3}} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} 2\pi \delta(\omega - (Q + G) \cdot \mathbf{v}_{\perp}) \times
\]

\[
e^{-iG_{0}e^{-it(\omega - Q)\cdot v_{\perp}}e^{it'(\omega - (Q + G)\cdot v_{\perp})} \chi_{\perp}^{R}(Q, Q + G; \omega) \tilde{v}(|Q|) \tilde{v}(|Q + G|)}
\]

\[
= \frac{i}{\tau} \int_{0}^{\tau} dt \sum_{G} \int \frac{d^{3}Q}{(2\pi)^{3}} e^{-iG_{0}e^{-it(\omega - Q)\cdot v_{\perp}}e^{it'(\omega - (Q + G)\cdot v_{\perp})} \chi_{\perp}^{R}(Q, Q + G; \omega) \cdot \mathbf{v}_{\perp} \chi_{\perp}^{R}(Q, Q + G; (Q + G) \cdot \mathbf{v}_{\perp})} \times
\]

\[
\tilde{v}(|Q|) \tilde{v}(|Q + G|).
\]

The integral over \( dt \) gives a \( \tau \delta_{G_{\|},0} \), where \( G_{\|} \) is the component of the vector \( G \) in the direction of the sliding velocity, here simply the \( z \) component of \( G \).

\[
P = \int_{G_{\perp}} e^{-iG_{\perp} \cdot x_{0}} \int \frac{d^{3}Q}{(2\pi)^{3}} (Q \cdot \mathbf{v}_{\perp}) \chi_{\perp}^{R}(Q, Q + G_{\perp}; Q \cdot \mathbf{v}_{\perp}) \tilde{v}(|Q|) \tilde{v}(|Q + G_{\perp}|). (51)
\]

Splitting the real part and the imaginary part of the response function we obtain

\[
P = \int_{G_{\perp}} e^{-iG_{\perp} \cdot x_{0}} \int \frac{d^{3}Q}{(2\pi)^{3}} (Q \cdot \mathbf{v}_{\perp}) \chi_{\perp}^{R}(Q, Q + G_{\perp}; Q \cdot \mathbf{v}_{\perp}) \tilde{v}(|Q|) \tilde{v}(|Q + G_{\perp}|) +
\]

\[
- \sum_{G_{\perp}} e^{-iG_{\perp} \cdot x_{0}} \int \frac{d^{3}Q}{(2\pi)^{3}} (Q \cdot \mathbf{v}_{\perp}) \chi_{\perp}^{R}(Q, Q + G_{\perp}; Q \cdot \mathbf{v}_{\perp}) \tilde{v}(|Q|) \tilde{v}(|Q + G_{\perp}|).
\]

\[
(52)
\]

4.2.1 Symmetries

In order to study the symmetries of the density density response function we consider each vector \( G_{\perp} \) together with the symmetric one \( -G_{\perp} \). In this way we can consider the function \( \chi_{\perp}(Q, Q + G_{\perp}, t - t') \) given by

\[
\chi_{\perp}^{R}(Q, Q + G_{\perp}, t - t') = \int d^{3}x \int d^{3}x' e^{iQ \cdot x} \chi_{\perp}^{R}(x, x', t - t') e^{-i(Q + G_{\perp}) \cdot x'}.
\]

(53)
together with the function \( \chi^R_{nn}(Q, Q - G_{\perp}, t - t') \) given by

\[
\chi^R_{nn}(Q, Q - G_{\perp}, t - t') = \int d^3x \int d^3x' e^{iQ\cdot x} \chi^R_{nn}(x, x', t - t') e^{-i(Q - G_{\perp})\cdot x'}. \tag{54}
\]

If we sum the contribution of Eq. (53) and (54) we obtain the expression

\[
\chi^R_{nn}(Q, Q + G_{\perp}, t - t') + \chi^R_{nn}(Q, Q - G_{\perp}, t - t') = \int d^3x \int d^3x' e^{iQ\cdot x} \chi^R_{nn}(x, x', t - t') [e^{-i(Q + G_{\perp})\cdot x'} + e^{-i(Q - G_{\perp})\cdot x'}]. \tag{55}
\]

Replacing \( Q \) with \(-Q\), the first exponential becomes its complex conjugate. We notice that the Fourier factors in the bracket behave in the same way. Explicitly they become:

\[
e^{-i(-Q + G_{\perp})\cdot x'} + e^{-i(-Q - G_{\perp})\cdot x'} = e^{i(Q - G_{\perp})\cdot x'} + e^{i(Q + G_{\perp})\cdot x'}. \tag{56}
\]

Consequently we obtain

\[
\chi^R_{nn}(Q, Q + G_{\perp}, t - t') + \chi^R_{nn}(Q, Q - G_{\perp}, t - t') = [\chi^R_{nn}(-Q, -Q + G_{\perp}, t - t') + \chi^R_{nn}(-Q, -Q - G_{\perp}, t - t')]^*. \tag{57}
\]

We note that the real part of this expression is an even function of \( Q \) while the imaginary part of this expression is odd.

