Electron-phonon interaction in Low-dimensional Systems

A thesis submitted for the degree of Doctor of Philosophy of the Australian National University

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September 5, 1995
Statement

This thesis reports the work carried out while I was a student in the Department of Theoretical Physics, Research School of Physical Sciences and Engineering of the Australian National University between March 1992 and September 1995, under the supervision of Dr. J. Mahanty and Dr. M. P. Das.

Chapter 1 is an introduction, Chapter 2 and part of Chapter 3 contain mostly review materials, whereas Chapters 4, 5, and 6, and Appendices A, B.2, and C present work done under the supervision of Dr. J. Mahanty and Dr. M. P. Das.

None of the work reported here has been submitted to any institution of learning for any degree.

In-Keun Oh

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Acknowledgements

My interest in the topic of my work has arisen through collaboration with Dr. J. Mahanty. I would like to thank one of my two supervisors, Dr. J. Mahanty, who has guided me in the ways of physics with kindness, interest and happiness even though he himself suffered great hardship when his lovely wife, the late Mrs. Sarojini Mahanty, passed away on the 28th of November 1994. He encouraged and supported me at every stage of my study. He has been guide and teacher in a personal sense; his friendship and encouragement have been invaluable. Unfortunately, he retired at the final stage of my research because of his cancer. He is still fighting his cancer. I wish him good health.

It is a pleasure to acknowledge my other supervisor, Dr. M. P. Das, for the stimulus and invaluable discussions and suggestions. He also guided me throughout my research, and supported me when I struck trouble.

I thank former head of department Dr. B. A. Robson, now Associate Director of the Research School of Physical Sciences and Engineering, for his assistance, kindness and warmth. Financial support for my work has been provided by the Australian National University and by the Harry Triguboff AM Research Syndicate. I thank my friend Graeme B. Honner for proofreading the manuscript and suggesting useful corrections.

I wish to thank my parents whose love and support was endless. Finally, it could not have been possible to complete this work without the full support and encouragement of my wife Min-Hwa Oh Kim; her love and forbearance did not waver.
Abstract

Low-dimensional electronic systems in semiconductor heterostructures, with the associated practical applications and basic scientific interest, have recently received a lot of attention. This thesis consists of studies of the electron-acoustic phonon interaction in low-dimensional systems, and has proceeded under the supervision of Dr. Jay Mahanty and Dr. Mukunda Das during the period from 5th of March, 1992, to 5th of September, 1995, at the Australian National University.

The aim of the research is to attempt to construct more feasible models for the electron-phonon interaction, and to explain experimental results for phonon generation in low-dimensional systems. In this context, this thesis deals with the strength of the electron-acoustic-phonon coupling, and with the acoustic phonon generation due to electronic transitions in low-dimensional systems. As model calculations, idealized deformable jellium and GaAs/GaAlAs heterostructures are chosen. Furthermore, only one-phonon processes, in which a single phonon is emitted or absorbed, are considered.

In Chapter 1, a motive for the study of low-dimensional systems is given, and relevant investigations and research are described. The dependence of physical properties on the dimensionality of a solid is the most interesting thing in this thesis. Chapter 2 deals with a model Hamiltonian in a solid. We review briefly how to construct a feasible Hamiltonian for electrons, phonons, and electron-phonon interactions. In Chapter 3, the general treatments of electron-acoustic phonon interaction due to deformation potential and piezoelectric couplings are also reviewed. These two chapters provide in depth review and necessary background
materials for understanding theory and results presented in later Chapters. Chapter 4 gives the dependence of deformation potential coupling on the dimensionality of a solid, where an idealised deformable jellium is considered, and also provides in detail deformation potential coupling constants in semiconductor heterostructures. Chapter 5 deals with phonon emissions from a 2DEG in GaAs/GaAlAs heterostructures. A mechanism for deformation coupling, which may explain the experimental results for phonon emissions in semiconductor heterostructures, is provided. We give numerical calculations for the intensity of phonons emitted from a 2DEG in GaAs/GaAlAs heterostructures using the elastic Green’s functions and a model deformation potential for the systems. In Appendices, some mathematical details are given, and the elastic Green’s functions for an overlayer system with a semi-infinite substrate are also derived.

This work has been supported by an ANU PhD scholarship and the Harry Triguboff AM Research Syndicate.

Most of material presented in Chapter 4 has been published as:
In-Keun Oh, J. Mahanty, and M. P. Das

*Deformation Potentials in 2D- and 3D-deformable jellium*


Parts of the work described in Chapters 4 and 5 have been presented in:
The 6TH APPC and the 11TH AIP Congress, Griffith University, Brisbane, QLD. (4th - 7th July, 1994)
In-Keun Oh, J. Mahanty, and M. P. Das

*Dependence of the Strength of the Deformation Potential on the Dimensionality of the Solid*

ANZIP 19th Condensed Matter Physics Meeting, Charles Sturt University, Wagga Wagga, NSW (7th - 10th February, 1995)
In-Keun Oh and J. Mahanty

*Phonon emission from 2DEG in heterostructures*
Papers, covering the materials presented in Chapter 5 including Appendix B.2, are under preparation for publication:

In-Keun Oh, M. P. Das, and J. Mahanty

*Phonon emission in a GaAs/GaAlAs heterojunction*

In-Keun Oh, M. P. Das, and J. Mahanty

*Acoustic phonon generation in a GaAs/GaAlAs quantum well*
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1.1 Introductory remarks on low-dimensional systems

There has been astonishing progress using modern techniques in the epitaxial growth of materials [Weisbuch (1987)], such as molecular-beam epitaxy (MBE), metal-organic chemical vapor deposition (MOCVD), liquid-phase epitaxy (LPE), migration enhanced epitaxy (MEE), hot-wall epitaxy (HWE), hydride vapor transport, and so on. Such techniques have made it possible to construct semiconductor devices and nanometer-scale heterostructures with accurately tailored physical properties, and to produce new high quality low-dimensional material structures (i.e. heterostructures) such as heterojunctions, quantum wells, superlattices, quantum wires, quantum dots, etc., which give rise to several interesting and unusual phenomena. Low-dimensional systems* have therefore attracted attention from the points of view of both basic research, and technological applications.

One of the most interesting structures is the two-dimensional system in which the charge carriers are free to move in a plane and have quantized energy levels in the direction perpendicular to the plane. These two-dimensional systems have received a lot of attention and our understanding has progressed significantly during the last couple of decades [Ando et al (1982), Beeby et al (1991)]. Quantum wires are examples of one-dimensional systems in which the charge carriers move freely in one direction and have quantized energy levels for the other two perpendicular directions. Quantum dots are examples of zero-dimensional systems in which the charge carriers in the solid are free to move.

*The dimensionality of a system (i.e. a solid) refers to the dimension in which the charge carriers in the solid are free to move.
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electronic energies are quantized in all three mutually perpendicular directions. The quantum dot seems to mimic an artificial atom with several electrons without a nuclear centre.

The dependence of physical properties on the dimensionality of the solid can be drastic. A good example is the electronic density of states which is shown in Figure 1.1 [Esaki (1990)]. The density of states is a parabolic curve $E^{1/2}$ for 3D, a step-like curve for 2D, a peaked curve $\sum_m (E - E_m - E_n)^{-1/2}$ for 1D, and a delta function for 0D systems. Another example is the polarization function of free electrons shown in Figure 1.2 [Kittel (1968), Isihara (1993)]. At $q = 2k_F$, the static normalized polarization function has a logarithmic singularity in 1D, a kink in 2D, and an infinite slope in 3D. As a final example consider the electronic mobility, as

![Figure 1.1: The dependence of the density of states on the dimensionality of the electronic system.](image)
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DIMENSIONLESS POLARIZATION FUNCTION

\[ V = \frac{q}{k r} \]

Figure 1.2: The dependence of the polarization function on the dimensionality of the solid.

Figure 1.3: Dependence of the mobility anomalies on dimensionality.
shown in Figure 1.3 [Bastard (1988)] where the calculations are carried out at zero temperature. The mobility anomalies occur when the Fermi energy coincides with the beginning of the first excited subband (i.e. second subband). In experiments, the mobility drops gradually rather than sharply because of thermal and collisional broadening.

Low-dimensional systems are usually realized near the surfaces of materials exposed to vacuum or interfaces between different materials. Such surfaces and interfaces influence the lattice vibrations of the materials. The lattice vibrations are periodic displacement of atomic constituents of materials about their equilibrium positions. They give rise to waves propagating along the surfaces or interfaces. Quantization of lattice vibrations give rise to phonons. Reflection, refraction, and localization of waves are common effects of the existence of surfaces and interfaces in materials.

The phenomena of interest are the localized modes of vibrations [Ewing (1957)] such as Rayleigh surface waves [Rayleigh (1887)], Love waves [Love (1911)], Lamb waves [Lamb (1917)], Stoneley waves [Stoneley (1924)], and Sezawa waves [Sezawa (1927)] which were first studied in the context of seismology. Such localized waves in solids can not only be applied to the devices for guided sound waves but also play a significant role in semiconductor heterostructure devices from a practical viewpoint. A Rayleigh surface wave is a wave localized near a free surface with an amplitude which decays exponentially away from the free surface. The elastic properties of Rayleigh surface waves in solids have been studied by several authors [Flores (1973), Maradudin and Mills (1976), García-Moliner (1977), Tamura and Yagi (1994)]. Djafari-Rouhani and Dobrzynski and coworkers [Djafari-Rouhani et al (1977a, 1977b), (1981)] have studied a Stoneley wave which is a localized wave at an interface between two different elastic media. They have also investigated localized elastic waves in several geometries such as an overlayer on a semi-infinite substrate (e.g. Love waves, Sezawa waves) [Djafari-Rouhani et al (1981)], a free surface solid slab (Lamb waves), a fluid sandwiched between two identical semi-infinite solids, a solid slab sandwiched between two different semi-infinite solids [Dobrzynski et al (1989), Dobrzynski (1990)], and semi-infinite superlattices [Camley et al (1983),

There has been a great deal of experimental and theoretical research on the electronic properties of low-dimensional systems. The electronic band structures of the low-dimensional systems have been investigated using several calculation tech­niques such as the variational wave function method [Fang and Howard (1966)], tight binding method [Schulman and McGill (1979), Bastard (1988)], LCAO method [Schulman and Chang (1981)], pseudopotential formalism [Jaros and Wong (1984)], Kronig-Penney model [Esaki and Tsu (1970)], self-consistent method using the density functional theory [Stern (1972), Stern and Das Sarma (1984), Marmorkos and Das Sarma (1993), Xu (1992), Xu and Mahanty (1994a)], etc. The self-consistent calculation and the variational wave function methods are applicable to hetero­structures containing free charge carriers. The variational wave function, Kronig-Penney, and self-consistent calculation methods use the envelope function approach with po­tential line-ups (confinement potentials) based on the bulk band structures of the materials. The tight-binding, pseudo-potential and LCAO methods are microscopic approaches based on the atomic wave functions.

Another electronic property thoroughly studied is the mobility of charge carriers, which is very important in determining the electronic and vibrational properties of practical devices. Also, the quantum Hall effect occurring in the two­dimensional electron gas has been investigated by measuring conductivity and by using phonon spectroscopy of the 2DEG [Eisenstein et al (1986)].

1.2 General remarks on the electron-phonon interaction

Energy and momentum in a solid may be exchanged between the electrons and the lattice ions via electron-phonon interactions. Electron-phonon interactions are composed of the following basic processes: (1) the absorption or emission of a phonon with an electronic transition from one state to another of an electron, (2) the recombination or creation of an electron-hole pair with the emission or absorp-
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tion of a phonon, (3) the emission and reabsorption of virtual phonons by electrons or the emission and reabsorption of virtual electron-hole pairs by phonons, and (4) an effective electron-electron interaction by exchange of a virtual phonon. The processes (1) and (2) are of first order whereas and (3) and (4) are of second order in the sense of a perturbation expansion. The process of absorption of a phonon with a consequent electronic transition leads to the attenuation of sound waves when the sound waves propagate in a conducting crystal. The emission of a phonon with an electronic transition is related to phonon generation, amplification of sound waves, and electrical resistance. The emission and reabsorption of virtual phonons by electrons bring about a shift of the one-electron energy (i.e. renormalization of the electron mass) and the emission and reabsorption of virtual electron-hole pairs by phonons give rise to a shift in phonon frequency (i.e. renormalization of the phonon frequency). The attractive effective electron-electron interaction in superconductivity theory has its origin in the electron-electron interaction by exchange of a virtual phonon. Thus the electron-phonon interaction plays an important role in electrical and thermal transport processes, in the renormalizations of electron effective mass and phonon frequency, in superconductor theory, in phonon generation, and in amplification and attenuation of sound waves. It also plays an important role in the Peierls phase transition as discussed below [see next page].

When external fields such as an electric field with or without a magnetic field, and a temperature gradient are applied to a solid, the equilibrium between the electrons and ions is disturbed and the external fields give rise to electrical or thermal transport. Such transport processes are described by several complicated interaction mechanisms in addition to the electron-phonon interaction. The transport properties of solids can be determined from the Boltzmann equation. The contribution of the electron-phonon interaction to the transport processes can be estimated by solving the Boltzmann equation with only electron-phonon scattering taken into account. In the transport process the contribution to the scattering of charge carriers with phonon emissions brings about the electrical resistance of materials (electrical transport).

In contrast with the phonon emission process, the electron-phonon interaction
leads to the attenuation of sound waves (or phonon decay) via the absorption of phonons by electrons when the drift velocity of the electrons is less than that of the sound waves. Conversely, the amplification of sound waves occurs when the drift velocity of the electrons exceeds the sound velocity of the solid. In the theory of superconductivity, the effective attraction between two electrons near the Fermi surface can occur due to the electron-phonon interaction; electrons exchange a virtual phonon which causes bound pairs of electrons to form.

Several experiments have been carried out on phonon generation and amplification using techniques such as drift-field pulse (or current-pulse) [Hutson et al. (1961)], heat-pulse [von Gutfeld and Nethercot (1964)], electromagnetic radiation [Houck et al. (1967)] and pulsed optical pumping [Ulbrich et al. (1980)]. These techniques are related to electron-phonon interactions. There are two main causes of phonon generation via electron-phonon interactions. The first is as in the traveling wave amplifiers in which the drift velocity of charge carriers exceeds the velocity of phonons. The second is the laser (or maser) type of amplification in which non-radiative downward electronic transitions are induced via optical pumping, where the phonon frequency is the same as energy difference between the two electronic states undergoing the transition. There are several other phonon generation techniques [see, e.g., Tucker and Rampton (1972)] using magnetostriction, piezoelectric transducer, paramagnetic resonance, piezoelectric surface excitation method, magnetic field pumping (spin-phonon interaction) [Tucker (1961)], and so on.

