# Chapter 7

## Lattice vibrations

#### 7.1 Introduction

Up to this point in the lecture, the crystal lattice was always assumed to be completely rigid, i.e. atomic displacements away from the positions of a perfect lattice were not considered. For this case, we have developed a formalism to compute the electronic ground state for an arbitrary periodic atomic configuration and therewith the total energy of our system. Although it is obvious that the assumption of a completely rigid lattice does not make a lot of sense (it even violates the uncertainty principle), we obtained with it a very good description for a wide range of solid state properties, among which were the electronic structure (band structure), the nature and strength of the chemical bonding, or low temperature cohesive properties like the stable crystal lattice. The reason for this success is that the internal energy U of the solid (or similarly of a molecule) can be written as

$$U = E^{\text{static}} + E^{\text{vib}} , \qquad (7.1)$$

where  $E^{\text{static}}$  is the electronic ground state energy with a fixed lattice (on which we have focused so far) and  $E^{\text{vib}}$  is the additional energy due to lattice motion. In general (and we will substantiate this below),  $E^{\text{static}} \gg E^{\text{vib}}$  and thus many properties are correctly obtained, even when simply neglecting  $E^{\text{vib}}$ .

There is, however, also a multitude of solid state properties, for which the consideration of lattice mobility is crucial. Mobility is in this respect already quite a big word, because for many of these properties it is enough to take small vibrations of the ions around their (ideal) equilibrium position into account. And although the amplitude of these vibrations is small, the important aspect about them is that they can describe deformations whose wavelength is comparable to the interatomic distances — which is thus outside of the validity of continuum elasticity theory. The vibrational modes of crystalline lattices are called phonons, and most salient examples of solid state properties for which they are of paramount importance are:

Heat capacity: In metals with a rigid perfect lattice, only the free electron like conduction electrons can take up small amounts of energy (of the order of thermal energies). The specific heat capacity due to these conduction electrons was computed to vary linearly with temperature for T→0 in the first exercise. In insulators with the same rigid perfect lattice assumption, not even these degrees of freedom are available. Correspondingly, the only excitations would be electronic excitations across the (huge) band gap E<sub>g</sub> ⇒ k<sub>B</sub>T. Their (vanishingly small) probability will be ~ exp(-E<sub>g</sub>/k<sub>B</sub>T), and the specific heat

# **Chapter 7 Crystals Lattices Lattice Vibrations And Phonons**

**AN Whitehead** 

#### **Chapter 7 Crystals Lattices Lattice Vibrations And Phonons:**

Semiconductor Optics Claus F. Klingshirn, 2012-07-06 The updated and enlarged new edition of this book provides an introduction to and an overview of semiconductor optics from the IR through the visible to the UV It includes coverage of linear and nonlinear optical properties dynamics magneto and electrooptics high excitation effects some applications experimental techniques and group theory The mathematics is kept as elementary as possible The subjects covered extend from physics to materials science and optoelectronics New or updated chapters add coverage of current topics while the chapters on bulk materials have been revised and updated **Introduction to Semiconductors** Peter Sutter, 2025-08-05 This textbook provides a new perspective on the classic topic of Semiconductor Materials and Devices It aims at undergraduate and beginning graduate students in the physical sciences and in engineering This book combines two unique aspects i Making quantum mechanical concepts broadly accessible Rather than avoiding fundamental concepts such as electronic band structure and phonons as is the case in the established texts on semiconductors the book embraces and incorporates them as key building blocks While conceptually sound and rigorous this textbook avoids unnecessary detail to provide students with a solid understanding of key concepts while enabling rapid progress toward the learning goals ii Extensive examples sourced from contemporary research Advanced topics from the current literature past 10 years are included as natural extensions to each chapter of the book These contemporary examples broaden the students knowledge beyond the typical content of an introductory textbook provide relevant literature references and encourage further reading and self study In this way the extensions help educate the students for careers in the post silicon era Provides a concise introduction to semiconductor materials and devices accessible to students of varying backgrounds Makes extensive use of current real examples to facilitate understanding and motivate further reading Prepares students for careers in semiconductor research and development device design and manufacturing **Excitons** Sergei Pyshkin, 2018-03-14 Excitons as part of the InTech collection of international works on optics and optoelectronics contains recent achievements of specialists from China France Japan Switzerland and Moldova jointly with Russia and the United States of America on properties and application of excitons in electronics. The growing number of countries participating in this endeavor and joint participation of the US Moldova Italy and Russian scientists in investigations of excitons in the edition of this book testify to the unifying effect of science An interested reader will find in the book the description of properties and possible applications of excitons as well as the methods of fabrication and analysis of operation and the regions of application of modern excitonic Fundamentals of Solid State Engineering Manijeh Razeghi, 2009-03-03 Fundamentals of Solid State devices Engineering 3rd Edition provides a multi disciplinary introduction to solid state engineering combining concepts from physics chemistry electrical engineering materials science and mechanical engineering Revised throughout this third edition includes new topics such as electron electron and electron phonon interactions in addition to the Kane effective mass method