This result applies (even more simply) to the \( G_{\perp} = 0 \) case. As a consequence, only the imaginary part contributes of \( \chi^R_{nn} \) to the integral of Eq. (52), then we can write

\[
P = -\sum_{G_{\perp}} e^{-iG_{\perp}\cdot x_0} \int \frac{d^3Q}{(2\pi)^3} (Q \cdot v_{SL}) Im \chi^R_{nn}(Q, Q + G_{\perp}; Q \cdot v_{SL}) \hat{v}(|Q|) \hat{v}(|Q + G_{\perp}|). \tag{58}
\]

Since we found no solution to use the Fluctuation-Dissipation theorem, which correlates the imaginary part of the response function to the structure factor when \( G_{\perp} \neq 0 \) we focus our analysis to the "central" term of this sum, the one with \( G_{\perp} = 0 \) assuming that the \( G \neq 0 \) are smaller. Thus, Eq. (58) becomes:

\[
P = -\int \frac{d^3Q}{(2\pi)^3} (Q \cdot v_{SL}) Im \chi^R_{nn}(Q, Q; Q \cdot v_{SL}) |\hat{v}(|Q|)|^2 \tag{59}
\]

\[
= -8 \int_{\Omega} \frac{d^3Q}{(2\pi)^3} (Q \cdot v_{SL}) Im \chi^R_{nn}(Q, Q; Q \cdot v_{SL}) |\hat{v}(|Q|)|^2,
\]

where \( \Omega \) is the subdomain given by \( (Q_x \geq 0, Q_y \geq 0, Q_z \geq 0) \).
Now we can use the Fluctuation-Dissipation Theorem and we can write the imaginary part of the response function as follows:

$$\text{Im} \chi_R^{nn}(Q; Q; v_{SL}) = -\frac{1}{2} S_{nn}(Q; Q; v_{SL})(1 - e^{-\beta \hbar |Q| v_{SL}}),$$  \hspace{1cm} (60)

where $S_{nn}(Q; Q; \omega)$ is the Fourier transform of the structure factor, see Eq.(19). Therefore the Eq. (59) becomes:

$$P = 4 \int_{\Omega} \frac{d^3Q}{(2\pi)^3} (Q \cdot v_{SL}) S_{nn}(Q; Q; v_{SL})(1 - e^{-\beta \hbar |Q| v_{SL}})|\tilde{\nu}(|Q|)|^2. \hspace{1cm} (61)$$

### 4.2.2 Response of the harmonic crystal

In this section we summarize the quantum theory of a three-dimensional harmonic crystal. We can express the position operator of the $j$-th atom as

$$\hat{x}_j = \mathbf{R}_j + \hat{u}^{(\mathbf{R}_j)}.$$  \hspace{1cm} (62)

where $\hat{u}^{(\mathbf{R}_j)}$ is the displacement from the equilibrium position $\mathbf{R}_j$. The harmonic Hamiltonian $\hat{H}_0$ is given by

$$\hat{H}_0 = \sum_j \hat{P}_{j}^2(\mathbf{R}_j) \frac{2M}{2} \sum_{j,j'} \hat{u}_\mu(\mathbf{R}_j) D_{\mu\nu}(\mathbf{R}_j - \mathbf{R}_{j'}) \hat{u}_\nu(\mathbf{R}_{j'})$$  \hspace{1cm} (63)

where $D_{\mu\nu}(\mathbf{R}_j - \mathbf{R}_{j'})$ is defined as:

$$D_{\mu\nu}(\mathbf{R}_j - \mathbf{R}_{j'}) = \frac{\partial^2 U}{\partial u_\mu(\mathbf{R}_j) \partial u_\nu(\mathbf{R}_{j'})}.$$  \hspace{1cm} (64)

and $U$ is the total crystal potential energy.

$\hat{H}_0$ can be expressed in terms of the phonon annihilation and creation operators $\hat{b}_{k\lambda}$ and $\hat{b}_{k\lambda}^\dagger$ in the following way:

$$\hat{H}_0 = \sum_k^{BZ} \sum_{\lambda=1}^3 h\omega_{\lambda}(k) \left( \hat{b}_{k\lambda}^\dagger \hat{b}_{k\lambda} + \frac{1}{2} \right)$$  \hspace{1cm} (65)

where $k$ belongs to the first Brillouin zone and $\lambda$ is the polarization of the phonon.

The annihilation operator is defined by

$$\hat{b}_{k\lambda} = \frac{1}{\sqrt{N}} \sum_j \epsilon_\lambda(k) \cdot \left[ \sqrt{\frac{M\omega_{\lambda}(k)}{2\hbar}} \hat{u}(\mathbf{R}_j) + i \sqrt{\frac{1}{2\hbar M\omega_{\lambda}(k)}} \hat{p}(\mathbf{R}_j) \right]$$  \hspace{1cm} (66)
and its adjoint, the creation operator is defined by

\[ \hat{b}^\dagger_{k\lambda} = \frac{1}{\sqrt{N}} \sum_j \epsilon_\lambda(k) \left[ \sqrt{\frac{M\omega_\lambda(k)}{2\hbar}} \hat{u}(R_j) - i \sqrt{\frac{1}{2\hbar M\omega_\lambda(k)}} \hat{p}(R_j) \right] \]  

(67)

where \( \epsilon_\lambda(k) \) are the eigenvectors of the dynamical matrix

\[ D_{\mu\nu}(k) = \sum_j D_{\mu\nu}(R_j)e^{ikR_j}. \]  

(68)

We can now express the displacement \( \hat{u}(R_j) \) in terms of the creation and annihilation operators:

\[ \hat{u}(R_j) = \frac{1}{\sqrt{N}} \sum_{k,\lambda} \sqrt{\frac{\hbar}{2M\omega_\lambda(k)}} \epsilon_\lambda(k)e^{ikR_j}(\hat{b}_{k\lambda} + \hat{b}^\dagger_{-k\lambda}). \]  