The Peierls phase transition occurs in solids with a partially filled electronic band when a distortion (Peierls distortion) of the lattice causes an energy gap to appear at the Fermi surface. The distortion leads to the metal becoming an insulator. Zhang et al. (1993) theoretically derived an expression for the Peierls phase temperature $T_p$ by using deformation potential theory in a 1D conductor such as TTF-TCNQ, where they claim the Peierls phase temperature ($T_p \propto \exp(-\frac{1}{\Xi})$, $\Xi$:deformation potential) is dominated by the electron-phonon interaction [Zhang et al. (1993)].
1.3 Remarks on phonon generation via electron-phonon interactions

Over the last forty years, there has been considerable interest in phonon generation in solids. In the early stages of phonon (ultrasonic waves) generation, piezoelectric materials such as quartz, CdS, and ZnO were employed using resonant transducer technique. This technique requires a very thin wafer where attenuation of sound waves can be severe. As mentioned in the previous section, there are several techniques for phonon generation depending on the particular phonon couplings, e.g. electron-phonon coupling, electron-magnon coupling, spin-phonon coupling, etc.

The effect of conduction electrons on the attenuation of acoustic waves in metals has been investigated by several authors [Pippard (1955, 1960), Holstein (1959), Khan and Allen (1987)] since Bömmel first measured the ultrasonic attenuation in lead [Bömmel (1954)]. Parmenter predicted theoretically the acoustoelectric effect, which is the generation of an electric current due to a traveling acoustic wave. The effect occurs in both metals and semiconductors [Parmenter (1953)]. The acoustoelectric effect was further developed both theoretically [Weinreich (1956)] and experimentally [Weinreich et al (1959)], and was first observed in germanium [Weinreich and White (1957)] by Weinreich and coworkers. Weinreich suggested that the acoustoelectric effect could be used to calculate the amount of attenuation of acoustic waves [Weinreich (1957)]. With the investigation of the attenuation of acoustic waves using the acoustoelectric effect, the possibility of the generation of acoustic waves by charge carriers was suggested by Weinreich based on the deformation potential coupling between electrons and phonons in semiconductors [Weinreich (1956)]. Also, the generation of ultrasonic waves via electron-phonon interactions was theoretically predicted by Tolpygo and Uritskii in 1956. Thenceforth there has been considerable interest in phonon generation using electronic transitions between two electronic states, where the phonon frequency corresponds to the energy difference between the electronic states involved.

From the experimental and practical points of view, phonon generation due to
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electronic transitions may provide a tunable ultrasonic source because the phonon frequency depends on the energy difference between the electronic levels undergoing the transition. From the theoretical point of view, the characteristics of phonon generation in a system can give clues for fundamental understanding on electronic structure, electron-phonon coupling, phonon dispersion in the system, and so on. Hutson and coworkers [Hutson et al (1961)] achieved experimentally the amplification of ultrasonic waves in a piezoelectric crystal by using a dc drift-field pulse. The concept of the amplification of acoustic phonons has been extended to semimetals using magnetoresistance, which is an electrical resistance due to electron-phonon interactions under the application of electric and magnetic fields [Esaki (1962), Dumke and Haering (1962)]. Pomerantz (1964) observed phonon amplification in germanium; in this case, the deformation potential plays an important role in the electron-phonon interaction. Direct generation of ultrasound by electromagnetic radiation in metals has also been studied by several authors [Houck et al (1967), Chimenti et al (1974), Ram Mohan et al (1979), Feyder et al (1982)].

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greater than LA signal for Si MOSFETS, a GaAs/AlGaAs heterojunction, and GaAs/AlGaAs quantum wells.

To fully describe the phonon generation via electron-phonon interactions in a solid, it is important to have some crucial information such as the deformation potential, piezoelectric coupling, and electron distribution, while to describe the transport processes, it is necessary to have complicated information such as deformation potential processes, polar scattering processes, piezoelectric scattering processes, impurity scattering processes, electron-electron scattering processes, etc. Therefore, it is more straightforward to study the phonon generation rather than the transport processes for research on the electron-phonon interaction.

1.4 Scope of the thesis

In this thesis, electron-acoustic-phonon interactions in several situations will be considered rather than the other type of electron-phonon interactions (i.e., electron-optical-phonon interactions). The interaction between localized-electrons and bulk-like phonons will be studied rather than the interactions between localized-electrons and localized phonons. This work will concentrate on the features of the phonon emissions arising from electronic transitions in semiconductor heterostructures and will attempt to explain experimental results using feasible models for the electron-phonon interaction. In Chapter 2, a feasible model Hamiltonian will be reviewed for electrons, phonons, and electron-phonon interactions in solids. As usual, we choose the adiabatic approximation where the processes take place slowly enough that the system under consideration remains almost in equilibrium without a change in entropy. Chapter 3 will deal with general treatments and characteristics of electron-acoustic-phonon interactions due to deformation potential and piezoelectric couplings. This review is necessary to examine further details in later Chapters. The dependence of the deformation potential on the dimensionality of the solid will be studied in Chapter 4. Finally, in Chapter 5, the intensity of phonons emitted from an electron gas will be studied where the surface and interface effects are taken into account by using the elastic Green's functions. In the last Chapter, a summary is provided with suggestion for future work.
2.1 Introduction to the model Hamiltonian for solids

Basically, the complete way to investigate the properties of solids would be the quantum-mechanical treatment, based on solving the Schrödinger equation of the system concerned. Unfortunately, it is not possible to exactly solve the Schrödinger equation of any solid system because in any system there are an enormous number of particles (~ $10^{23}$) and several complicated interactions between them. One or more approximations are therefore essential in any investigation of the properties of a solid. Before introducing any approximation, it is important to construct a proper Hamiltonian for the solid. For completeness, we discuss some very basic aspects of electrons, phonons, and their interaction in the following sections.

The Hamiltonian of a solid is made up of the kinetic energy of all particles in the solid and their interaction energies. The electrons in the solid can usually be classified into two groups [Madelung (1978)]—the valence electrons which mediate the chemical bond, and the core electrons which are tightly bound in the closed shells of the lattice ions and which scarcely influence the properties of the solid. Therefore, we can approximately consider the valence electrons and the lattice ions as independent constituents. A suitable model of the total Hamiltonian for the solid is then [Haug (1972)]

$$\mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{ion}} + \mathcal{H}_{\text{el}} + \mathcal{H}_{\text{ion-\text{el}}}$$

(2.1)

with

$$\mathcal{H}_{\text{ion}} = T_{\text{ion}} + V_{\text{ion}} \equiv \sum_{\ell} \frac{p_{\ell}^2}{2M_{\ell}} + \sum_{\ell \neq \ell'} V_{\text{ion-\text{ion}}} (\mathbf{R}_{\ell} - \mathbf{R}_{\ell'})$$,

$$\mathcal{H}_{\text{el}}$$

$$\mathcal{H}_{\text{ion-\text{el}}}$$
2. The Hamiltonian for Solids

\[ \mathcal{H}_{el} = T_{el} + V_{el} \equiv \sum_{i} \frac{P_{i}^{2}}{2m} + \sum_{i<j} \frac{e^{2}}{|r_{i} - r_{j}|}, \]

and

\[ \mathcal{H}_{ion-el} = \sum_{i} V_{ion-el}(r_{i} - R_{\ell}), \]

where \( P_{\ell} \) is the momentum of the \( \ell \)-th ion, \( M_{\ell} \) is the mass of \( \ell \)-th ion, and \( V_{ion} \) is the interaction of the collection of ions, which is assumed to be through the direct ion-ion coupling \( V_{ion-ion}(R_{\ell} - R_{\ell'}) \) that depends only on the distance between pairs of ions. Here we neglect ion-ion interactions beyond two body interaction. \( V_{el} \) is the interaction of the valence electrons via the Coulomb interaction. \( \mathcal{H}_{ion-el} \) describes the interaction between the electrons and ions. In this approximation, we have neglected the structure of ions and coupling between the closed-shell electrons on different ions. It is not possible to rigorously solve the Schrödinger equation for the total Hamiltonian (2.1). There are several possible choices of approximations, depending on the physical circumstances and the behaviour of the solid to be studied. Following Born and Oppenheimer \([e.g. \ see \ Haug \ (1972), Jones and March \ (1973)]\), the total Hamiltonian can be divided into two components—that dealing with the motion of the valence electrons together with stationary ions, and that dealing with the motion of the ions. From the viewpoint of the electrons, the ions appear nearly stationary because the ions respond only slowly to a change in the electron configuration, while the electrons respond adiabatically to a change in the positions of the ions \([Jones and March \ (1973)]\). So the Schrödinger equation for the electrons can be approximated by

\[ \mathcal{H}_{e}(\{r_{\ell}\}, \{R_{\ell}\})\Phi_{\kappa}(\{r_{\ell}\}, \{R_{\ell}\}) = \mathcal{E}_{\kappa}(\{R_{\ell}\})\Phi_{\kappa}(\{r_{\ell}\}, \{R_{\ell}\}), \quad (2.2) \]

with

\[ \mathcal{H}_{e}(\{r_{\ell}\}, \{R_{\ell}\}) = \mathcal{H}_{el}(\{r_{\ell}\}) + \mathcal{H}_{ion-el}(\{r_{\ell}\}, \{R_{\ell}\}) \]

in which the coordinates \( \{R_{\ell}\} \) of the ions are taken as fixed parameters, and where \( \kappa \) stands for all the quantum numbers describing the electrons. The wavefunctions \( \Phi_{\kappa} \) form a complete set in \( r \) space. Therefore the total wavefunction \( \Psi_{tot} \) can be
2. The Hamiltonian for Solids

expanded in terms of the $\Phi_\kappa$:

$$\Psi_{tot} = \sum_\kappa \varphi_\kappa(\kappa, \{R_\ell\}) \Phi_\kappa(\{r_1\}, \{R_\ell\})$$.

where $\Lambda$ denotes all the quantum numbers for the total ions. The total Schrödinger equation is now given by

$$\mathcal{H}_{tot} \Psi_{tot} = \mathcal{E}_{tot} \Psi_{tot}. \quad (2.3)$$

Taking the inner product with $\Phi^*_\kappa$ of both sides of equation (2.3), we have

$$(\mathcal{H}_{ion} + \mathcal{E}_\kappa) \varphi_\kappa(\kappa, \{R_\ell\}) + \sum_{\kappa'} C_{\kappa\kappa'}(\{R_\ell\}) \varphi_{\kappa'}(\kappa', \{R_\ell\}) = \mathcal{E}_{tot} \varphi_\kappa(\kappa, \{R_\ell\}), \quad (2.4)$$

where

$$C(\kappa \kappa') = A(\kappa \kappa') + B(\kappa \kappa')$$

with

$$A(\kappa \kappa') = -\sum_\ell \frac{\hbar^2}{2m_\ell} \int \Phi^*_\kappa \nabla R_\ell \Phi_{\kappa'} \, dr \nabla R_\ell,$$

$$B(\kappa \kappa') = -\sum_\ell \frac{\hbar^2}{2m_\ell} \int \Phi^*_\kappa \nabla^2 R_\ell \Phi_{\kappa'} \, dr.$$

The first term ($\mathcal{H}_{ion} + \mathcal{E}_\kappa$) in the left side of equation (2.4) is the effective Hamiltonian $\mathcal{H}_p$ of the ions which is given by

$$\mathcal{H}_p = T_{ion} + V_{ion} + \mathcal{E}_\kappa \equiv T_{ion} + V^{eff}_{ion}.$$

The second term in the left side of equation (2.4) corresponds to the electron-phonon interactions which can be ignored in the adiabatic approximation. Thus the Schrödinger equation for the total system in the adiabatic approximation is given by

$$\mathcal{H}_p \varphi_\kappa(\kappa, \{R_\ell\}) = \mathcal{E}_{tot}(\Lambda) \varphi_\kappa(\kappa, \{R_\ell\}). \quad (2.5)$$

2.2 Phonons

The Schrödinger equation (2.5) describes the motion of the ions which is governed by the effective potential $V^{eff}_{ion}$. The electrons are treated as instantaneous objects because they respond so quickly to the motion of the ions that their states
are always a function of the positions of the ions. So far we have used $\mathbf{R}_\ell$ to refer to the positions of the ions in which $\ell$ stands for the lattice position and the basis atom positions together. Generally, the positions of the ions in a solid with $N$ unit cells and $r$ basis atoms in each unit cell, can be described by

$$\mathbf{R}_{\ell\alpha} = \mathbf{R}_\ell + \mathbf{R}_\alpha, \quad (\ell = 1, \ldots, N; \quad \alpha = 1, \ldots, r)$$

where $\mathbf{R}_\ell$ is the Bravais lattice vector and $\mathbf{R}_\alpha$ denotes the vector from the Bravais lattice site to the $\alpha$th basis atom. Let us now consider a small ionic displacement $\mathbf{u}_{\ell\alpha}$ from the equilibrium position $\mathbf{R}_{\ell\alpha}^0$.

$$\mathbf{R}_{\ell\alpha}(t) = \mathbf{R}_{\ell\alpha}^0 + \mathbf{u}_{\ell\alpha}(t), \quad (2.6)$$

with

$$\mathbf{u}_{\ell\alpha} = \mathbf{u}_\ell + \mathbf{u}_\alpha,$$

where $\mathbf{u}_\ell$ is the displacement of the cell as a whole and $\mathbf{u}_\alpha$ is a relative displacement of the $\alpha$th basis atom. From equation (2.6) we have

$$\nabla \mathbf{R}_{\ell\alpha} = \nabla \mathbf{u}_{\ell\alpha}.\]

Thus the kinetic energy of the ions is given by

$$T_{\text{ion}} = \sum_{\ell\alpha i} \frac{M_\alpha}{2} \dot{\mathbf{u}}_{\ell\alpha i}^2, \quad (2.7)$$

where $M_\alpha$ is the mass of the $\alpha$th basis atom and $i$ is a Cartesian coordinate index. We expand the total potential energy of the ions in a Taylor series in powers of the displacement $u_{\ell\alpha i}$ and terminate the expansion at the first non-vanishing term within the harmonic approximation. The first term in the expansion is a constant corresponding to the static equilibrium energy and may be chosen as zero in the dynamics of lattice vibrations.

