INTRODUCTION
to the Computational Laboratory

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Thomas Young Centre:
the London Centre for Theory and Simulation of Materials

AUTUM 2014
Outline

1. TIMETABLE and DEADLINE
2. AIMS and SYSTEMS
3. VIBRATIONS
4. HOW
5. SIMULATION TYPES
6. CLASSICAL SIMULATION
7. FIRST STEP
8. HOW TO WRITE A REPORT
## TIMETABLE and DEADLINE

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- **Demonstrator**
  - **1:00-4:00**
  - **Mon**
  - **Tue**
  - **Thur**
  - **Fri**

**DEADLINE:**

- **when?** 12:00am on next Friday
- **where?** Blackboard - bb.imperial.ac.uk
AIM:
The Thermal Expansion of MgO

- to predict how the material expands when heated;
- to calculate the thermal expansion coefficient:
  \[ \alpha = \frac{1}{V_0} \left( \frac{\partial V}{\partial T} \right)_P \]
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- **QUASI-HARMONIC APPROXIMATION** (LD)
  to compute vibrational energy levels of MgO;
  to understand the **phonon dispersion** of a material and the vibrational density of state;
AIM:
The Thermal Expansion of MgO

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  to compute vibrational energy levels of MgO;
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- MOLECULAR DYNAMICS (MD)
  to simulate the vibrations as random motions of atoms
  inside a cell;
AIM:
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- **QUASIS-HARMONIC APPROXIMATION (LD)**
  to compute vibrational energy levels of MgO;
  to understand the **phonon dispersion** of a material and
  the vibrational density of state;
- **MOLECULAR DYNAMICS (MD)**
  to simulate the vibrations as random motions of atoms
  inside a cell;
- to compare QUASIS-HARMONIC APPROXIMATION with
  MOLECULAR DYNAMICS results.
SYSTEMS: MgO crystal (fcc)

IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

- **CONVENTIONAL CELL**
  \[ \mathbf{a}_c = \mathbf{b}_c = \mathbf{c}_c; \quad \alpha_c, \beta_c, \gamma_c \]
  \[ N_c: \text{number of atoms} \]
  \[ V_c: \text{volume} \]
SYSTEMS: MgO crystal (fcc)

IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

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- PRIMITIVE CELL
  \[ \mathbf{a}_p = \mathbf{b}_p = \mathbf{c}_p; \ \alpha_p, \ \beta_p, \ \gamma_p \]
  \( N_p \): number of atoms
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SYSTEMS: MgO crystal (fcc)

IDEAL, NON DEFECTIVE, PERIODIC SYSTEM IN 3D

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- **PRIMITIVE CELL**
  \[ \mathbf{a}_p = \mathbf{b}_p = \mathbf{c}_p ; \ \alpha_p, \ \beta_p, \ \gamma_p \]
  \[ N_c : \text{number of atoms} \]
  \[ V_p : \text{volume} \]

- **SUPERCELL**
  \[ \mathbf{a}_s = \mathbf{b}_s = \mathbf{c}_s = 2 \times \mathbf{a}_c \]
  \[ \alpha_s, \ \beta_s, \ \gamma_s \]
  \[ N_s : \text{number of atoms} \]
  \[ V_s : \text{volume} \]
What is the lattice parameter of MgO?
What is the lattice parameter of MgO?

CONVENTIONAL CELL

\[ a_c = b_c = c_c; \ \alpha_c, \ \beta_c, \ \gamma_c \]
What is the lattice parameter of MgO?

**CONVENTIONAL CELL**

\[ a_c = b_c = c_c; \alpha_c, \beta_c, \gamma_c \]
Is it possible to move from the CONVENTIONAL CELL to the PRIMITIVE CELL?
Is it possible to move from the CONVENTIONAL CELL to the PRIMITIVE CELL?
VIBRATIONS
Atoms vibrate around their equilibrium positions.

- thermal properties: heat capacity, expansion
- phase transitions, including melting
- transport: thermal conductivity, sound
- electrical properties, e.g., superconductivity
- dielectric phenomena at low frequencies

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1From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
VIBRATIONS: FROM A FINITE SYSTEM TO AN INFINITE SYSTEM

1 From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
In this case, as $k$ increases, the energy of vibration increases and the frequency too.

$\lambda = 2a, k = \frac{\pi}{a}$

$\lambda = 3a, k = \frac{2\pi}{3a}$

$\lambda = \infty, k = 0$

$k = \frac{2\pi}{\lambda}$

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1From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
VIBRATIONS: PHONON DISPERSION

VIBRATIONAL FREQUENCY $\omega$ AS A FUNCTION OF $k$

$\omega_k$

$-\pi/a$  $\Gamma$  $\pi/a$

$^1$From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
VIBRATIONS: PHONON DISPERSION

VIBRATIONAL FREQUENCY $\omega$ AS A FUNCTION OF $k$

SIMILARLY, ELECTRONIC BAND STRUCTURE OF THE HYDROGEN POLYMER

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1From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
VIBRATIONS: PHONON?

electron: WAVE or PARTICLE
radiation: WAVE or PARTICLE
VIBRATIONS: PHONON?

electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE (photon)
**VIBRATIONS: PHONON?**

electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE *(photon)*

vibration: WAVE or PARTICLE
VIBRATIONS: PHONON?

electron: WAVE or PARTICLE

radiation: WAVE or PARTICLE (photon)

vibration: WAVE or PARTICLE (phonon)
VIBRATIONS:
1D MONOATOMIC CHAIN (OR POLYMER)