(69)

It is useful to express the density operator \( \hat{n}(x) = \sum_j \delta_\lambda(x - \hat{x}_j) \) in terms of the phonon operators. We can introduce

\[ \hat{n}_q = \int_V d^3x \hat{n}(x)e^{-iq\cdot x} = \int_V d^3x \sum_j \delta_\lambda(x - \hat{x}_j)e^{-iq\cdot x} = \sum_j e^{-iq\cdot R_j}e^{-iq\cdot \hat{u}(R_j)}. \]  

(70)

In terms of \( \hat{n}_q \),

\[ \hat{n}(x) = \frac{1}{V} \sum_q \hat{n}_q e^{iq\cdot x} = \frac{1}{V} \sum_q \sum_j e^{iq\cdot (x-R_j)}e^{iq\cdot \hat{u}(R_j)}. \]  

(71)

We can then calculate the Heisenberg free time evolution of the operator \( \hat{u}_j \), which is

\[ \hat{u}(R_j, t) = e^{\frac{i}{\hbar}H_0t}\hat{u}(R_j)e^{-\frac{i}{\hbar}H_0t} = \frac{1}{\sqrt{N}} \sum_{k,\lambda} \sqrt{\frac{\hbar}{2M\omega_\lambda(k)}} \epsilon_\lambda(k)e^{ikR_j}(e^{-i\omega_\lambda(k)t}\hat{b}_{k\lambda} + e^{i\omega_\lambda(k)t}\hat{b}^\dagger_{-k\lambda}). \]  

(72)

As a consequence the time evolution for the density operator is expressed by the formula:

\[ \hat{n}(x, t) = \frac{1}{V} \sum_q \sum_j e^{iq\cdot (x-R_j)}e^{iq\cdot \hat{u}(R_j, t)} \]  

(73)

and in the Fourier space we obtain:

\[ \hat{n}_q(t) = \sum_j e^{-iq\cdot R_j}e^{iq\cdot \hat{u}(R_j, t)}. \]  

(74)
4.2.3 Dynamic structure factor for the harmonic crystal

In this section we calculate the dynamical structure factor in order to obtain an expression for the friction force. Using the Fourier transform of the structure factor we obtain:

$$ S_{nn}(Q, Q', \omega) = \frac{1}{\hbar} \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3 x' e^{-iQ \cdot x'} \frac{1}{V} \int d^3 x \langle \hat{n}(\mathbf{x} + \mathbf{x}', t) \hat{n}(\mathbf{x}, 0) \rangle, \quad \text{(75)} $$

where $V$ is the volume of the crystal. Taking into consideration an infinite crystal we obtain:

$$ S_{nn}(Q, Q', \omega) \simeq \frac{1}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \int \frac{d^3 q}{(2\pi)^3} \frac{d^3 q'}{(2\pi)^3} \langle \hat{n}_{\mathbf{q}}(t) \hat{n}_{\mathbf{q}'}(0) \rangle \int d^3 x' e^{i(Q - Q') \cdot x'} $$

$$ \times \frac{1}{V} \int d^3 x e^{i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{x}} = \frac{1}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3 q d^3 q' \langle \hat{n}_{\mathbf{q}}(t) \hat{n}_{\mathbf{q}'}(0) \rangle \delta_3(\mathbf{q} - Q) \delta_3(\mathbf{q} + \mathbf{q}') $$

$$ = \frac{1}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{n}_{\mathbf{Q}}(t) \hat{n}_{-\mathbf{Q}}(0) \rangle. \quad \text{(76)} $$

Using the formula (74) the previous expression becomes:

$$ S_{nn}(Q, Q', \omega) \simeq \frac{1}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_{j, j'} e^{-iQ \cdot (\mathbf{R}_j - \mathbf{R}_{j'})} \langle e^{-iQ \cdot \hat{u}(\mathbf{R}_j, t)} e^{iQ \cdot \hat{u}(\mathbf{R}_{j'}, 0)} \rangle = $$

$$ = \frac{N}{\hbar V} \int_{-\infty}^{\infty} dt e^{i\omega t} \sum_j e^{-iQ \cdot \mathbf{R}_j} \langle e^{-iQ \cdot \hat{u}(\mathbf{R}_j, t)} e^{iQ \cdot \hat{u}(\mathbf{R}_0, 0)} \rangle, \quad \text{(77)} $$

where in the last line we used the discrete translational symmetry of the crystal.

To evaluate the averages we use the Gaussian identity $\langle e^{A} e^{B} \rangle = e^{\frac{1}{2} \langle A^2 \rangle} e^{\frac{1}{2} \langle B^2 \rangle} e^{\langle AB \rangle}$ valid for harmonic oscillator operators.