A chapter devoted to quantum mechanics has been expanded to cover topics such as the harmonic oscillator the hydrogen atom the quantum mechanical description of angular momentum and the origin of spin This textbook also features an improved transport theory description which now goes beyond Drude theory discussing the Boltzmann approach Introducing students to the rigorous quantum mechanical way of thinking about and formulating transport processes this textbook presents the basic physics concepts and thorough treatment of semiconductor characterization technology designed for solid state engineers *Phonons in Perfect Lattices and in Lattices with Point Imperfections* Raymond W. H. Stevenson,1966

**Principles of Solid State Physics** Robert M Levy, 2012-12-02 Principles of Solid State Physics presents a unified treatment of the basic models used to describe the solid state phenomena This book is divided into three parts Part I considers mechanical or geometrical properties that are describable by a lattice of mass points What happens if the electric charge and magnetic moment are to be associated with the lattice points is explained in Part II Part III discusses the application of the band theory and imperfections in solids This publication is recommended for a one semester senior course in solid state physics for students majoring in physics chemistry and electrical engineering Survey of Semiconductor Physics, Electrons and Other Particles in Semiconductors Karl W. Böer, 2002-04-05 A comprehensive treatment of the fundamentals of semiconductor physics and materials science The first edition of the Survey of Semiconductor Physics set the standard for the multifaceted exploration of semiconductor physics Now Dr Karl B er one of the world's leading experts in solid state physics with assistance from a team of the fields top researchers expands this coverage in the Second Edition Completely updated and substantially expanded the Survey of Semiconductor Physics Second Edition covers the basic elements in the entire field of semiconductor physics emphasizing the materials and surface science involved The Second Edition uses similar theoretical approaches and analyses for the basic material classes crystalline amorphous quantum structures and organics The first volume provides thorough coverage of the structure of semiconductors including Phonons Energy bands Photons as they interact with the semiconductor and other particles Defects Generation and recombination Kinetics In both volumes extensive appendices simplify searches for important formulae and tables An elaborate word index and reference listings allow readers to use the reference in multiple ways to discover expanding literature to explore similarities and connecting principles in other fields to find out how others in adjacent fields came up with intriguing solutions to similar problems and to obtain a broad overview of the entire field of semiconductor physics An **Introduction to Lattice Dynamics** Ajoy K. Ghatak, L. S. Kothari, 1972 Sci-tech Book Profiles ,1965 Includes title page table of contents list of contributors preface and all indexes of each book Acta Physica Hungarica ,1968 **Solid-State Physics** James D. Patterson, Bernard C. Bailey, 2019-02-20 This book teaches solid state physics in a comprehensive way covering all areas It begins with three broad topics how and why atoms bind together to form solids lattice vibrations and phonons and electrons in solids It then applies this knowledge to interactions especially those between electrons and

phonons metals the Fermi surface and alloys semiconductors magnetism superconductivity dielectrics and ferroelectrics optical properties defects layered materials quantum Hall effect mesoscopics nanophysics and soft condensed matter Further important topics of the book are the evolution of BEC to BCS phenomena conducting polymers graphene iron pnictide superconductors light emitting diodes N V centers nanomagnetism negative index of refraction optical lattices phase transitions phononics photonics plasmonics quantum computing solar cells spin Hall effect and spintronics In this 3rd edition topics such as topological insulators quantum computing Bose Einstein transitions highly correlated electron systems and several others have been added New material on magnetism in solids as well as a discussion of semiconductors and a changed set of problems with solutions are also included The book also discusses folk theorems to remind readers of the essence of the physics without mathematics and includes 90 mini biographies of prominent solid state physicists of the past and present to put a human face on the subject An extensive solutions manual rounds out the book Physics and **Chemistry of Glasses** ,1963 Condensed Matter Physics Michael P. Marder, 2000-01-27 Problems after each chapter Zeitschrift Für Kristallographie ,2006 Handbook of Elastic Properties of Solids, Liquids, and Gases: Dynamic methods for measuring the elastic properties of solids Moises Levy, Henry E. Bass, Richard R. Stern, Veerle Keppens, 2001 This book will discuss the propagation of sound in newly discovered or created materials and in common materials which are being investigated with a fresh outlook This four volume set is intended for university industrial and government libraries serving engineering and research personnel working in acoustics Midwest Energy Research Abstracts ,1979 INIS **Solid Hydrogen** J. Van Kranendonk, 1983 The solid molecular hydrogens are the simplest and most Atomindex ,1987 fundamental molecular solids Except at ultrahigh pressures on the order of a few mega bars where a transition to a metallic atomic phase is expected these solids are true molecular crystals in which the molecules retain their identity with properties not too different from those of the free molecules At energies below the electronic excitation energy the thermal and spectroscopic pro perties of these solids are determined by the translational rotational and intramolecular vibrational motions of the interacting molecules The theo retical analysis of the solid state properties in terms of the free molecules and the intermolecular interactions forms the main topic of this book The available detailed knowledge of the properties of the free molecules makes it feasible to carry out this program to a large extent on the basis of first principles and this is one of the attractive features of these systems The solid hydrogens are dominated by quantum effects the most out standing property being that the rotation of the molecules is free down to the lowest temperatures in the sense that the rotational quantum number I characterizing the rotational motion of the free molecules remains a good quantum number in all of the solid state phases except at ultrahigh pressures Quarterly of Applied Mathematics ,1963 Physics Briefs ,1993

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