INFINITE NUMBER OF VIBRATIONS $\rightarrow$ \textbf{BRANCH}
VIBRATIONS:
1D MONOATOMIC CHAIN (OR POLYMER) \(^1\)

\[ \omega_k = \sqrt{\frac{4J}{M}} |\sin(ka/2)| \]
VIBRATIONS:  
1D MONOATOMIC CHAIN (OR POLYMER) \(^1\)

\[ \omega_k = \sqrt{\frac{4J}{M}} |\sin(ka/2)| \]

INFINITE NUMBER OF VIBRATIONS $\rightarrow$ BRANCH

\[ k = 0 \text{ (} \Gamma \text{ point)}: \omega_{k=0} = 0 \]
\[ k = \pi/a: \omega_{\pi/a} = \sqrt{\frac{4J}{M}} \]
\[ k = \pi/2a: \omega_{\pi/2a} = \sqrt{\frac{2J}{M}} \]
VIBRATIONS: DIRECT AND RECIPROCAL SPACE

1 PERIODIC DIRECTION IN THE DIRECT SPACE!

\[ a \]

1 PERIODIC DIRECTION IN THE RECIPROCAL SPACE!

\[ a^* = \frac{2\pi}{a} \]
VIBRATIONS: 1D DIATOMIC CHAIN

(SIMILARLY TO THE POLYMER WITH H$_2$ PER CELL)

FOLDING PROCESS!!!
VIBRATIONS:
1D HETERO DIATOMIC CHAIN

From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
VIBRATIONS:
OPTIC AND ACOUSTIC MODES

OPTIC:
1) has a frequency that is in the vicinity of the optical region of the electromagnetic spectrum
2) the atomic motions associated are the same as the response to an oscillating electromagnetic field

ACOUSTIC:
1) has acoustic frequency
VIBRATIONS: LONGITUDINAL AND TRANSVERSE MODES

From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
Neutron data for GaAs

\[\text{From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals}\]
HOW?

**COMPUTATIONAL EXPERIMENT / SIMULATION**

- program
- input

**Environment:**
the choice of the Operating System → **linux**

**Interface:**
**DLV** = package for the visualisation of materials structures and properties.
SIMULATION TYPES

- CLASSICAL SIMULATION
  
  Newton law $\rightarrow$ GULP

- QUANTUM-MECHANICAL SIMULATION
  
  Schroedinger equation $\rightarrow$ CRYSTAL

Systems under investigation
- Properties
- Accuracy
- Computational time
- Resources
CLASSICAL SIMULATION
INTERATOMIC POTENTIAL

- coulombic interaction
- short term repulsive contribution
- Morse-like potential
HELMHOLTZ FREE ENERGY

\[
F = E_0 + \frac{1}{2} \sum_{k,j} \hbar \omega_{j,k} + k_B T \sum_{k,j} \ln \left[ 1 - \exp \left( -\frac{\hbar \omega_{j,k}}{k_B T} \right) \right]
\]

\(1\)From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
QUASI-HARMONIC APPROXIMATION I

HELMHOLTZ FREE ENERGY

\[ F = E - TS \]

\[ F = F(T, V) \]
MOLECULAR DYNAMICS

Initial configuration and initial velocities:
the initial configuration will be that of ideal MgO
the velocities will be random but scaled to produce
roughly the target temperature.

- Compute the forces on the atoms \(F\).
- Compute the accelerations \(a = F/m\)
- Update the velocities: \(V_{\text{new}} = V_{\text{old}} + a \times dt\)
- Update the positions of the atoms: \(R_{\text{new}} = R_{\text{old}} + V_{\text{new}} \times dt\)
- Repeat until average properties like \(E\) and \(T\) settle down
- Once settled measure some properties.

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\(^1\)From Prof N. M. Harrison’s Lecture Notes: Vibrations in crystals
What does it mean?
What does it mean?

Minimization of the energy as a function of the atomic position 
\((x_i, y_i, z_i, \text{ with } i = 1, N, \text{ and } N \text{ is the number of atoms})\) and of the lattice parameters 
\((a, b, c, \alpha, \beta, \gamma)\)
How many variables for MgO?
FIRST STEP

1. Restart the PCs that are running Windows;
2. Once you have a black screen with the following line:
   
   > boot:
   Type linux
   > boot: linux
   Press Enter
3. Use your login and passwd as in Window
4. Open firefox: the web browser
Introduction

- the system
- the methodology (theory in use)
- the aims of the exercise
- the tools in use (programs)

Body of the text

- write it like a scientific paper (well-articulated sentences, NOT a list of two-word answers)
- analyse critically obtained data and given answers
- round numerical answers to a specific number of decimal places (i.e. 4)
- add literature/web citations whenever a comparison with experimental data is required
- add explicitly every formula used one to obtain results
- check spelling
HOW TO WRITE A REPORT II
by Giulia C. De Fusco

Pictures

- max 20
- reasonably sized (NOT one-page sized pictures, but still readable)
- white background (follow the instructions given on the website clicking on the link 'How to save a picture for your report')
- described in caption or in the text

Graphs

- add labels and units
- add a critical comment whenever required (NOT a merely descriptive comment)
Tables
- add labels and units
- round numerical answers to a specific number of decimal places (i.e. 4)
- repeat heading if the table cannot fit in a single page

Conclusions
- give a general description of your calculations and your main findings
- outline the differences between the methods in use and the results obtained
- analyse critically these differences
THANK YOU!!!