A direct application of this formula with $\hat{A} = -i\mathbf{Q} \cdot \hat{u}(\mathbf{R}_j, t)$ and $\hat{B} = i\mathbf{Q} \cdot \hat{u}(\mathbf{R}_0, 0)$ leads us to

$$ \langle e^{-iQ \cdot u(\mathbf{R}_j, t)} e^{iQ \cdot u(\mathbf{R}_0, 0)} \rangle = e^{-\frac{1}{2} \langle Q \cdot u(\mathbf{R}_j, t) \rangle \langle Q \cdot u(\mathbf{R}_j, t) \rangle} e^{-\frac{1}{2} \langle Q \cdot u(\mathbf{R}_0, 0) \rangle \langle Q \cdot u(\mathbf{R}_0, 0) \rangle} e^{\langle Q \cdot u(\mathbf{R}_j, t) \rangle \langle Q \cdot u(\mathbf{R}_0, 0) \rangle} \quad \text{(78)} $$

where the first term represents the fluctuations from the equilibrium position of the $j$th atom at the time $t$, the second represents the fluctuations from the equilibrium position of the atom at the origin at $t = 0$ and the third the correlation of two different atoms at different time.
Using the expression (72) for the displacements we can write:

\[
\langle \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_j, t) \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_j, t) \rangle = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}', \lambda, \lambda'} \mathbf{Q} \cdot \epsilon_\lambda(\mathbf{k}) \mathbf{Q} \cdot \epsilon_{\lambda'}(\mathbf{k}') \frac{\hbar}{2M \sqrt{\omega_\lambda(\mathbf{k}) \omega_{\lambda'}(\mathbf{k}')}} e^{i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{R}_j} \\
\langle e^{-i\omega_\lambda(\mathbf{k}) t} \hat{b}_{\mathbf{k}\lambda} + e^{i\omega_\lambda(\mathbf{k}) t} \hat{b}_{\mathbf{k}\lambda}^\dagger \rangle \langle e^{-i\omega_{\lambda'}(\mathbf{k}') t} \hat{b}_{\mathbf{k}'\lambda'} + e^{i\omega_{\lambda'}(\mathbf{k}') t} \hat{b}_{\mathbf{k}'\lambda'}^\dagger \rangle = \\
= \frac{1}{N} \sum_{\mathbf{k}, \mathbf{k}', \lambda, \lambda'} \mathbf{Q} \cdot \epsilon_\lambda(\mathbf{k}) \mathbf{Q} \cdot \epsilon_{\lambda'}(\mathbf{k}') \frac{\hbar}{2M \sqrt{\omega_\lambda(\mathbf{k}) \omega_{\lambda'}(\mathbf{k}')}} e^{i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{R}_j} \\
\langle e^{-i\omega_\lambda(\mathbf{k}) t} e^{-i\omega_{\lambda'}(\mathbf{k}') t} \hat{b}_{\mathbf{k}\lambda} \hat{b}_{\mathbf{k}'\lambda'} + e^{-i\omega_\lambda(\mathbf{k}) t} e^{i\omega_{\lambda'}(\mathbf{k}') t} \langle \hat{b}_{\mathbf{k}\lambda} \hat{b}_{\mathbf{k}'\lambda'}^\dagger \rangle + \\
e^{i\omega_\lambda(\mathbf{k}) t} e^{-i\omega_{\lambda'}(\mathbf{k}') t} \langle \hat{b}_{\mathbf{k}\lambda}^\dagger \hat{b}_{\mathbf{k}'\lambda'} \rangle + e^{i\omega_\lambda(\mathbf{k}) t} e^{i\omega_{\lambda'}(\mathbf{k}') t} \langle \hat{b}_{\mathbf{k}\lambda} \hat{b}_{\mathbf{k}'\lambda'}^\dagger \rangle \rangle = \\
= \frac{1}{N} \sum_{\mathbf{k}} \sum_{\lambda} \mathbf{Q} \cdot \epsilon_\lambda(\mathbf{k}) \mathbf{Q} \cdot \epsilon_\lambda(-\mathbf{k}) \frac{\hbar}{2M \omega_\lambda(\mathbf{k})} \\
\langle \hat{b}_{\mathbf{k}\lambda} \hat{b}_{\mathbf{k}\lambda}^\dagger + \langle \hat{b}_{\mathbf{k}\lambda}^\dagger \hat{b}_{\mathbf{k}\lambda} \rangle \rangle = \\
= \frac{1}{N} \sum_{\mathbf{k}} \sum_{\lambda} |\mathbf{Q} \cdot \epsilon_\lambda(\mathbf{k})|^2 \frac{\hbar}{2M \omega_\lambda(\mathbf{k})} \langle \hat{b}_{\mathbf{k}\lambda} \hat{b}_{\mathbf{k}\lambda}^\dagger + \langle \hat{b}_{\mathbf{k}\lambda}^\dagger \hat{b}_{\mathbf{k}\lambda} \rangle \rangle \\
(79)
\]

where in the last two lines we used the orthonormality of quantum states, the parity of \( \omega_\lambda(\mathbf{k}) \) and the fact that \( \epsilon_\lambda(-\mathbf{k}) = \epsilon_\lambda^*(\mathbf{k}) \) (in a monoatomic Bravais lattice, as in our model, the dynamical matrix, Eq. (64), is real, so we can take \( \epsilon_\lambda(-\mathbf{k}) = \epsilon_\lambda(\mathbf{k}) \)). Observe that \( \langle \hat{b}_{\mathbf{k}\lambda}^\dagger \hat{b}_{\mathbf{k}\lambda} \rangle = 1 \) and \( \langle \hat{b}_{\mathbf{k}\lambda}^\dagger \hat{b}_{\mathbf{k}\lambda} \rangle \) is the average number of quanta \( n_\lambda(\mathbf{k}) \) in that oscillator. The equilibrium average number of quanta follows the Bose-Einstein formula and is therefore a function of the ratio \( \hbar \omega_\lambda(\mathbf{k})/k_B T \). As a consequence \( n_\lambda(\mathbf{k}) \) is an even function of \( \mathbf{k} \). We obtain:

\[
\langle \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_j, t) \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_j, t) \rangle = \frac{1}{N} \sum_{\mathbf{k}} \sum_{\lambda} |\mathbf{Q} \cdot \epsilon_\lambda(\mathbf{k})|^2 \frac{\hbar}{2M \omega_\lambda(\mathbf{k})} (2n_\lambda(\mathbf{k}) + 1) = \\
= \langle \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_0, 0) \mathbf{Q} \cdot \hat{\mathbf{u}}(\mathbf{R}_0, 0) \rangle. \tag{80}
\]

As expected, the obtained result depends neither on \( j \) nor on time, because the equilibrium fluctuations of each atom of the crystal are the same at all times.