$$V_{\text{ion}}^{\text{eff}}(\mathbf{R}_{\ell\alpha}) = V_{\text{ion}}^{\text{eff}}(\mathbf{R}_{\ell\alpha}^0) + \frac{1}{2} \sum_{\ell\alpha i} \nu_{\ell\alpha i}^{\ell'\alpha' i'} u_{\ell\alpha i} u_{\ell'\alpha' i'}, \quad (2.8)$$

with

$$\nu_{\ell\alpha i}^{\ell'\alpha' i'}(\mathbf{R}_{\ell\alpha}^0; \mathbf{R}_{\ell'\alpha'}^0) = \frac{\partial^2 V_{\text{ion}}^{\text{eff}}}{\partial u_{\ell\alpha i} \partial u_{\ell'\alpha' i'}} \bigg|_{u_{\ell\alpha i} = 0, u_{\ell'\alpha' i'} = 0}. \quad (2.9)$$
where $V_{\text{t}a}^{\ell \alpha \ell' \alpha'}$ is called atomic force constant (coupling constant) which is the force in the $i$-direction on the $\alpha$th atom in the $\ell$th unit cell when the $\alpha'$th atom in the $\ell'$th cell is displaced by unit distance in the $i'$-direction. The equation of motion is derived classically from equations (2.7) and (2.8)

$$M_{\alpha} \ddot{u}_{\text{t}a} = - \frac{\partial V_{\text{ion}}^{\ell \alpha \ell' \alpha'}}{\partial u_{\text{t}a}} = - \sum_{\ell' \alpha'} V_{\text{t}a}^{\ell \alpha \ell' \alpha'} u_{\ell' \alpha' \ell' \alpha'}. \quad (2.10)$$

The coupling constants $V_{\text{t}a}^{\ell \alpha \ell' \alpha'}$ have the following properties:

1. Because $V_{\text{t}a}^{\ell \alpha \ell' \alpha'}$ is a second-order differential, equation (2.9) gives

$$V_{\text{t}a}^{\ell \alpha \ell' \alpha'} = V_{\text{t}a}^{\ell' \alpha' \ell \alpha}$$

2. $V_{\text{t}a}^{\ell \alpha \ell' \alpha'}$ has lattice translational invariance which means that $V_{\text{t}a}^{\ell \alpha \ell' \alpha'}$ depends only on $(R_{\ell}^0 - R_{\ell'}^0 = R_{\ell}^m)$ and not on $R_{\ell}^0, R_{\ell'}^0$ separately. Thus we have

$$V_{\text{t}a}^{\ell \alpha \ell' \alpha'} = V(m)^{\alpha \alpha'}_{\alpha \alpha'}$$

3. Under a rigid body displacement of the lattice ($i.e.$, all $u_{\text{t}a}$ are independent of $\ell, \alpha$), there is no acceleration. Therefore, from equation (2.10) we have

$$\sum_{\ell \alpha} V_{\text{t}a}^{\ell \alpha \ell' \alpha'} = \sum_{m \alpha} V(m)^{\alpha \alpha'}_{\alpha \alpha'} = 0$$

Let us now consider a periodic solution of the equation of motion (2.10),

$$u_{\text{t}a} = \frac{1}{\sqrt{M_{\alpha}}} w_{\alpha}(q) e^{i(q \cdot R_{\ell}^0 - \omega t)} \quad (2.11)$$

where $w_{\alpha}(q)$ is independent of $R_{\ell}^0$. Substituting equation (2.11) into equation (2.10), we obtain

$$\omega^2 w_{\alpha}(q) = \sum_{\ell' \alpha'} \frac{1}{\sqrt{M_{\alpha} M_{\alpha'}}} V_{\text{t}a}^{\ell \alpha \ell' \alpha'} e^{i(q \cdot (R_{\ell}^0 - R_{\ell'}^0))} w_{\alpha'}(q) = \sum_{\alpha'} D_{\alpha \alpha'}^{\ell \alpha} (q) w_{\alpha}(q) \quad (2.12)$$

where

$$D_{\alpha \alpha'}^{\ell \alpha} (q) = \frac{1}{\sqrt{M_{\alpha} M_{\alpha'}}} \sum_{\ell'} V_{\text{t}a}^{\ell \alpha \ell' \alpha'} e^{i(q \cdot (R_{\ell}^0 - R_{\ell'}^0))} = \frac{1}{\sqrt{M_{\alpha} M_{\alpha'}}} \sum_{m} V(m)^{\alpha \alpha'}_{\alpha \alpha'} e^{i(q \cdot R_{\ell}^m)} \quad (2.13)$$

and has the Hermitian property

$$D_{\alpha \alpha'}^{\ell \alpha} (q) = D_{\alpha \alpha'}^{\ell \alpha} (-q) = D_{\alpha \alpha'}^{\ell \alpha} (q).$$
The equations (2.12) give the secular equation

\[ \omega^2 \delta_{ii'} \delta_{\alpha \alpha'} - D_{\alpha i}^{\alpha' i'}(q) = 0, \]

involving a $3r \times 3r$ determinant which has $3r$ eigenvalues, $\omega_\lambda^2(q)(\lambda = 1, \cdots, 3r)$. The eigenvalues correspond to the longitudinal and transverse acoustic waves when the lattice has one basis in the unit cell, and in addition, the longitudinal and transverse optical waves when the lattice has more than one basis in the unit cell. The equation

\[ \omega = \omega_\lambda(q) \quad (\lambda = 1, \cdots, 3r) \]

is called the phonon dispersion relation of the solid. Since $D_{\alpha i}^{\alpha' i'}(q)$ is Hermitian, the eigenvalues are real

\[ \omega_\lambda^2(q) = \omega_\lambda^2(-q), \quad (2.14) \]

which implies time reversal symmetry. To each $\omega_\lambda(q)$ corresponds an eigenvector $e_{\alpha i}^{(\lambda)}(q)$ satisfying

\[ \omega_\lambda^2(q) e_{\alpha i}^{(\lambda)}(q) = \sum_{\alpha' i'} D_{\alpha i}^{\alpha' i'}(q) e_{\alpha' i'}^{(\lambda)}(q). \quad (2.15) \]

The eigenvectors $e_{\alpha i}^{(\lambda)}$ contain a suitable phase factor depending on $\alpha$ to describe the motion of the different atoms in the unit cell. They are complex, and obey both orthonormality and completeness relations:

\[ \sum_{\alpha i} e_{\alpha i}^{(\lambda)*}(q) e_{\alpha i}^{(\lambda')}(q) = \delta_{\lambda \lambda'}, \quad (\text{orthonormality}) \]

\[ \sum_{\lambda} e_{\alpha i}^{(\lambda)*}(q) e_{\alpha i'}^{(\lambda)}(q) = \delta_{\alpha \alpha'} \delta_{ii'}. \quad (\text{completeness}) \]

Multiplying equation (2.15) by $e_{\alpha i}^{(\lambda)*}(q)$ and summing over $\alpha$ and $i$ with the use of the orthonormality, we obtain

\[ \omega_\lambda^2(q) = \sum_{\alpha' i'} e_{\alpha i}^{(\lambda)*}(q) D_{\alpha i}^{\alpha' i'}(q) e_{\alpha' i'}^{(\lambda)}(q). \]

For the displacement $u_{i\alpha}$ we now have a solution of the equation of motion (2.10),

\[ u_{i\alpha}^{(\lambda)} = \frac{1}{\sqrt{M_\alpha}} e_{\alpha}^{(\lambda)}(q) e^{i(q \cdot R_\alpha - \omega_\lambda(q)t)}. \quad (2.17) \]
Any lattice displacement is a linear combination of the eigenvectors of the dynamical matrix

\[ u_{\alpha i} = \frac{1}{\sqrt{NM}} \sum \mathcal{Q}_\lambda (q, t) \epsilon^{(\lambda)}_{\alpha i}(q) e^{iq \cdot R_0^2}, \tag{2.18} \]

where \( \mathcal{Q}_\lambda (q, t) \) for different \( q \) and \( \lambda \) are called normal coordinates, including the time-dependent exponential factor in equation (2.17). Since the displacement \( u_{\alpha i} \) must be real, we have

\[ \epsilon^{(\lambda)}_{\alpha i}^*(q) \mathcal{Q}_\lambda^*(q, t) = \epsilon^{(\lambda)}_{\alpha i}(-q) \mathcal{Q}_\lambda(-q, t). \]

This is satisfied by the requirements

\[ \epsilon^{(\lambda)}_{\alpha i}^*(q) = \epsilon^{(\lambda)}_{\alpha i}(-q) \quad \text{and} \quad \mathcal{Q}_\lambda^*(q, t) = \mathcal{Q}_\lambda(-q, t). \tag{2.19} \]

Let us now consider the effective Hamiltonian \( \mathcal{H}_{ph} \) for the lattice vibrations

\[ \mathcal{H}_{ph} = \sum_{\alpha i} \frac{M \dot{u}_{\alpha i}^2}{2} + \frac{1}{2} \sum_{\alpha i, \alpha i'} \gamma_{\alpha i, \alpha i'} u_{\alpha i} u_{\alpha i'} \tag{2.20} \]

In order to express the Hamiltonian in terms of the normal coordinates, \( \mathcal{Q}_\lambda (q, t) \), we need the following condition in addition to the equations (2.13), (2.14), (2.15), (2.16), and (2.19)

\[ \sum_\xi e^{i(q+q') \cdot R_\xi} = N \sum_{G_m} \delta_{q+q', G_m} = N \delta_{q+q', 0} \tag{2.21} \]

where \( G_m \) is a reciprocal lattice vector, and any phonon wave vector (i.e. \( q \) and \( q' \)) must be inside the first Brillouin zone. Because \( q + q' \) can not equal a nonzero reciprocal lattice vector, we have only \( q + q' = 0 \) in equation (2.21). Thus the Hamiltonian \( \mathcal{H}_{ph} \) becomes

\[ \mathcal{H}_{ph} = \frac{1}{2} \sum_{q, \lambda} \left[ \dot{\mathcal{Q}}_\lambda^*(q, t) \dot{\mathcal{Q}}_\lambda(q, t) + \omega_\lambda^2(q) \mathcal{Q}_\lambda^*(q, t) \mathcal{Q}_\lambda(q, t) \right] \tag{2.22} \]

The coupled Hamiltonian (2.20) is now replaced by the decoupled Hamiltonian (2.22). From the Lagrangian \( L = T - V \), the conjugate momentum \( P_\lambda (q, t) \) is given by

\[ P_\lambda (q, t) = \frac{\partial L}{\partial \mathcal{Q}_\lambda^*(q, t)} = \dot{\mathcal{Q}}_\lambda (q, t) \]
Thus the Hamiltonian (2.20) can be written

\[ \mathcal{H}_{ph} = \frac{1}{2} \sum_{\mathbf{q}, \lambda} \left[ P_{\lambda}(\mathbf{q}, t)^2 + 2 \omega_{\lambda}(\mathbf{q}) P_{\lambda}(\mathbf{q}, t) Q_{\lambda}^*(\mathbf{q}, t) Q_{\lambda}(\mathbf{q}, t) \right] \]

and the equation of motion from \( \dot{P}_{\lambda}(\mathbf{q}, t) = -\partial \mathcal{H}_{ph}/\partial Q_{\lambda}^*(\mathbf{q}, t) \) is

\[ \ddot{Q}_{\lambda}(\mathbf{q}, t) + \omega_{\lambda}^2(\mathbf{q}) Q_{\lambda}(\mathbf{q}, t) = 0 \]

which is just a simple harmonic oscillator of frequency \( \omega_{\lambda}(\mathbf{q}) \). Introducing creation and annihilation operators \( a_{\lambda}^{\dagger}(\mathbf{q}) \), \( a_{\lambda}(\mathbf{q}) \) for phonons by

\[ Q_{\lambda}(\mathbf{q}, t) = \sqrt{\frac{\hbar}{2\omega_{\lambda}(\mathbf{q})}} [a_{\lambda}(\mathbf{q}) e^{i\omega_{\lambda}(\mathbf{q}) t} + a_{\lambda}^{\dagger}(-\mathbf{q}) e^{-i\omega_{\lambda}(\mathbf{q}) t}] \]

\[ P_{\lambda}(\mathbf{q}, t) = i \sqrt{\frac{\hbar\omega_{\lambda}(\mathbf{q})}{2}} [a_{\lambda}^{\dagger}(-\mathbf{q}) e^{-i\omega_{\lambda}(\mathbf{q}) t} - a_{\lambda}(\mathbf{q}) e^{i\omega_{\lambda}(\mathbf{q}) t}] \]

the Hamiltonian (2.22), is given by

\[ \hat{\mathcal{H}}_{ph} = \sum_{\mathbf{q}, \lambda} \left[ a_{\lambda}^{\dagger}(\mathbf{q}) a_{\lambda}(\mathbf{q}) + \frac{1}{2} \right] \hbar \omega_{\lambda}(\mathbf{q}) , \]

in which the creation and annihilation operators for the phonons satisfy the commutation relations,

\[ [a_{\lambda}(\mathbf{q}), a_{\lambda}^{\dagger}(\mathbf{q}')] = \delta_{\lambda,\lambda'} \delta_{\mathbf{q}, \mathbf{q'}} \]

and the total energy of phonon system is given by

\[ E_{ph} = \sum_{\mathbf{q}, \lambda} (n_{\mathbf{q}}^{(\lambda)} + \frac{1}{2}) \hbar \omega_{\lambda}(\mathbf{q}) , \quad N_{ph} = \sum_{\mathbf{q}, \lambda} n_{\mathbf{q}}^{(\lambda)} \]

where \( n_{\mathbf{q}}^{(\lambda)} \) is the phonon occupation number and \( N_{ph} \) is the total number of phonons in the system. For a system in thermal equilibrium, the average number of phonons in the state \((\mathbf{q}, \lambda)\) is given by the Bose-Einstein distribution

\[ < n_{\mathbf{q}}^{(\lambda)} > = \frac{1}{e^{\hbar \omega_{\lambda}(\mathbf{q})/k_B T} - 1} \]

and the average energy due to phonons in the state \((\mathbf{q}, \lambda)\) is

\[ < E_{ph}(\omega_{\lambda}(\mathbf{q})) >= ( < n_{\mathbf{q}}^{(\lambda)} > + \frac{1}{2} ) \hbar \omega_{\lambda}(\mathbf{q}) \]
2.3 Electrons in solids