Now we calculate the correlation of two different atoms at different times, setting
\( R_0 = 0 \), for simplicity:

\[
\langle Q \cdot \hat{u}(R_j, t) Q \cdot \hat{u}(R_0, 0) \rangle = \frac{1}{N} \sum_{k,k',\lambda,\lambda'} Q \cdot \epsilon_\lambda(k) Q \cdot \epsilon_{\lambda'}(k') \frac{\hbar}{2M \sqrt{\omega_\lambda(k)\omega_{\lambda'}(k')}} e^{i k R_j} \\
\langle e^{-i \omega_\lambda(k)t} \hat{b}_{k\lambda} + e^{i \omega_\lambda(k)t} \hat{b}_{k\lambda}^\dagger \rangle (\hat{b}_{k'\lambda'} + \hat{b}_{k'\lambda'}^\dagger) = \\
\frac{1}{N} \sum_{k,k',\lambda,\lambda'} Q \cdot \epsilon_\lambda(k) Q \cdot \epsilon_{\lambda'}(k') \frac{\hbar}{2M \sqrt{\omega_\lambda(k)\omega_{\lambda'}(k')}} e^{i k R_j} \\
\langle e^{-i \omega_\lambda(k)t} \hat{b}_{k\lambda} \hat{b}_{k'\lambda'} + e^{-i \omega_\lambda(k)t} \hat{b}_{k\lambda}^\dagger \hat{b}_{k'\lambda'} + e^{i \omega_\lambda(k)t} \hat{b}_{k\lambda} \hat{b}_{k'\lambda'} + e^{i \omega_\lambda(k)t} \hat{b}_{k\lambda}^\dagger \hat{b}_{k'\lambda'}^\dagger \rangle = \\
\frac{1}{N} \sum_{k,\lambda} \langle Q \cdot \epsilon_\lambda(k) \rangle^2 \frac{\hbar}{2M \omega_\lambda(k)} [\cos(k \cdot R_j) + i \sin(k \cdot R_j)] \\
\langle (n_\lambda(k) + 1)(\cos(\omega_\lambda(k)t) - i \sin(\omega_\lambda(k)t)) + \\
+ n_\lambda(k)(\cos(\omega_\lambda(k)t) + i \sin(\omega_\lambda(k)t)) \rangle = \\
\frac{1}{N} \sum_{k,\lambda} \langle Q \cdot \epsilon_\lambda(k) \rangle^2 \frac{\hbar}{2M \omega_\lambda(k)} \cos(k \cdot R_j) [2n_\lambda(k) + 1] \langle \cos(\omega_\lambda(k)t) - i \sin(\omega_\lambda(k)t) \rangle \],
\]

(81)

where in the last line we used the fact that \( \sin(k \cdot R_j) \) does not contribute to the sum, since it is an odd factor in \( k \), that multiplies only even function of \( k \).

By combining these results we can rewrite the dynamical structure factor as follows:

\[
S_{mn}(Q, Q, \omega) = \frac{N}{\hbar V} \int_{-\infty}^{\infty} dt e^{i \omega t} \sum_j e^{-i Q \cdot R_j} e^{-\Phi_j(Q, t, \beta)},
\]

(82)

where we introduced the function \( \Phi_j(Q, t, \beta) \) defined as:

\[
\Phi_j(Q, t, \beta) = \frac{1}{N} \sum_{k,\lambda} \langle Q \cdot \epsilon_\lambda(k) \rangle^2 \frac{\hbar}{2M \omega_\lambda(k)} \times \\
\{(2n_\lambda(k) + 1)[1 - \cos(\omega_\lambda(k)t) \cos(k \cdot R_j)] + i \sin(\omega_\lambda(k)t) \cos(k \cdot R_j) \}.
\]

(83)
Since we are interested in an infinite crystal (thermodynamic limit) the previous expression becomes:

\[ \Phi_j(Q, t, \beta) = a^3 \sum_\lambda \int_{BZ} \frac{d^3k}{(2\pi)^3} |Q \cdot \epsilon_\lambda(k)|^2 \frac{\hbar}{2M\omega_\lambda(k)} \times \]

\( \{(2n_\lambda(k) + 1)[1 - \cos(\omega_\lambda(k)t) \cos(k \cdot R_j)] + i \sin(\omega_\lambda(k)t) \cos(k \cdot R_j)\} \).

(84)

4.2.4 Evaluation of the dissipated power

We can now combine Eq. (61) with the expression (82) of the dynamic structure factor and write the dissipated power as follow:

\[ P = \frac{4N}{\hbar V} \int\int d^3Q e^{iQ \cdot v_{SL}t} \sum_j Q \cdot v_{SL} e^{-iQ \cdot R_j} e^{-\Phi_j(Q, t, \beta)} (1 - e^{-\beta\hbar Q \cdot v_{SL}}) |\tilde{\nu}(|Q|)|^2. \]

(85)

Since we can find no way to evaluate this expression we resort to an expansion of the \( e^{-\Phi_j(Q, t, \beta)} \) exponential.

\[ e^{-\Phi_j(Q, t, \beta)} = \sum_{m=0}^\infty \frac{1}{m!} [-\Phi_j(Q, t, \beta)]^m. \]

(86)

As is done in the theory of neutron scattering one can classify the expansion terms according to the number \( m \) of phonons emitted and/or absorbed by the moving particle: It can be shown that the \( m \)th term in this expansion gives the contribution of the excitation of \( m \) phonons to the total scattering cross section.

Here we resort to the one phonon expansion, i.e. we approximate the exponential in the following way:

\[ e^{-\Phi_j(Q, t, \beta)} \simeq 1 - \Phi_j(Q, t, \beta). \]

(87)

We can easily show that the zero-phonon term, the one associated to Bragg scattering, does not contribute to the integral:

\[ P^{(0)} = \frac{4N}{\hbar V} \int\int d^3Q e^{iQ \cdot v_{SL}t} \sum_j Q \cdot v_{SL} e^{-iQ \cdot R_j} (1 - e^{-\beta\hbar Q \cdot v_{SL}}) |\tilde{\nu}(|Q|)|^2 = \]

\[ = \frac{4N}{\hbar V} \int\int d^3Q e^{iQ \cdot v_{SL}t} \sum_j Q \cdot v_{SL} e^{-iQ \cdot R_j} (1 - e^{-\beta\hbar Q \cdot v_{SL}}) |\tilde{\nu}(|Q|)|^2 = 0. \]

(88)
Since $\Phi_j(Q,t,\beta)$ is a complex function it is useful to calculate separately the contribution to the 1-phonon power dissipated due to its real part and to its imaginary part. We start from the real part:

$$P_{Re} = -\frac{4N}{\hbar V} \sum_{\lambda} \int_{\Omega} \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{\infty} dt \int_{\mathcal{BZ}} \frac{d^3k}{(2\pi)^3} e^{iQ \cdot v_{SL} t} \sum_j Q \cdot v_{SL} e^{-iQ \cdot R_j} (1 - e^{-\beta \hbar Q \cdot v_{SL}})$$

$$|\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2 \frac{\hbar}{2M \omega_\lambda(k)} (2n_\lambda(k) + 1) [1 - \cos(\omega_\lambda(k)t) \cos(k \cdot R_j)]$$

$$= \frac{2}{M} \sum_{\lambda} \int_{\Omega} \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{\infty} dt \int_{\mathcal{BZ}} \frac{d^3k}{(2\pi)^3} e^{iQ \cdot v_{SL} t} \sum_j Q \cdot v_{SL} e^{-i(Q \cdot R_j)} (1 - e^{-\beta \hbar Q \cdot v_{SL}})$$

$$|\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2 \frac{1}{\omega_\lambda(k)} (2n_\lambda(k) + 1) \cos(\omega_\lambda(k)t) \cos(k \cdot R_j)$$

(89)

Now we use the identity $\cos(x) = \frac{e^{ix} + e^{-ix}}{2}$ and we obtain:

$$= \frac{1}{2M} \sum_{\lambda} \int_{\Omega} \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{\infty} dt \int_{\mathcal{BZ}} \frac{d^3k}{(2\pi)^3} e^{iQ \cdot v_{SL} t} \sum_j Q \cdot v_{SL} e^{-iQ \cdot R_j} (1 - e^{-\beta \hbar Q \cdot v_{SL}})$$

$$|\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2 \frac{1}{\omega_\lambda(k)} (2n_\lambda(k) + 1) (e^{i\omega_\lambda(k)t} + e^{-i\omega_\lambda(k)t}) (e^{iR_j} + e^{-iR_j}) =$$

$$= \frac{1}{2M} \sum_{\lambda} \int_{\Omega} \frac{d^3Q}{(2\pi)^3} \int_{-\infty}^{\infty} dt \int_{\mathcal{BZ}} \frac{d^3k}{(2\pi)^3} \sum_j Q \cdot v_{SL} (1 - e^{-\beta \hbar Q \cdot v_{SL}}) |\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2$$

$$\frac{1}{\omega_\lambda(k)} (2n_\lambda(k) + 1) (e^{i(\omega_\lambda(k)+Q \cdot v_{SL})t} + e^{-i(\omega_\lambda(k)-Q \cdot v_{SL})t}) (e^{-i(Q-K) \cdot R_j} + e^{-i(Q+K) \cdot R_j})$$

(90)

Now we observe that $e^{iG \cdot R} = 1$ if $R$ belongs to the direct lattice and $G$ belongs to the reciprocal lattice, while $\sum_R e^{iR \cdot q} = 0$ if $q \neq G$. A direct application of this fact leads us to the so called Dirac comb:

$$\sum_j e^{-i(Q + K) \cdot R_j} = \frac{(2\pi)^3}{V_c} \sum_G \delta(G - (Q + K))$$

where $V_c$ is the volume of the primitive cell, which for a simple cubic lattice is $a^3$. 