Let us first consider the ground state of $N_e$ electrons in a solid when the ions are in their equilibrium positions $\{R^0_\ell\}$. From equation (2.2) the Hamiltonian for the $N$ electrons in the solid is given by

$$\mathcal{H}_e = \sum_i \frac{p_i^2}{2m} + \sum_i V_e^0(r_i) + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

with

$$V_e^0(r_i) = \sum_\ell V_{\text{ion-el}}(r_i - R^0_\ell).$$

If we choose a wavefunction $\Phi$ of $\mathcal{H}_e$ as a determinant (Slater determinant)

$$\Phi(1, \ldots, N_e) = \frac{1}{\sqrt{N_e!}} \begin{vmatrix} \psi_1(r_1, \sigma_1) & \cdots & \psi_1(r_{N_e}, \sigma_{N_e}) \\ \vdots & \ddots & \vdots \\ \psi_{N_e}(r_1, \sigma_1) & \cdots & \psi_{N_e}(r_{N_e}, \sigma_{N_e}) \end{vmatrix},$$

where $\sigma$ indicates the spin of the electron, then using the variational principle we can write the one-electron Schrödinger equation in the Hartree-Fock form,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_e^0(r) - e \int \frac{\rho(r') - \rho^\text{HF}_n(r, r')}{|r - r'|} dr' \right] \psi_n(r) = E_n \psi_n(r)$$

with

$$\rho(r) = -e \sum_n |\psi_n(r)|^2$$

$$\rho^\text{HF}_n(r, r') = -e \sum_{n', \text{spin}} \frac{\psi_n^*(r') \psi_n(r') \psi_{n'}^*(r) \psi_{n'}(r)}{\psi_n^*(r) \psi_n(r)} ,$$

where $\rho(r)$ is the electron density and $\rho^\text{HF}_n(r, r')$ is the exchange charge density. The one-electron Schrödinger equation can self-consistently be solved using equations (2.25), (2.26), and (2.27) with the exchange interaction. Furthermore, taking into account the correlation interaction in addition to the exchange interaction, the Schrödinger equation can self-consistently be solved using the density functional theory (e.g. local density functional theory). Generally, the one-electron Schrödinger equation in the solid is described by

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi_n(r) = E_n \psi_n(r)$$
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where \( V(r) \) contains not only the periodic potential \( V^0_e \) due to the ions alone, but also effects due to the interaction of the electron with all the other electrons (e.g., the third term of equation (2.25) in the HF approximation). The effective one-electron potential in the solid has the periodicity of the underlying Bravais lattice with lattice vector \( \mathbf{R}_0^2 \);

\[
V(r + \mathbf{R}_0^2) = V(r) = \sum_{\kappa} V_{ei}^{\text{eff}}(r - \mathbf{R}_0^2),
\]

where \( V_{ei}^{\text{eff}} \) is the effective interaction of an electron with both a ion and the other electrons. The eigenfunctions of the one-electron Hamiltonian are generally given as Bloch functions with a spin wavefunction \( \chi(\sigma) \);

\[
\psi_{\kappa\kappa\sigma}(r) = e^{ik\cdot r} u_{\kappa\kappa\sigma}(r) \chi(\sigma)
\]

with

\[
u_{\kappa\kappa\sigma}(r + \mathbf{R}_0^2) = u_{\kappa\kappa\sigma}(r) \quad \text{for any } \mathbf{R}_0^2,
\]

and the corresponding eigenvalues have the form \( E_{n\kappa}(k) \) where \( n \) denotes the band index, \( \sigma \) the spin, and \( k \) the wave vector of the electron. In this one-electron approximation, the electrons in the solid occupy one-electron states. Introducing creation and annihilation operators \( c^\dagger_{\kappa\kappa\sigma}, c_{\kappa\kappa\sigma} \) for the electrons, the system of electrons can be described by

\[
\hat{\psi} = \sum_{n\kappa\sigma} c_{\kappa\kappa\sigma} \psi_{\kappa\kappa\sigma}(r), \quad \hat{\psi}^\dagger = \sum_{n\kappa\sigma} c_{\kappa\kappa\sigma}^\dagger \psi_{\kappa\kappa\sigma}^*(r),
\]

which give the appropriate Bloch wave second-quantized Hamiltonian for the electrons

\[
\hat{\mathcal{H}}_e = \sum_{n\kappa\sigma} E_{n\kappa}(k) c_{\kappa\kappa\sigma}^\dagger c_{\kappa\kappa\sigma}.
\]

Here the creation and annihilation operators satisfy the anticommutation relations

\[
\{c_{\kappa\kappa\sigma}, c_{\kappa\kappa'\sigma'}^\dagger\} = \delta_{\kappa,\kappa'} \delta_{\sigma,\sigma'}. \]

The total energy of the electrons in the solid is given by

\[
\mathcal{E}_e = \sum_{n\kappa\sigma} E_{n\kappa}(k) n_{n\kappa\sigma}^e,
\]
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with

\[ N_e = \sum_{nk\sigma} n_{nk\sigma}^e \]

where \( N_e \) is the total number of electrons and \( n_{nk\sigma}^e \) is the electron occupation number. If the electrons are in thermal equilibrium, the average number of electrons in the Bloch state \((n, k, \sigma)\) is given by the Fermi-Dirac distribution

\[ n_{nk\sigma}^e = \langle c_{nk\sigma}^+ c_{nk\sigma} \rangle = \frac{1}{e^{[\varepsilon_{nk\sigma} - E_F]/k_BT} + 1} \]

where \( E_F \) is the Fermi energy and \( T \) is the temperature.

2.4 Electron-phonon interactions in solids

Let us now consider the electron-phonon interactions whose Hamiltonian is included in equation (2.4). In fact, the electron-phonon interaction term in equation (2.4), which was neglected in the adiabatic approximation, plays a major role in properties other than the energy eigenvalues of the ions, e.g. the transport of charge carriers, phonon emission, etc. In addition, there are some unusual effects that arise when electrons move in systems of reduced dimensionality. The electron-phonon interaction in the solid determines the matrix element for a simultaneous transition of the ions and the electrons

\[ M_{\Lambda \Lambda'}(\kappa \kappa'; R_{\ell}) = \int \varphi_{\Lambda}(\kappa', R_{\ell})C_{\kappa'\kappa}(R_{\ell})\varphi_{\Lambda}(\kappa, R_{\ell})dR_{\ell}, \quad (2.30) \]

where \( \varphi_{\Lambda}(\kappa, R_{\ell}) \) is a solution of equation (2.5). However, this approach has the disadvantage that the eigenfunctions \( \varphi_{\Lambda}(\kappa, R_{\ell}) \) depend on the ionic positions, which are vibrating, and the determination of the \( \varphi_{\Lambda}(\kappa, R_{\ell}) \) is very difficult. We therefore need an alternative method that uses a fixed set of eigenfunctions. Let us consider an idealized system in which the ions are fixed in their equilibrium positions, and the energy levels \( E_n^0(k) \) and eigenfunctions \( \psi_n^0(k, \mathbf{r}) \) are determined in a one-electron approximation. The small ionic displacement \( \mathbf{u}_n \) due to lattice vibrations gives rise to a change in the potential energy of an electron from that with the ions in their equilibrium positions. We can expand the potential energy of an electron in powers of the displacement up to the linear term
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\[ V(r) = \sum_{\ell \alpha} V_{ei}^{\text{eff}}(r - R_{\ell \alpha}) = \sum_{\ell \alpha} \left[ V_{ei}^{\text{eff}}(r - R_{\ell \alpha}^0) - u_{\ell \alpha} \cdot \nabla V_{ei}^{\text{eff}}(r - R_{\ell \alpha}^0) \right] \]

\[ = V^0(r) - \sum_{\ell \alpha} u_{\ell \alpha} \cdot \nabla V_{ei}^{\text{eff}}(r - R_{\ell \alpha}^0). \]

The second term on the right is the Hamiltonian for the electron-phonon interaction. Thus the electron-phonon interaction Hamiltonian is given by

\[ H_{ep} = \delta V(r) = V(r) - V^0(r) = -\sum_{\ell \alpha} u_{\ell \alpha} \cdot \nabla V_{ei}^{\text{eff}}(r - R_{\ell \alpha}^0). \] (2.31)

In order to find the matrix element of the electronic transition from \((n, k, \sigma)\) to \((n', k', \sigma')\), it is convenient to express \(V_{ei}^{\text{eff}}\) as a Fourier series,

\[ V_{ei}^{\text{eff}}(r - R_{\ell \alpha}^0) = \sum_{\kappa} V_{ei,\alpha}^{\text{eff}}(\kappa) e^{i\kappa \cdot (r - R_{\ell \alpha}^0)}. \] (2.32)

From equations (2.18), (2.23), and (2.32), the electron-phonon interaction Hamiltonian (2.31) can be written as

\[ H_{ep} = -\sum_{\ell \alpha} \frac{1}{\sqrt{NM_0}} \sum_{\ell \alpha} Q_\lambda(q) e^{i(q - \kappa) \cdot R_{\ell \alpha}^0} e^{(\lambda)}(q) \cdot (i\kappa) V_{ei,\alpha}^{\text{eff}}(\kappa) e^{i\kappa \cdot r}. \]

Summing over \(\ell\) and using the relation

\[ \sum_{\ell} e^{i(q - \kappa) \cdot R_{\ell \alpha}^0} = N \sum_{\mathbf{G}_m} \delta_{\kappa, \mathbf{q} + \mathbf{G}_m}, \]

where \(\mathbf{G}_m\) denotes a reciprocal lattice vector, we can calculate the matrix element of the transition from \((n, k, \sigma)\) to \((n', k', \sigma')\);

\[ < n', k', \sigma' | H_{ep} | n, k, \sigma > = \int \psi_{n',k',\sigma'}^* (r) H_{ep} \psi_{nk\sigma} (r) dr. \]

Thus, using equation (2.23) for \(Q_\lambda(q)\) we can write \(H_{ep}\) for a normal process \((\mathbf{G}_m = 0)\) in second-quantized form as

\[ \hat{H}_{ep} = < \hat{\psi}^\dagger | H_{ep} | \hat{\psi} > = \sum_{\lambda\sigma\sigma' n'kq} M_{\lambda\sigma\sigma' n'kq} [a_{\lambda}(q) + a^\dagger_{\lambda}(-q)] c^\dagger_{n'k+q\sigma'} c_{nk\sigma}, \]

where
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\[ M_{\lambda\sigma\nu',\kappa'\kappa} = -i \sum_{\alpha} \sqrt{\frac{N\hbar}{2M_{\alpha}\omega_{\lambda}(q)}} V_{\epsilon_{\alpha}}^{\text{eff}}(q)[q \cdot e_{\alpha}(q)] \]

\[ \times \int u_{\alpha',\kappa'\sigma'}(r)u_{\alpha,\kappa\sigma}(r) < \chi(\sigma') | \chi(\sigma) > dr. \]

Let us now calculate the probability of an electronic transition from a state \(|k\rangle\) to a state \(|k + q\rangle\) in the same electronic band and the spin conservation process. Using Fermi's golden rule the transition probability is given by

\[ W(i \rightarrow f) = \frac{2\pi}{\hbar} |< f | \hat{H}_{\text{ep}} | i >|^2 \delta(E_f - E_i). \]

Using the following matrix elements

\[ < n^{\epsilon}_{k+q} + 1, n^{\epsilon}_{k} - 1; n^{(\lambda)}_{q} - 1 | c^\dagger_{k+q} c_{k}\lambda(q) | n^{\epsilon}_{k+q}, n^{\epsilon}_{k}; n^{(\lambda)}_{q} > \]

\[ = \sqrt{(1 - n^{\epsilon}_{k+q})n^{\epsilon}_{k}n^{(\lambda)}_{q}}, \quad E_f - E_i = E(k + q) - E(k) - \hbar\omega_{\lambda}(q) \]

(for absorption of a phonon)

and

\[ < n^{\epsilon}_{k+q} + 1, n^{\epsilon}_{k} - 1; n^{(\lambda)}_{q} - 1 | c^\dagger_{k+q} c_{k}\lambda(\bar{q}) | n^{\epsilon}_{k+q}, n^{\epsilon}_{k}; n^{(\lambda)}_{q} > \]

\[ = \sqrt{(1 - n^{\epsilon}_{k+q})n^{\epsilon}_{k}(n^{(\lambda)}_{q} + 1)}, \quad E_f - E_i = E(k + q) - E(k) + \hbar\omega_{\lambda}(q) \]

(for emission of a phonon)

we have

\[ W(k \rightarrow k + q) = \frac{2\pi}{\hbar} |M_{\lambda k q}|^2 \left( 1 - n^{\epsilon}_{k+q} \right) \{ n^{(\lambda)}_{q} \delta(E(k + q) - E(k) - \hbar\omega_{\lambda}(q)) \}

\[ + (n^{(\lambda)}_{q} + 1) \delta(E(k + q) - E(k) + \hbar\omega_{\lambda}(q)) \}

where

\[ M_{\lambda k q} = -2i \sum_{\alpha} \sqrt{\frac{N\hbar}{2M_{\alpha}\omega_{\lambda}(q)}} V_{\epsilon_{\alpha}}^{\text{eff}}(q)[q \cdot e_{\alpha}(q)] \]

\[ \times \int u^*_{q+k}(r)u_{k}(r)dr. \]
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2.5 Effect of dimensionality on the electronic bands of a solid

As mentioned in Chapter 1, the dimensionality of a solid means the dimension in which the charge carriers in the solid are free to move. The dimension may be less than that of the bulk semiconductor (3D) due to quantum confinement produced at interfaces between different semiconductors as in semiconductor heterostructures. This Section deals with the effect of dimensionality on the electronic band structure of these heterostructures. For a heterostructure with no free charge carries, it generally suffices to use the envelope function method, which is a textbook quantum mechanics problem [Bastard (1988)], using a known band line-up from the bulk band structure of of the material. For heterostructures with free charge carriers e.g., modulation-doped heterostructures, self-consistent calculations are required.

Here we consider a heterostructure whose potential depends only on the \( x_3 \)-direction, as in 2D systems, and whose states are built up from the same extrema in both types of layers. However, if the heterostructure is built from the different band extrema in the two layers, we can not use the envelope function approximation but use microscopic methods such as tight-binding or pseudopotential method. Once the eigenstates of the bulk semiconductors, which compose the heterostructure, are known, the electronic band structure of the heterostructure can be determined from the envelope function framework [Bastard (1988)]. In the envelope function framework, the electron wave function can be expressed in terms of the Bloch functions of the edge (e.g. \( k_0 \)) under consideration

\[
\psi(r) = \sum_n \frac{1}{\sqrt{A_0}} e^{ik_n \cdot r} u_{n,k_0}(r) \zeta_n(x_3)
\]

where \( A_0 \) is the area of the sample and \( k_n \) is the 2D wave vector measured from the band extrema \( k_0 \). Then the envelope wave function \( \zeta_n(x_3) \) satisfies the one-dimensional Schrödinger and Poisson equations:

\[
\left[ -\frac{\hbar^2}{2m^*(x_3)} \frac{\partial}{\partial x_3} \frac{1}{m^*(x_3)} \frac{\partial}{\partial x_3} + E_{n,k_0} + \frac{\hbar^2}{2m^*(x_3)} k_\parallel^2 + V_e(x_3) \right] \zeta_n(x_3) = E_n(k_\parallel) \zeta_n(x_3) \tag{2.33}
\]

\[
\frac{d^2 V_{sc}(x_3)}{dx_3^2} = \frac{\epsilon \rho(x_3)}{\epsilon} \tag{2.34}
\]
where \( V_c(x_3) \) is the confinement potential and \( V_{s.c}(x_3) \) is the self-consistent potential. The energy eigenvalue and electron charge density are given by

\[
E_n(k_{||}) = E_{n,k_0} + E_n + \frac{\hbar^2 k_{||}^2}{2m^*(x_3)}
\]

\[
\rho(x_3) = -e \sum_{n \text{ occupied}} n_n |\zeta_n(x_3)|^2 + N_a^-(x_3) - N_d^+(x_3),
\]

with

\[
n_n = \begin{cases} 
(m_n^*/k_B T/\pi \hbar^2) \ln[1 + e^{(E_F - E_n)/k_B T}] & \text{if } T \neq 0 \\
(m_n^*/\pi \hbar^2)(E_F - E_n) \Theta(E_F - E_n) & \text{if } T = 0
\end{cases}
\]

where \( n_n \) is the areal concentration of electrons in the \( n \)-th subband, \( N_a^- \) and \( N_d^+ \) are the acceptor and donor concentrations respectively, \( E_F \) is the Fermi energy of the electrons, \( E_{n,k_0} \) is the \( n \)-th band edge energy at the zone centre, and \( E_n \) is the \( n \)-th subband energy. The dependence of the effective mass \( m^* \) on position is hardly distinguishable from the band non-parabolicity of host materials [Bastard (1988)]. In a parabolic band approximation, the energy eigenvalues are given by

\[
E_n(k_{||}) = E_{n,k_0} + E_n + E_{n,K.E}^{2D}.
\]

with

\[
E_{n,K.E}^{2D} = \frac{\hbar^2 k_{||}^2}{2m_n^*},
\]

where the subband energy \( E_n \) satisfies

\[
\left[ -\frac{\hbar^2}{2m_n^*} \frac{d^2}{dx_3^2} + V_c(x_3) \right] \zeta_n(x_3) = E_n \zeta_n(x_3)
\]

and \( m_n^* \) is the in-plane effective mass in the \( n \)-th subband, defined by

\[
\frac{1}{m_n^*} = \int dx_3 |\zeta_n(x_3)|^2 \frac{1}{m^*(x_3)}.
\]

The confinement potential may be expressed as

\[
V_c(x_3) = \Delta E_c f(x_3) + V_{s.c}(x_3) + V_{xc}(x_3)
\]

where \( f(x_3) \) depends on the grading effect of the interface in the heterostructure and \( V_{xc}(x_3) \) is the exchange-correlation potential. A simple analytic form of the exchange-correlation potential, which was parameterised from the local-density-functional theory [Hedin and Lundqvist, (1971)], has been used for several heterostructures such as GaAs-Ga_{1-x}Al_{x}As heterojunctions [Stern and Das Sarma...
The analytic form of the exchange-correlation potential (in units of the effective Rydberg, $R_\ast^* = (e^2/8\pi\varepsilon a_B^*)$) is given by

$$V_{xc}(x_3) = -\left[1 + 0.7734\frac{r_s}{21}\ln(1 + \frac{21}{r_s})\right]\frac{2}{\pi\alpha r_s},$$

with

$$\alpha = \left(\frac{4}{9\pi}\right)^{\frac{1}{3}}; \quad r_s^\ast = r_s(x_3) = \left(\frac{4}{3}\pi a_B^* n(x_3)\right)^{-\frac{1}{3}}.$$

Here $a_B^* = (4\pi\varepsilon\hbar^2/m^*e^2)$ is the effective Bohr radius. The electronic band structure can be evaluated self-consistently through the equations (2.33), (2.34), (2.35), (2.38), and (2.39).

In Si surface inversion layers and modulation doped GaAlAs/GaAs heterojunctions, the band bending has a quasi-triangular shape near the surface and the interface. In these cases, we can use a triangular potential approximation. The simplest approach to the confinement potential is the exact triangular potential which gives a constant electric field $F_s$ and an exact solution for the wave functions [Stern (1972), Ando et al (1982)]:

$$V_c(x_3) = \begin{cases} 
\infty & \text{for } x_3 \leq 0 \\
eF_s x_3 & \text{for } x_3 \geq 0
\end{cases}$$

$$F_s = \begin{cases} 
e(N_{\text{depl}} + N_s)/\varepsilon_A & \text{at the interface} \\
eN_{\text{depl}}/\varepsilon_A & \text{the depletion layer contribution only} \\
e(N_{\text{depl}} + N_s/2)/\varepsilon_A & \text{average field in the inversion layer}
\end{cases}$$

$$\zeta_n(x_3)^{11} = \text{Ai}\left[\left(\frac{2m^*_n eF_s^{\ast}}{\hbar^2}\right)^{1/3} \left(x_3 - \frac{E_n}{eF_s}\right)\right]$$

where $N_s$ and $N_{\text{depl}}$ are the areal electron concentrations in the inversion layer and the depletion charge concentration in the depletion layer of the well region respectively, and where $\varepsilon_A$ is the dielectric constant in the well side, and Ai is the Airy function. Then the energy eigenvalues are approximately given by

$$E_n \approx \left(\frac{\hbar^2}{2m^*_n}\right)^{1/3} \left[\frac{3}{2}\pi eF_s(n + 3/4)\right]^{2/3} \quad n = 0, 1, 2, \ldots$$

**In equation (2.3) of reference [Marmorkos and Das Sarma, (1993)], there is a misprint. The superscript in the equation should read $-\frac{1}{3}$.**

**There is a misprint in the reference [Ando et al (1982)]. The argument of the Airy function in equation (3.23) of the reference should read $\left[\left(\frac{2m^*_n eF_s^{\ast}}{\hbar^2}\right)^{1/3} (z - \frac{E_n}{eF_s})\right]$.**
Furthermore, a simple analytic variational wave function method using the Fang-Howard trial wave function [Fang and Howard (1966)] is available. In Si inversion layers, a triangular well with an infinite barrier is most widely used [Ando et al (1982)] with the Fang-Howard wave function:

$$\zeta(x_3) = \begin{cases} 
0 & \text{for } x_3 \leq 0 \\
\left(\frac{b^3}{2}\right)^{1/2} x_3 \exp\left(-bx_3/2\right) & \text{for } x_3 \geq 0
\end{cases}$$

From the minimization of the total energy per electron, we have the lowest subband energy $E_0$ for the exact triangular potential model (2.40):

$$E_0 = \frac{\hbar^2 b^2}{8m^*_z} + \frac{3eF_s}{b}$$ (2.43)

with

$$b = \left(\frac{6m^*_z eF_s}{\hbar^2}\right)^{1/3}$$ (2.44)

and for the quasi-triangular potential $V_c(x_3) = V_d(x_3) + V_s(x_3) + V_f(x_3)$ which is given in the reference [Ando et al (1982)], we have

$$E_0 = \frac{\hbar^2 b^2}{8m^*_z} + \frac{3e^2 N_{depl}}{\varepsilon_A b^2} - \frac{6e^2 N_a}{\varepsilon_A b^2} + \frac{33e^2 N_s}{16\varepsilon_A b} + \frac{\varepsilon_A - \varepsilon_B}{\varepsilon_A + \varepsilon_B} \left(\frac{e^2 b}{32\pi \varepsilon_A}\right)$$ (2.45)

with

$$b = \left[\frac{12m^*_z e^2}{\varepsilon_A \hbar^2} (N_{depl} + \frac{11}{32}N_a)\right]^{1/3}$$ (2.46)

where $N_a$ is the acceptor charge concentrations and $\varepsilon_B$ is the dielectric constant in the barrier region. The image potential contribution (i.e. $V_f$, the last term in equation (2.45)) and a part of the depletion layer potential contribution (i.e. the third term in equation (2.45)) are neglected to find the minimization parameter $b$ in equation (2.46).

In modulation doped GaAlAs/GaAs heterojunctions [see Figure 2.1], penetration of electrons into the GaAlAs barrier occurs because the height of the barrier in GaAlAs/GaAs heterojunctions is much smaller than that in Si inversion layers. The modified Fang-Howard wave function used for GaAlAs/GaAs heterojunctions is then [Ando (1982), Bastard (1984, 1988)]:

$$\zeta(x_3) = \begin{cases} 
M' \exp(b'x_3/2) & \text{for } x_3 \leq 0 \\
M(x_3 + z_0) \exp(-bx_3/2) & \text{for } x_3 \geq 0
\end{cases}$$
2. The Hamiltonian for Solids

Here $M$, $M'$, and $z_0$ can be determined from the usual boundary and normalization conditions in terms of the two independent variational parameters, $b$ and $b'$. As an approximation, the standard wave-function penetration in the barrier, $b'$, has been taken in the form [Bastard (1988)]:

$$b' = 2\sqrt{\frac{2m_B^\ast \Delta E_c}{\hbar^2}}$$

where $m_B^\ast$ is the effective mass in GaAlAs layer. From the boundary and normalization conditions, we have

$$z_0 = \frac{2}{b + b'(m_A^\ast/m_B^\ast)}$$

$$M = \left(\frac{b^3}{2}\right)^{1/2} \left[1 + b z_0 + \frac{1}{2} b^2 z_0^2 \left(1 + \frac{b}{b'}\right)\right]^{-1/2}$$

$$M' = M z_0$$

Figure 2.1: Band-extrema configurations in a selectively modulation-doped GaAlAs/GaAs single heterojunction (A) before charge transfer (B) after charge transfer. $E_c$ and $E_v$ are the conduction- and valence-band edges. $E_0$ and $E_1$ are the subbands, and $E_F$ is the Fermi energy. $E_{g1}$ and $E_{g2}$ are the band gaps in GaAlAs and GaAs, respectively. $\Delta E_c$ and $\Delta E_v$ are the conduction band offset and the valence band offset.
where $m^*_A$ is the effective mass in GaAs layer. Then we obtain the lowest subband energy as
\[
E_0 = -\frac{\hbar^2}{8m^*_B} M'^2 b' + \frac{\hbar^2 M^2}{2m^*_A} \left( \frac{1}{2b} + \frac{1}{2z_0} - \frac{1}{4b^2z_0^2} \right) + \frac{e^2}{\varepsilon_A} \frac{M^2 z_0^2}{b'^2} \left[ M^2 N_s \left( \frac{2z_0}{b^2} + \frac{4}{b^3} - \frac{z_0^2}{b} - \frac{4z_0}{b^2} - \frac{6}{b^3} \right) - N_{\text{depl}} \right]
\]
where the variational parameter $b$ is determined from the following minimization condition of the total energy per electron:
\[
\frac{\partial \tilde{E}(b)}{\partial b} = 0
\]
where
\[
\tilde{E}(b) = \frac{E(b)}{N} = -\frac{\hbar^2}{8m^*_B} M'^2 b' + \frac{\hbar^2 M^2}{2m^*_A} \left( \frac{1}{2b} + \frac{1}{2z_0} - \frac{1}{4b^2z_0^2} \right) + \frac{1}{2\varepsilon_A} N_s \frac{M^4}{b^7} \left( \frac{33}{4} + \frac{25}{2} b z_0 + \frac{17}{2} b^2 z_0^2 + 3b^3 z_0^3 + \frac{1}{2} b^4 z_0^4 \right) + \frac{e^2}{\varepsilon_A} N_{\text{depl}} M^2 \frac{6}{b^4} \left( 1 + \frac{2}{3} b z_0 + \frac{1}{6} b^2 z_0^2 \right).
\]

The modulation doping technique makes it possible to obtain conducting charge carriers in high-purity, -mobility, and -performance semiconductor devices due to the spatial separation between charge carriers in the channel and impurity atoms in the barrier material. However, the charge mobility is limited by several scattering mechanisms whose contributions to the mobility can be determined by using electronic wave functions as mentioned above, and interaction Hamiltonians depending on scattering mechanisms. One of the important mechanisms is the electron-phonon interaction which is more important in phonon emissions from electronic transitions in low-dimensional system. The effect of electron-phonon coupling on low-dimensionality will be discussed in Chapter 4.
CHAPTER 3

Electron-acoustic Phonon Coupling

3.1 Introduction

Low-dimensional systems have the interesting applicability both to basic research (e.g. 2D physics, quantum Hall effect, etc.) and to high-performance devices (e.g. MOSFET, HEMT, TEGFET, etc) [Weisbuch (1987)]. It therefore becomes very important to understand the various basic mechanisms related to the physical properties in low-dimensional systems. As pointed out in Chapter 1 one of the most important mechanisms is the electron-acoustic phonon interaction which is closely related to the electron mobility and the mechanical wave (i.e. phonon) generation in low-dimensional systems. We shall consider the problems of electron-acoustic phonon couplings in the context of phonon generation.