29
The integral over $dt$ gives a delta function for $\omega_\lambda(k)$:

$$\begin{align*}
P_{Re} &= \frac{1}{2Ma^3} \sum_\lambda \int_\Omega \frac{d^3Q}{(2\pi)^3} \int_{BZ} d^3k \sum_G Q \cdot v_{SL} \left(1 - e^{-\beta h Q \cdot v_{SL}}\right)|\tilde{\nu}(|Q|)|^2|Q \cdot \epsilon_\lambda(k)|^2 \frac{1}{\omega_\lambda(k)} \\
&= 2n_\lambda(k) \left[\delta(\omega_\lambda(k) + Q \cdot v_{SL}) + \delta(\omega_\lambda(k) - Q \cdot v_{SL})\right] \\
&= 2n_\lambda(k) \left[\delta(\omega_\lambda(k) + Q \cdot v_{SL}) + \delta(\omega_\lambda(k) - Q \cdot v_{SL})\right] \\
&= \left(2n_\lambda(k) + 1\right) \left[\delta(\omega_\lambda(k) + Q \cdot v_{SL}) + \delta(\omega_\lambda(k) - Q \cdot v_{SL})\right] \\
&= \left(2n_\lambda(k) + 1\right) \delta(\omega_\lambda(k) - Q \cdot v_{SL}) \delta(G - (Q + k)) + \delta(\omega_\lambda(k) - Q \cdot v_{SL}) \delta(G - (Q - k)).
\end{align*}$$

In the last line we considered the fact that, since $\omega_\lambda(k)$ is a positive number and $Q \cdot v_{SL} > 0$ if $Q$ belongs to $\Omega$, the function $\delta(\omega_\lambda(k) + Q \cdot v_{SL})$ does not contribute to the integral. Now we evaluate the contribution of the imaginary part of the function.
Thus the contribution to the dissipated power due to $P_{Re}$ and to $P_{Im}$ turns out the same, except for the factor $(2n_\lambda(k) + 1)$ in Eq. (91) which is replaced by unity in Eq.
(92). Calling \( f(Q, k, G) \) the integrand of Eq. (92) we can write:

\[
P = P^{Re} + P^{Im} = \frac{1}{Ma^3} \sum_{\lambda} \int_\Omega \frac{d^3Q}{(2\pi)^3} \int_{BZ} d^3k \sum_G f(Q, k, G)(n_\lambda(k) + 1) =
\]

\[
= \frac{1}{Ma^3} \sum_{\lambda} \int_\Omega \frac{d^3Q}{(2\pi)^3} \int_{BZ} d^3k \sum_G Q \cdot v_{SL} \left(1 - e^{-\beta h Q \cdot v_{SL}}\right) |\tilde{\nu}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2 \frac{1}{\omega_\lambda(k)}
\]

\[
\delta(\omega_\lambda(k) - Q \cdot v_{SL}) |\delta(Q - (Q + k)) + \delta(Q - (Q - k))| (n_\lambda(k) + 1) =
\]

\[
= \frac{1}{Ma^3} \sum_{\lambda} \int_\Omega \frac{d^3Q}{(2\pi)^3} \int_{BZ} d^3k Q \cdot v_{SL} \left(1 - e^{-\beta h Q \cdot v_{SL}}\right) |\tilde{\nu}(|Q|)|^2 |Q \cdot \epsilon_\lambda(k)|^2 \frac{1}{\omega_\lambda(k)}
\]

\[
\delta(\omega_\lambda(k) - Q \cdot v_{SL}) |\delta(-Q - k) + \delta(-Q + k)| (n_\lambda(k) + 1)
\]

(93)

The contribution of the two delta functions in the bracket is the same because of the parity of the eigenvalues and the eigenvectors of the dynamical matrix, so we can execute the \( k \) integration obtaining:

\[
P = \frac{2}{Ma^3} \sum_{\lambda} \int_\Omega \frac{d^3Q}{(2\pi)^3} Q \cdot v_{SL} \left(1 - e^{-\beta h Q \cdot v_{SL}}\right) |\tilde{\nu}(|Q|)|^2 |Q \cdot \epsilon_\lambda(Q)|^2 \frac{1}{\omega_\lambda(Q)}
\]

\[
\delta(\omega_\lambda(Q) - Q \cdot v_{SL})(n_\lambda(Q) + 1).
\]

(94)

To perform the integral over \( Q \) we use the well-known property of the Dirac Delta:

\[
\int d^3Q g(Q) \delta(f(Q)) = \int_S d^2Q \frac{g(Q)}{|\nabla f(Q)|},
\]

(95)

where \( S \) are the 2D manifolds in \( Q \)-space where one finds the solutions of the equation \( f(Q) = 0 \). Substituting and simplifying, we conclude that

\[
P = \frac{2}{Ma^3} \sum_{\lambda} \int_{S_\lambda} d^2Q |\tilde{\nu}(|Q|)|^2 |Q \cdot \epsilon_\lambda(Q)|^2 \frac{1}{|v_{SL} - \nabla(Q)|},
\]

(96)

Here we defined \( v_\lambda(Q) = \nabla \omega_\lambda(Q) \) and \( S_\lambda \) is a set of 2-dimensional manifolds in \( Q \) space, that are consistent with the solution of the momentum conservation equation

\[
\omega_\lambda(Q) = Q \cdot v_{SL}.
\]

(97)

Note that, like in the 1 dimensional case, both \( \hbar \), and the inverse of temperature \( \beta \) have disappeared from the final expression of Eq. (96).

The result (96) holds in a perfectly conservative context, where the phonons are infinitely-long-lived excitations. In any realistic situation some weak amount of dispersion will have phonons decay. We can introduce this effect phenomenologically, like
in [3], by adding a decay of the density-density correlation function for large $t$, so we have:

$$S_{nn}^{\text{diss}}(x, x', t) = S_{nn}(x, x', t)e^{-\frac{\gamma}{2}|t|}. \quad (98)$$

This decay leads to a broadening of the $\delta(\omega_\lambda(Q) - Q \cdot v_{SL})$ in Eq. (94):

$$\delta(\omega_\lambda(Q) - Q \cdot v_{SL}) \to \frac{1}{\pi} \frac{\gamma/2}{(\omega_\lambda(Q) - Q \cdot v_{SL})^2 + (\gamma/2)^2}. \quad (99)$$

Hence, taking into consideration this dissipation, equation (96) becomes:

$$P = 2Ma^3 \sum_\lambda \int_\Omega d^3Q |\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(Q)|^2 \frac{1}{\pi} \frac{\gamma/2}{(\omega_\lambda(Q) - Q \cdot v_{SL})^2 + (\gamma/2)^2}. \quad (100)$$

From this equation we obtain the friction force dividing by $v_{SL}$:

$$F = 2Ma^3v_{SL} \sum_\lambda \int_\Omega d^3Q |\tilde{v}(|Q|)|^2 |Q \cdot \epsilon_\lambda(Q)|^2 \frac{1}{\pi} \frac{\gamma/2}{(\omega_\lambda(Q) - Q \cdot v_{SL})^2 + (\gamma/2)^2}. \quad (101)$$

### 4.3 Numerical calculation of Eq. (101)

In this section we report the result of the numerical calculation of the main result of the present work, Eq. (101). We use the Fourier Transform of the potential $\tilde{v}(q)$ in Eq. (47), and the dynamical matrix of a simple cubic crystal, with harmonic springs of stiffness $K$ and $K'$ counting the 6 nearest and the 12 next nearest neighbours [8].

We take $K' = 0.2K$ and for the damping rate we adopt $\gamma = 0.1(M/K)^{1/2}$. Our program executes the integration and summation in Eq. (101) using the so called rectangle method: we sample the $\Omega$ region with a grid of spacing $\Delta q = 0.15/a$. We integrate in a cube $0 \leq Q_i \leq Q_{\text{max}} = 35/a$ checking that thanks to the rapid decay of $\tilde{v}_q$, 4, the results are independent of this cutoff. We report calculation for velocities in the range $[0 - 1.2]$.

Figure 7 reports the friction force.

As expected the force exhibits peaks, in correspondence to the regions where each component the group velocity of the phonons is equal to the respective component of the slider velocity. The huge value obtained for the friction force can be explained by the fact that, during the calculation, we set $\epsilon/(Ka^2) = 1$ and it suggests that the weak-coupling could start when $\epsilon/(Ka^2) \leq 10^{-4}$.

### 5 Conclusions and future developments

The aim of this thesis was to use the LRT to find an analytic formula which permits to calculate the power dissipated by a slider channelling in a crystal and interacting with its phonons.
For this periodic problem it is convenient to work in the Fourier domain. We express
the dissipated power as a sum over all the perpendicular components of the vectors
of the reciprocal lattice involving integrals of many elements including the imaginary
part of the response function evaluated at two points of the reciprocal space, differing
precisely by a perpendicular $\mathbf{G}$ vector. Eq.(58). We could calculate analytically only
the "central term" of this sum, the one for $\mathbf{G}_\perp = 0$, because we could not obtain a
generalization the Fluctuation-Dissipation Theorem, Eq.(60), for correlation functions
evaluated at two different points of the reciprocal space.

The analytic formula for the contribution the "central term", Eq. (101), involves
the Fourier Transform of the interaction potential, the phonon polarization vectors
and the phonon dispersion relations. Given these quantities it allows us to evaluate friction
as a function of the velocity of the slider. There are no thermodynamic effects, and
no quantum effects: this is due to the fact that we used the one-phonon expansion
for the calculation of the dynamic structure factor. Like in the one-dimensional case
the formula shows friction peaks when the velocity of the slider matches to the group
velocity of the phonons of the crystals.

This thesis can have some interesting future development. Firstly it would be im-
portant, if is possible, to connect the imaginary part of the density-density response
function to the structure factor of the crystal, when they are evaluated at different
points in the reciprocal space, in order the calculate also the other terms in the fric-
tion sum. Then one can extend this work by considering the slider moving along the
surface of truncated crystal, rather than inside a bulk crystal in order to address more conventional sliding friction.
Ringraziamenti

Ho tante persone da ringraziare. In primo luogo il mio relatore, il prof. Manini per la pazienza che ha avuto con me quest’anno e per i sempre utili consigli che mi ha dato, poi il mio correlatore, il prof. Santoro per il materiale sulla teoria della risposta lineare che mi ha fornito, il prof. Molinari per il tempo che mi ha dedicato quando ero in difficoltà nel trovare le simmetrie di alcune funzioni nello spazio di Fourier e Mattia per i consigli che mi ha dato su python (e non solo).

Vorrei inoltre ringraziare la mia famiglia, che mi ha sempre supportato e stimolato anche nei momenti più difficili.

Infine vorrei ringraziare gli amici, in particolare modo Marco, José, Alessandro, Sara, Francesco, Stefania, Lorenzo, Riccardo e tutti gli altri che in questo momento sto dimenticando per il supporto morale, anche condito da qualche birra, che mi hanno sempre dato.
References


http://materia.fisica.unimi.it/manini/theses/riva_g.pdf


[8] E. Meisterhofer - Phonon dispersion relation and density of states of a simple cubic lattice- Bachelor Degree theses (Technische Universitat Graz, 2015)