In semiconductors whose lattices lack inversion symmetry such as GaAs, CdS, and ZnO, both the deformation potential coupling and the piezoelectric coupling play an important role in the electron-acoustic phonon interaction [Mahan (1972, 1990), Ridley (1993)]. In general, the relative strengths of the couplings vary from material to material. For example, it has been found that in n-doped GaAs the piezoelectric coupling does not dominate because electric fields are shielded out by free charge carriers to nearly within the Debye length [Kaufmann et al (1994)]. In the long wavelength region, the screening due to conduction electrons contributes quite significantly to the phonon frequencies, while the screening in the short wavelength region does not [Agarwal and Kachhava (1993)].

In this Chapter, we shall discuss electron-acoustic phonon coupling when free electrons are undergoing electronic transitions in piezoelectric semiconductors. We
shall also discuss the relations between this coupling and the equations of motion for the acoustic (or elastic) and electric fields. First, we consider the basic equations, which will be used in the following Sections, for the electron-acoustic phonon interactions. When acoustic waves are generated due to electronic transitions in non-piezoelectric semiconductors such as Si and Ge, the total Lagrangian density in a quasistatic approximation can be separated into the elastic kinetic part $\mathcal{L}_K$, the elastic potential part $\mathcal{L}_L$, the electric part $\mathcal{L}_D$, and the deformation potential coupling part $\mathcal{L}_d$ in the following form:

$$\mathcal{L} = \mathcal{L}_K + \mathcal{L}_L + \mathcal{L}_D + \mathcal{L}_d$$  \hspace{1cm} (3.1)

with

$$\mathcal{L}_K = \frac{1}{2}\rho_m \left( \frac{\partial u}{\partial t} \right)^2$$  \hspace{1cm} (3.2)

$$\mathcal{L}_L = -\frac{1}{2} \mathbb{T} : \mathbb{\varepsilon}$$  \hspace{1cm} (3.3)

$$\mathcal{L}_D = \frac{1}{2} \mathbf{E} \cdot \mathbf{D} - \rho_e^F \varphi$$  \hspace{1cm} (3.4)

$$\mathcal{L}_d = -n_e(t, \mathbf{r}) \mathbb{\varepsilon}_d : \mathbb{\varepsilon}$$  \hspace{1cm} (3.5)

and

$$\mathbf{E} = -\nabla \varphi \quad \nabla \cdot \mathbf{D} = \rho_e^F = -e n_e,$$

where $\rho_m$ is the mass density of the material, $\mathbf{u}$ is the displacement vector, $\mathbb{\varepsilon}$ the second rank strain tensor\*, $\mathbb{T}$ the second rank stress tensor, $\mathbf{E}$ the electric field vector, $\mathbf{D}$ the electric displacement vector, $\rho_e^F$ the free electron density, $\varphi$ the electrostatic potential, $n_e$ the number density of electrons undergoing the transition, and where $\mathbb{\varepsilon}_d$ is the second rank deformation potential tensor. Double dot product represents summation over pairs of subscripts [see, e.g., equation (3.35)]. For a piezoelectric material, the stress tensor and the electric displacement vector, which will be discussed in detail in Sections 3.2 and 3.3, are expressed as

$$\mathbb{T} = \mathbb{C}^F : \mathbb{\varepsilon} - \mathbf{E} \cdot \mathbf{h},$$  \hspace{1cm} (3.6)

$$\mathbf{D} = \mathbb{\varepsilon}_e \cdot \mathbf{E} + \mathbf{h} : \mathbb{\varepsilon}$$  \hspace{1cm} (3.7)

\*In this thesis, an under-tilde stands for a tensor [cf. upper-tilde as in equation (3.19)].
3. Electron-acoustic Phonon Coupling

where $h$ is the third rank piezoelectric tensor and $Q^E$ is the fourth rank elastic tensor at constant electric field. From equations (3.1) through (3.7), the Lagrangian density for the piezoelectric semiconductor, when electronic transitions occur, may be expressed in the form

$$L = \frac{1}{2} \rho_m \left( \frac{\partial \mathbf{u}}{\partial t} \right)^2 - \frac{1}{2} (Q^E : \mathbf{u}) : \mathbf{u} + \mathbf{E} \cdot h : \mathbf{u}$$

$$+ \frac{1}{2} \mathbf{E} : \varepsilon \cdot \mathbf{E} - \rho_e \varepsilon - n_e \Phi : \mathbf{u}. \quad (3.8)$$

In the next section the thermodynamic functions and thermal variables will be discussed. Section 3.3 deals with continuum approximation for lattice vibrations. In Section 3.4 we give a brief discussion of interface effects on acoustic waves. Sections 3.5 and 3.6 deal with deformation potential and piezoelectric couplings, respectively. Finally, we give brief comments on electron-phonon couplings in low dimensions in Section 3.7.

3.2 Thermodynamic functions and thermal variables

There are several possible choices for thermodynamic functions depending on the independent variables of interest. The Gibbs function $G$ and the electric Gibbs function* $G_2$ are most frequently used for a piezoelectric crystal [Mason (1966)]. Let us choose the electric Gibbs function in which the stresses, electric displacements, and the entropy are the dependent variables while the strains, electric fields, and temperature are the independent ones. In this case, we may express the electric Gibbs function and its differential form as

$$G_2 = U - E_m D_m - \sigma T$$

$$dG_2 = T_{ij} du_{ij} - D_m dE_m - \sigma dT \quad (3.9)$$

where $U$ is the internal energy, $E_m$ are the components of the electric field, $D_m$ are the components of the electric displacement, $\sigma$ is the entropy, and $T$ is the temperature in the crystal. From the differential form of the electric Gibbs function

*Here we follow Mason's notations for the Gibbs functions [Mason (1966)].
3. Electron-acoustic Phonon Coupling

we have

\[ T_{ij} = \left( \frac{\partial G_2}{\partial u_{ij}} \right)_{E,T}, \quad D_m = - \left( \frac{\partial G_2}{\partial E_m} \right)_{y,T}, \quad \sigma = - \left( \frac{\partial G_2}{\partial T} \right)_{y,E} \]  \hspace{1cm} (3.10)

where the subscripts mean that the variables remain constant in the processes. Since the above dependent variables are functions of the independent variables, \( u_{ij}, E_m, \) and \( T, \) we have the following total differentials:

\[

dT_{ij} = \left( \frac{\partial T_{ij}}{\partial u_{kl}} \right)_{E,T} du_{kl} + \left( \frac{\partial T_{ij}}{\partial E_n} \right)_{y,T} dE_n + \left( \frac{\partial T_{ij}}{\partial T} \right)_{y,E} dT, \\

dT, = \left( \frac{\partial D_m}{\partial u_{kl}} \right)_{E,T} du_{kl} + \left( \frac{\partial D_m}{\partial E_n} \right)_{y,T} dE_n + \left( \frac{\partial D_m}{\partial T} \right)_{y,E} dT, \\

d\sigma = \left( \frac{\partial \sigma}{\partial u_{kl}} \right)_{E,T} du_{kl} + \left( \frac{\partial \sigma}{\partial E_n} \right)_{y,T} dE_n + \left( \frac{\partial \sigma}{\partial T} \right)_{y,E} dT. \hspace{1cm} (3.11)
\]

Using equations (3.10) and (3.11), we may write the Maxwell relations for the system as

\[
\left( \frac{\partial T_{ij}}{\partial u_{kl}} \right)_{E,T} = C_{ijkl}^{E,T}, \quad \left( \frac{\partial \sigma}{\partial T} \right)_{y,E} = \frac{\rho_m C_{ij}^{y,E}}{T}, \quad \left( \frac{\partial D_m}{\partial E_n} \right)_{y,T} = \varepsilon_{nm}^{T}, \\

\left( \frac{\partial T_{ij}}{\partial E_n} \right)_{y,T} = - \left( \frac{\partial D_m}{\partial u_{ij}} \right)_{E,T} = -h_{nij}^{T}, \\
\left( \frac{\partial T_{ij}}{\partial T} \right)_{y,E} = - \left( \frac{\partial \sigma}{\partial u_{ij}} \right)_{E,T} = -\lambda_{ij}^{E}, \\
\left( \frac{\partial D_m}{\partial T} \right)_{y,E} = \left( \frac{\partial \sigma}{\partial E_m} \right)_{y,T} = \rho_m^{U}. \hspace{1cm} (3.12)
\]

Here \( C_{ijkl}^{E,T} \) denotes the elastic constant measured at constant electric field and temperature, \( C_{ij}^{y,E} \) is the specific heat at constant strain and electric field, \( \varepsilon_{nm}^{T} \) is the dielectric constant at constant strain and temperature, \( h_{nij}^{T} \) is the piezoelectric constant at constant temperature, \( \lambda_{ij}^{E} \) is the thermal stress constant at constant electric field, and \( \rho_m^{U} \) is the pyroelectric constant for the crystal at constant strain.

On introducing the constants (3.12) in equation (3.11), we obtain the following equations:

\[ T_{ij} = C_{ijkl}^{E,T} u_{kl} - h_{nij}^{T} E_m - \lambda_{ij}^{E} \delta T \]
3. Electron-acoustic Phonon Coupling

\[ D_m = \hbar \tau_{mij} u_{ij} + \varepsilon_{mn} E_m + p_m \delta T \]

\[ \delta \sigma = \lambda_{ij} u_{kl} + \frac{\varepsilon_{mn} E_m}{\rho_m C_{ij} E} \delta T. \]  

(3.13)

For a rapidly vibrating crystal, there is no change in heat. We may therefore use the adiabatic condition \((\delta Q = T \delta \sigma = 0)\) to eliminate \(\delta T\) from equation (3.13). This gives the relation between adiabatic and isothermal values of elastic, piezoelectric and dielectric constants as follows:

\[ T_{ij} = C_{ijkl} u_{kl} - h_{mij} E_m \]  

(3.14)

\[ D_m = h_{mij} u_{ij} + \frac{\varepsilon_{mn} E_m}{\rho_m C_{ij} E} \]  

(3.15)

with*

\[ C_{ijkl}^E = C_{ijkl}^E + \frac{\lambda_{ij} E_k^T}{\rho_m C_{ij} E}, \quad h_{mij}^E = h_{mij}^T - \frac{\lambda_{ij} p_m E_k^T}{\rho_m C_{ij} E}, \quad \varepsilon_{mn} = \varepsilon_{mn}^T - \frac{p_m p_n E_k^T}{\rho_m C_{ij} E}. \]

Unless the crystal is pyroelectric (only the crystal classes—1, \( \bar{1} \), 2, \( \bar{2} = m \), 2/m, 3, \( \bar{3} \), 4, \( \bar{4} / m \), 6, \( \bar{6} \), 6/m), the piezoelectric and dielectric constants are identical for isothermal and adiabatic processes.

3.3 Continuum approximation for lattice vibrations

At low temperatures \((T \ll \Theta_D)\), only elastic waves (or acoustic phonons) with small \(q\) \((i.e.\ long\ wavelength)\) will be excited [Bardeen (1937)]. In such situations, the lattice can be considered to be a continuous medium which is the long wavelength limiting case. In this case, the lattice displacements as in (2.17) can be described as a slowly changing continuous displacement field \(u(r,t)\) which corresponds to the discrete \(u^{(\lambda)}_{\kappa\alpha}\) as in (2.17) at the lattice points:

\[ u^{(\lambda)}(r,t) = u^{(\lambda)}_0 e^{(\lambda) q}(q)e^{i(q \cdot r - \omega\tau - q(t)} , \]  

(3.16)

where \(u^{(\lambda)}_0\) denotes the amplitude of the displacement for a mode \((\lambda, q)\). Even though we do not have any periodic structure of positive ions in a continuum, we

*In the equations just below equation (4.21) on page 87 in reference [Mason (1966)], there is a misprint. The constant \(C_{ij}^E\) should read \(C_{ij}^U\) which is the specific heat at constant strain and electric field rather than constant stress and electric field. In the reference, the superscript \(T\) is used for the process at constant stress instead of \(T\).
3. Electron-acoustic Phonon Coupling

can define a strain tensor associated with lattice vibrations along the lines of the theory of elasticity in continuous media [Landau and Lifshitz (1986)]. Furthermore, the equation of motion (2.10) for the discrete lattice can be reduced to the equation of motion of an elastic continuum in a non-piezoelectric material as

$$
\rho_m \ddot{u}_i = \sum_j \frac{\partial T_{ij}}{\partial x_j} = \sum_{jkl} \frac{\partial}{\partial x_j} (C_{ijkl} u_{kl})
$$

(3.17)

where general strain for small deformations is given by

$$
u_{ij} = \frac{1}{2} \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right),
$$

(3.18)

with $u_i$ the $x_i$-axis component of the displacement vector $\mathbf{u}$. Let us introduce the following simpler notations [Auld (1973)] which treat a tensor as a matrix:

$$
\mathbf{S} = \tilde{\nabla} \mathbf{u}
$$

(3.19)

with

$$
\tilde{\nabla} = \begin{pmatrix}
\frac{\partial}{\partial x_1} & 0 & 0 & 0 & \frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_2}
0 & \frac{\partial}{\partial x_2} & 0 & \frac{\partial}{\partial x_3} & 0 & \frac{\partial}{\partial x_1}
0 & 0 & \frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} & 0
\end{pmatrix}
$$

and

$$
\tilde{\mathbf{u}} = (u_1, u_2, u_3)
$$

where $\mathbf{S}$, called the engineering strain, is a six component column vector [$\mathbf{S}_r$ $(r = 1, 2, \ldots, 6)$], $\mathbf{u}$ is a three component column vector, a bold nabla ($\tilde{\nabla}$) is the $3 \times 6$ matrix-differential operator, and an upper-tilde (e.g. $\tilde{\mathbf{S}}$) stands for a transposed matrix. Using the engineering strain and equations (3.14) and (3.15), the Lagrangian density (3.8) for a piezoelectric semiconductor can be written in the form

$$
\mathcal{L} = \frac{1}{2} \rho_m \left( \frac{\partial \tilde{\mathbf{u}}}{\partial t} \right) \left( \frac{\partial \mathbf{u}}{\partial t} \right) - \frac{1}{2} \tilde{\mathbf{S}} (\mathbf{C} \mathbf{E} \mathbf{S}) + \tilde{\mathbf{E}} (\mathbf{h} \mathbf{S}) + \frac{1}{2} (\tilde{\mathbf{E}} (\varepsilon \mathbf{E}) - \rho_e \phi - n_e (\mathbf{r}, t) \tilde{\mathbf{E}} \mathbf{S},
$$

(3.20)

or

$$
\mathcal{L} = \frac{1}{2} \rho_m \left( \frac{\partial \tilde{\mathbf{u}}}{\partial t} \right) \left( \frac{\partial \mathbf{u}}{\partial t} \right) - \frac{1}{2} (\tilde{\nabla} \mathbf{u}) (\mathbf{C} \mathbf{E} \tilde{\nabla} \mathbf{u}) - (\tilde{\nabla} \phi) (\mathbf{h} \tilde{\nabla} \mathbf{u})
$$

$$
+ \frac{1}{2} (\tilde{\nabla} \phi) (\varepsilon \tilde{\nabla} \phi) - \rho_e \phi - n_e (\mathbf{r}, t) \tilde{\mathbf{E}} \tilde{\nabla} \mathbf{u}
$$

(3.21)
3. Electron-acoustic Phonon Coupling

with

\[ \vec{\nabla}_c = \left( \frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3} \right), \]

where \( C^E \) is a 6 x 6 matrix, \( \Xi \) is the deformation potential with the six component column matrix [\( \Xi_{r} = 1, 2, \ldots, 6, (\Xi_1 = \Xi_{11}, \Xi_2 = \Xi_{22}, \Xi_3 = \Xi_{33}, \Xi_4 = \Xi_{23} = \Xi_{32}, \Xi_5 = \Xi_{31} = \Xi_{13}, \Xi_6 = \Xi_{12} = \Xi_{21}) \], \( h \) is a 3 x 6 matrix, and \( \varepsilon \) is a 3 x 3 matrix.

For cubic crystals without inversion symmetry, \( C^E, h, \) and \( \varepsilon \) are given by [Cady (1946)],

\[
C^E = \begin{pmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44}
\end{pmatrix}, \tag{3.22}
\]

\[
h = \begin{pmatrix}
0 & 0 & 0 & h_{14} & 0 & 0 \\
0 & 0 & 0 & 0 & h_{14} & 0 \\
0 & 0 & 0 & 0 & 0 & h_{14}
\end{pmatrix}, \tag{3.23}
\]

\[
\varepsilon = \varepsilon \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix}, \tag{3.24}
\]

It is easy to derive equations of motions for the elastic and electric fields using the Lagrangian density (3.21);

\[ \rho_m \frac{\partial^2 u}{\partial t^2} - \nabla (C^E \nabla u + h \nabla \varphi + n_e \Xi) = 0 \tag{3.25} \]

\[ \nabla_c (-h \nabla u + \varepsilon \nabla \varphi) + \rho_e^F = 0 \tag{3.26} \]

which are Newton's equation of motion and Poisson's equation, respectively. From equation (3.7), we have the following relation for the electric field in matrix form;

\[ E = -\nabla \varphi = \varepsilon^{-1}D - \varepsilon^{-1}h \nabla u \tag{3.27} \]

with

\[ \varepsilon \varepsilon^{-1} = \varepsilon^{-1} \varepsilon = I \]

where \( I \) is the unit matrix. Therefore, the equation of motion (3.25) for the elastic field may be expressed as

\[ \rho_m \frac{\partial^2 u}{\partial t^2} - \nabla (C^D \nabla u) = F^{(e)} = F^{(d)} + F^{(p)} \tag{3.28} \]
3. Electron-acoustic Phonon Coupling

with

$$C^D = C^E + \hbar \varepsilon^{-1}$$

(3.29)

and

$$F^{(d)} = \nabla (n_e \Phi) \quad F^{(p)} = -\nabla (\hbar \varepsilon^{-1} D)$$

(3.30)

where $C^D$ is the stiffened elastic constant which is measured under a constant electric displacement $D$, $F^{(d)}$ is the source force matrix via deformation potential couplings, and $F^{(p)}$ is the source force matrix via piezoelectric couplings under electronic transitions. The stiffened elastic constant $C^D$ is greater than the elastic constant $C^E$ in piezoelectric materials. Hence piezoelectric couplings enhance the velocity of acoustic waves. For a cubic crystal which lacks inversion symmetry, the stiffened elastic constant $C^D$ is given by

$$C^D = 
\begin{pmatrix}
C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\
C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\
0 & 0 & 0 & C_{44} + (h_{22}^2/\varepsilon) & 0 & 0 \\
0 & 0 & 0 & 0 & C_{44} + (h_{14}^2/\varepsilon) & 0 \\
0 & 0 & 0 & 0 & 0 & C_{44} + (h_{14}^2/\varepsilon)
\end{pmatrix}.$$  

(3.31)

Using Fourier transformations, the equation of motion (3.28) can be written

$$-\rho_m \omega^2 \mathbf{u}(k, \omega) + k(C^D \mathbf{k} \mathbf{u}(k, \omega)) = F^{(s)}(k, \omega) = F^{(d)}(k, \omega) + F^{(p)}(k, \omega)$$

(3.32)

with

$$k = \begin{pmatrix}
k_1 & 0 & 0 & 0 & k_3 & k_2 \\
k_2 & 0 & k_3 & 0 & k_1 & 0 \\
k_3 & k_2 & k_1 & 0 & 0 & 0
\end{pmatrix} \quad \text{and} \quad k = \begin{pmatrix}
k_1 \\
k_2 \\
k_3
\end{pmatrix}$$

(3.33)

where

$$f(k, \omega) = \int dt \int dr f(r, t) e^{-i(kr - \omega t)}.$$  

The source force via piezoelectric couplings can be determined using Poisson's equation (3.26). Let us define a potential $\varphi_D$ which satisfies Poisson's equation;

$$\nabla n_e \varphi_D = -\rho_0 e = e n_e \quad D = -\nabla \varphi_D.$$  

Therefore, the electric displacement $D$ in Fourier space can be written

$$D(k, \omega) = i e \frac{k}{k^2} n_e(k, \omega).$$
3. Electron-acoustic Phonon Coupling

Using the above relations, the source force matrices may be written in the following forms

\[
F^{(d)}(k, \omega) = i k n_e(k, \omega) \Xi \
F^{(p)}(k, \omega) = e k [\hbar \epsilon^{-1}(k^2) n_e(k, \omega)].
\]  (3.34)

3.4 Surface and interface acoustic modes

The role of the localization of lattice vibrations may be significant in heterostructures. From the viewpoint of the long wavelength limit (continuum model of solids), the localization of the elastic waves at the surface of a half space or at the interface of two solids is determined from the elastic properties of the system. Localized modes of elastic waves such as Rayleigh waves, Stoneley waves, Sezawa waves and Love waves were first studied in the context of seismology many years ago [Ewing et al (1957)]. With development of epitaxial crystal growth techniques, the localized modes of lattice vibrations in solids became basic topics for scientific research and technical applications. The localization of phonons in low-dimensional systems (e.g. Rayleigh waves near a surface [Ezawa (1971)], Stoneley waves near an interface [Djafari-Rouhani et al (1977a)]) is very important in the study of surface phonon propagation [Aleksandrov et al (1994a, 1994b)] and electrical transport [Prange (1969)] through a semiconductor heterojunction, where the electron-phonon interaction could cause most of the scattering. Recently, the confined acoustic phonons within a 2DEG due to the electron-phonon interaction have been investigated [Kochelap and Gülseren (1993), Bannov et al (1994)].

3.5 Deformation potential coupling

The energy band structure of a solid determines the energy distribution of the electrons in the solid and their properties in external fields. When the \(N_a\) identical atoms comprising the solid are far enough apart, the coupling between them may be weak enough that the quantum states of the system will be \(N_a\)-fold degenerate. As the atoms come closer together, the wave functions of adjacent atoms develop significant overlap and the degenerated energy levels spread out into a band of levels as in Figure 3.1 [Shockley (1950)]. The electronic state occupations...
3. Electron-acoustic Phonon Coupling

Figure 3.1: Dependence of energy levels on lattice constant.

Figure 3.2: Shift of band edges with lattice spacing.
of electrons and the band structure in a solid determine whether the solid is a metal, a semiconductor, or an insulator. In general, the position of the conduction and valence band extrema in a semiconductor depend on the lattice spacing as in Figure 3.2 [Nag (1972)]. Since the spacing of the lattice atoms shift when they vibrate, the conduction band minimum and the valence band maximum change from one point to another. As the lattice atoms vibrate they are displaced in position and at the same time strains are produced. In the limit in which only phonons whose wavelength is long compared to the lattice spacing are considered, the vibrations of the solid resemble those of an elastic continuum, and their effects may be described using the theory of elasticity. The basic concept of the theory is that when the solid is subject to a strain (tensor) $\mathbf{u}$, which is a slowly varying function of position, there will be a change in the energy of each electronic state, and that this change will be proportional to the strain as long as the strain is small. Therefore, we may write for the change in energy of an electron in a state with wave vector $\mathbf{k}$ in band $n$,

$$
\Delta E(n, \mathbf{k}) = \sum_{ij} \Xi_{ij}(n, \mathbf{k})u_{ij} = \mathbf{\Xi} : \mathbf{u} 
$$

(3.35)

where the $\Xi_{ij}$ is the deformation potential tensor. In the classical sense the change in electron energy can be set equal to the change in the potential energy. So the deformation potential is obtained as an interaction term:

$$
V_D = \Delta E(n, \mathbf{k}) = \sum_{ij} \Xi_{ij}(n, \mathbf{k})u_{ij}.
$$

Generally, the deformation potential tensor $\Xi_{ij}(n, \mathbf{k})$ depends on the crystal structure and the band structure of the solid. For instance, in the case of a cubic crystal with spherical energy surfaces, the deformation potential has a simple form:

$$
V_D = \Xi_h \nabla \cdot \mathbf{u} = \Xi_h (u_{xx} + u_{yy} + u_{zz})
$$

where $\Xi_h$ is the hydrostatic deformation potential as in Bardeen and Shockley’s paper (1950). Deformation potentials for ellipsoidal energy surfaces were investigated by several authors [Dumke (1956), Herring and Vogt (1956, 1957)].
3. Electron-acoustic Phonon Coupling

3.5.1 Effect of strain on energy eigenvalues

In order to determine the effect of strain on the energies of the electronic levels in crystals, we must first consider the Hamiltonian representing the change in the electronic energy due to a uniform strain. The Hamiltonian for an electron in an unstrained crystal is

\[ H_0 = \frac{p^2}{2m} + V_0(r) \]

with \( p = -i\hbar \nabla \). Its eigenfunctions and eigenvalues are

\[ \psi_{nk}(r) = u_{nk}(r)e^{ik \cdot r} \]

and \( E_n^0(k) \), respectively. \( V_0(r) \) and \( u_{nk}(r) \) are periodic functions of \( R^0 = a_1^0 + a_2^0 + a_3^0 \) where \( \{a_i^0\} \) are lattice basis vectors. Under a strain \( \mathbf{u} \), the lattice point \( R_0^m \) (i.e., \( m_1a_1^0 + m_2a_2^0 + m_3a_3^0 \)) in the unstrained crystal is displaced to the point \( R_m \):

\[ R_m = (I + \mathbf{u}) \cdot R_0^m \]

The Hamiltonian of the strained crystal can be written [Bir and Pikus (1974)] as

\[ H(\mathbf{u}) = \frac{p^2}{2m} + V_\mathbf{u}(r) \]

where \( V_\mathbf{u}(r) \) is the potential in the strained crystal. The eigenfunctions and eigenvalues [Bir and Pikus (1974), Kartheuser and Rodriguez (1986)] are

\[ \phi_{nk\mathbf{u}}(r) = u'_{nk\mathbf{u}}(r)e^{ik \cdot r} \]

and \( E_n(k_\mathbf{u}) \), respectively. \( V_\mathbf{u}(r) \) and \( u'_{nk\mathbf{u}}(r) \) have the periodicity of \( R = (I + \mathbf{u}) \cdot R^0 \). If an eigenstate of the unstrained crystal has wave vector \( k \) and band index \( n \), the corresponding eignestate in the strained crystal has wave vector \( k_\mathbf{u} = (I - \mathbf{u}) \cdot k \) and the same band index \( n \). The effect of a small strain, \( \mathbf{u} \), may be treated as a perturbation. However, we can not directly apply ordinary perturbation theory [Pikus and Bir (1959)] because we can not regard the difference \( V_\mathbf{u}(r) - V_0(r) \) as a small perturbation of \( H_0 \). This difficulty may be avoided by using an inverse transformation of coordinates, making the lattice positions of the strained crystal in the new coordinate system coincide with those of the unstrained crystal in the old coordinate system:

\[ r' = (I + \mathbf{u})^{-1} \cdot r = (I - \mathbf{u}) \cdot r \]
3. Electron-acoustic Phonon Coupling

\[ p' = (\mathbf{I} + \mathbf{y}) \cdot p \]  (3.36)

In the new coordinate system, \( H'(\mathbf{y}) \) has the same symmetry as \( H_0 \). Under the transformation,

\[
H'(\mathbf{y}) = \frac{p'^2}{2m} - \frac{1}{m} \sum_{ij} u_{ij} p'_i p'_j + V_\mathbf{y}((\mathbf{I} + \mathbf{y}) \cdot r')
\]

\[ = \frac{p'^2}{2m} + V_0(r') + \sum_{ij} u_{ij}[V_{ij} - \frac{1}{m} p'_i p'_j]
\]

\[ = \frac{p'^2}{2m} + V_0(r') + \sum_{ij} u_{ij} D_{ij}
\]

\[ = H_0(r', p') + H_\mathbf{y}(r', p'),
\]

where

\[ H_0(r', p') = \frac{p'^2}{2m} + V_0(r') \]

\[ H_\mathbf{y}(r', p') = \sum_{ij} u_{ij} D_{ij}
\]

\[ V_{ij}(r') = \frac{1}{2 - \delta_{ij}} \lim_{u_{ij} \to 0} \frac{V_\mathbf{y}((\mathbf{I} + \mathbf{y}) \cdot r') - V_0(r')}{u_{ij}}
\]

and

\[ D_{ij} = V_{ij} - \frac{1}{m} p'_i p'_j.
\]

In other words, the Schrödinger equation of the strained crystal in the new coordinate system can be written as

\[ H'(\mathbf{y}) \Phi_{nk'}((\mathbf{I} + \mathbf{y}) \cdot r') = E_n((\mathbf{I} - \mathbf{y}) \cdot k') \Phi_{nk'}((\mathbf{I} + \mathbf{y}) \cdot r') \]

where

\[ E_n((\mathbf{I} - \mathbf{y}) \cdot k') = E_n((\mathbf{I} - \mathbf{y}) \cdot k)
\]

because we have \( k_\mathbf{y} = (\mathbf{I} + \mathbf{y}) \cdot k' \) from the coordinate transformation and \( k_\mathbf{y} = (\mathbf{I} + \mathbf{y}) \cdot k \) from the effect of the strain.

\( H_\mathbf{y} \) is now the desired perturbation on \( H_0 \) due to the strain. The wavefunctions of \( H_0(r', p') \) are of the Bloch form \( u_{nk}(r')e^{ikr'}. \) When written in terms of the original coordinate system of the strained crystal, the wavefunctions are

\[ \psi_{nk}(r') = u_{nk}((\mathbf{I} - \mathbf{y}) \cdot r)e^{ik((\mathbf{I} - \mathbf{y}) \cdot r)} \]
3. Electron-acoustic Phonon Coupling

Therefore, \( \psi_{nk} \) belongs to the wave vector \( \mathbf{k}_U = (\mathbf{I} - \mathbf{u}) \cdot \mathbf{k} \) and to energy \( E^0_n(\mathbf{k}_U) \).

The energy eigenvalue of \( H'(\mathbf{u}) \) associated with the solution of

\[
H_0(r', p') \psi_{nk}(r') = E^0_n(k) \psi_{nk}(r')
\]

is

\[
E_n((\mathbf{I} - \mathbf{u}) \cdot \mathbf{k}) = E^0_n(k) + \sum_{ij} u_{ij} < n, k | D_{ij} | n, k > .
\]

There is no unique definition of the deformation potential for a strain \( \mathbf{u} \). If we compare the energies at the wave vector \( \mathbf{k}_U \) in the strained system and the wave vector \( \mathbf{k} \) in the unstrained system [Gibson and Keller (1957)], then the deformation potential is given by

\[
\Xi^b_{ij}(k) = \lim_{u_{ij} \rightarrow 0} \frac{\mathcal{E}((\mathbf{I} - \mathbf{u}) \cdot \mathbf{k}) - \mathcal{E}^0(k)}{u_{ij}} = < D_{ij} > ,
\]

where \( \Xi^b_{ij}(k) \) is called the band structure deformation potential [Khan and Allen (1984, 1986)]. If we compare the energies at the same value of \( \mathbf{k} \), the deformation potential is defined by

\[
\Xi^e_{ij}(k) = \lim_{u_{ij} \rightarrow 0} \frac{\mathcal{E}(k) - \mathcal{E}^0(k)}{u_{ij}} = \frac{1}{2} \left[ k_i \frac{\partial \mathcal{E}^0}{\partial k_j} + k_j \frac{\partial \mathcal{E}^0}{\partial k_i} + D_{ij} \right].
\]

Suppose now that there is a phonon with a wave vector \( \mathbf{q} \). The displacement \( \mathbf{u} \) at the point \( \mathbf{r} \) gives rise to a change in the density of electrons, and the change in density induces a change in potential \( \delta \mathcal{V} (\mathbf{r}) = \mathcal{V}(\mathbf{r} - \mathbf{u}) - \mathcal{V}(\mathbf{r}) = \sum_{ij} V_{ij} u_{ij} \).

The deformation potential theorem introduced by Bardeen and Shockley (1950) is the relation of the change per macroscopic strain in the energy of an electron level to the matrix elements of the electron-phonon interaction. The theorem for phonons with wave vector \( \mathbf{q} \) is

\[
\langle \mathbf{k} + \mathbf{q} | H_{ep} | \mathbf{k} \rangle = \sum_{ij} \Xi^e_{ij}(k) u_{ij} = \sum_{ij} \left( \Xi^b_{ij}(k) + m v_i(k) v_j(k) \right) u_{ij},
\]

where \( H_{ep} = \delta \mathcal{V}(\mathbf{r}) \) is the change in the potential energy of an electron under the strain \( \mathbf{u} \) and \( v_i(k) \) is the group velocity of the electron. The theorem was proved by Khan and Allen (1984) within a rigid-ion model of \( \delta \mathcal{V}(\mathbf{r}) \), by Kartheuser and Rodriguez (1986) within both a rigid-ion and deformable-ion model of \( \delta \mathcal{V}(\mathbf{r}) \),
and by Resta (1991) within the Kohn-Sham potential of $\delta V(r)$ in the density-functional theory. In fact, the theorems of Khan and Allen (1984) and Kartheuser and Rodriguez (1986) are valid only for metals. Resta extended the theorem to both metals and dielectrics and is valid for any long-wavelength phonon, by generalizing deformation potentials to take into account the long-range nature of the Coulomb interaction which has a fourth-rank tensor term. He showed that the deformation potential theorem has different aspects in metals and dielectrics. In the case of deformable jellium [see Chapter 4], there is no effect due to the long-range Coulomb interaction, so that the deformation potential theorem is reduced to equation (3.38).

When we calculate the electronic energy shift due to a single acoustic phonon with wave vector $\mathbf{q}$ and mode ($\lambda$), we use the effective deformation potential because the energy shift of the electronic energy depends on the direction of propagation and the polarization of the phonon. From equations (3.16) and (3.18), we obtain

$$u_{ij}^{(\lambda)}(\mathbf{q}) = u_0^{(\lambda)} \frac{1}{2} \left[ e_1^{(\lambda)}(\mathbf{q}) q_j + e_2^{(\lambda)}(\mathbf{q}) q_i \right].$$

or from equation (3.19), we also have a strain associated with the phonon ($\lambda, \mathbf{q}$) in matrix form

$$\mathbf{S}^{(\lambda)}(\mathbf{q}) = i\mathbf{q} \mathbf{u}^{(\lambda)}(\mathbf{q})$$

with

$$\mathbf{q} = \begin{pmatrix} q_1 & 0 & 0 & q_3 & q_2 \\ 0 & q_2 & 0 & q_3 & 0 \\ 0 & 0 & q_3 & q_2 & q_1 \end{pmatrix}$$

(3.39)

and where

$$\mathbf{u}^{(\lambda)}(\mathbf{q}) = u_0^{(\lambda)} \mathbf{e}^{(\lambda)}(\mathbf{q})$$

$$\mathbf{e}^{(\lambda)}(\mathbf{q}) = (e_1^{(\lambda)}(\mathbf{q}), e_2^{(\lambda)}(\mathbf{q}), e_3^{(\lambda)}(\mathbf{q})).$$

Then the energy shift due to the acoustic phonon with wave vector $\mathbf{q}$ and mode ($\lambda$) can be written as

$$V_D^{(\lambda)}(\mathbf{q}) = \Xi \mathbf{S}^{(\lambda)}(\mathbf{q}) = i\Xi [\mathbf{q} \mathbf{u}^{(\lambda)}(\mathbf{q})] = u_0^{(\lambda)} \left( \Xi_{\mathbf{e}_f}(\mathbf{q}) i\mathbf{q} \right)$$

where $\Xi_{\mathbf{e}_f}(\mathbf{q})$ is called the effective deformation potential due to a phonon in the state ($\lambda, \mathbf{q}$),

$$\Xi_{\mathbf{e}_f}(\mathbf{q}) = \left( \Xi [\mathbf{q} e^{(\lambda)}(\mathbf{q})] / q \right)$$

(3.40)
3. Electron-acoustic Phonon Coupling

3.6 Piezoelectric coupling

Materials lacking a centre of symmetry usually manifest piezoelectric phenomena, i.e. an electric field is induced when the materials deform and conversely, the electric field induces an elastic deformation. Let us consider a piezoelectric semiconductor where there are no free charge carriers. The electric potential \( \varphi \) can be determined from Poisson’s equation (3.26) with the condition \( \rho_e^F = 0 \)

\[
\nabla \varepsilon \varphi = \nabla \phi (h \nabla u)
\]

(3.41)

Using Fourier transformations, the electric potential due to piezoelectric couplings associated with the strain due to a single acoustic phonon in a state \(( \lambda, \mathbf{q} )\) may be written as

\[
\varphi^{(\lambda)} (\mathbf{q}) = \left( \frac{\hat{q} (h \left[ \hat{q} \mathbf{u}^{(\lambda)} (\mathbf{q}) \right])}{\hat{q} \varepsilon \mathbf{q}} \right)
\]

(3.42)

with

\[
\hat{q} = (q_1, q_2, q_3).
\]

(3.43)

We can write the electric potential (3.42) as

\[
\varphi^{(\lambda)} (\mathbf{q}) = \frac{h_{e_{\mathbf{q}}^{(\lambda)}} (\mathbf{q}) u_0^{(\lambda)}}{\varepsilon_0}
\]

with

\[
h_{e_{\mathbf{q}}^{(\lambda)}} (\mathbf{q}) = \varepsilon_0 \left( \frac{\hat{q} (h \left[ \hat{q} \mathbf{e}^{(\lambda)} (\mathbf{q}) \right])}{\hat{q} \varepsilon \mathbf{q}} \right)
\]

(3.44)

where \( \varepsilon_0 \) is the permittivity of the vacuum, and \( h_{e_{\mathbf{q}}^{(\lambda)}} (\mathbf{q}) \), which depends on the direction of propagation and the polarization of the phonon as in the case of deformation potential, is called effective piezoelectric constant associated with a single acoustic phonon with a state \(( \lambda, \mathbf{q} )\). Now the potential via piezoelectric couplings due to all of the phonons can be obtained by [Mahan (1972)]

\[
\varphi_p (\mathbf{r}) = \sum_{\lambda, \mathbf{q}} \varphi^{(\lambda)} (\mathbf{q}) e^{i\hat{\mathbf{q}} \cdot \mathbf{r}}.
\]

If free electrons are introduced in the piezoelectric semiconductors, the free electrons will interact with the above potential \( \varphi_p (\mathbf{r}) \). Hence the electron-phonon interaction Hamiltonian due to piezoelectric couplings can be written as

\[
H_{ep}^{(F)} = \int d^3 \mathbf{r} \rho_e^F (\mathbf{r}) \varphi_p (\mathbf{r}) = -e \int d^3 \mathbf{r} n_e (\mathbf{r}) \varphi_p (\mathbf{r})
\]
Using the classical Hamiltonian equations of motion, the force density due to the piezoelectric couplings is given by

$$F^{(p)}(r) = -\frac{\partial}{\partial u} \left[ \rho^{F}_{e}(r)\varphi_{p}(r) \right] = e\frac{\partial}{\partial u} \left[ n_{e}(r)\varphi_{p}(r) \right]$$

or in a matrix form with Fourier transformation

$$F^{(p)}(k) = e\left( \frac{\partial}{\partial u} \left[ n_{e}(k) \left( \frac{k}{\hbar} [\hat{u}(k)] \right) \right] \right) = e \left[ n_{e}(k) \left( \frac{(k\hbar)k}{(k\varepsilon)k} \right) \right]$$

where superscript $t$ denotes a transposed matrix as in the upper-tilde e.g., $\hbar$.

### 3.7 Comments on electron-phonon coupling in low dimensions

The determination from first principles of deformation potentials in lower-dimensional systems has not been pursued prior to Oh et al (1994). Most physical quantities associated with the deformation potential have used 3D results. However, it has been suggested that the deformation potential in 2D systems for GaAs should be greater than that in 3D systems in order to explain the experimental results reported by several authors [Vinter (1986a, 1986b), Kawamura and Das Sarma (1990), Das Sarma (1991)], where they have used the electron mobility. From an experimental point of view, measurements of electron mobility include several mechanisms due to carrier-carrier scattering, acoustic phonon scattering, piezoelectric scattering, optical phonon scattering, polar optical scattering, and impurity atom scattering. Figure 3.3 [Bockelmann (1994)] is a theoretical result for the electron scattering rate due to longitudinal phonons in low-dimensional systems. The dependence of the scattering rate on dimensionality is due to the different electronic states in each case. Interface effects are ignored and the same electron-phonon coupling constants as in 3D are used in each case for the calculation of Figure 3.3.

Recently, the time-of-flight method for detecting phonons and for distinguishing between the different polarisations of phonons has been developed. The method has also provided the phonon intensity as a function of emission angle. A comparison of the experimental phonon distribution with the theoretical calculation of phonon intensity will provide much information on the effect of electron-phonon
couplings in low-dimensional systems. For instance, the deformation potential and the piezoelectric constant due to an arbitrary strain, and the dielectric constant for 3D GaAs are known to be

\[
\Xi = \Xi_h(1,1,1,0,0,0)
\]

\[
h = h_{14}\begin{pmatrix}
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\]

\[
\varepsilon = \varepsilon\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix},
\]

where \(\Xi_h = 7\ eV\) [Shur, (1987)], \(h_{14} = 0.16\ C/m^2\) [Ridley (1993)], and \(\varepsilon = 13.18\varepsilon_0\) [Adachi (1985)]. From equations (3.40) and (3.44), we can obtain the effective deformation potential \(\Xi_{eff}(q)\) and the effective piezoelectric constant \(h_{eff}(q)\) associated

---

Figure 3.3: Scattering rates for LA phonons in 0D, 1D, and 2D systems, \((L_z = 10\ nm, T=4\ K, for\ InGaAs/InP)\) [Bockelmann (1994)].
3. Electron-acoustic Phonon Coupling

with a single acoustic phonon in a state \((\lambda, \mathbf{q})\) as

\[
\Xi^{(\lambda)}_{\text{eff}}(\mathbf{q}) = \Xi_h \left[ \frac{q_1}{q} e_1^{(\lambda)}(\mathbf{q}) + \frac{q_2}{q} e_2^{(\lambda)}(\mathbf{q}) + \frac{q_3}{q} e_3^{(\lambda)}(\mathbf{q}) \right] = \Xi_h \cos(\mathbf{q}, e^{(\lambda)}(\mathbf{q}))
\]

\[
k^{(\lambda)}_{\text{eff}}(\mathbf{q}) = 2 \hbar \frac{\xi_0}{\varepsilon} \left[ \frac{q_2}{q} \frac{q_3}{q} e_1^{(\lambda)}(\mathbf{q}) + \frac{q_3}{q} \frac{q_1}{q} e_2^{(\lambda)}(\mathbf{q}) + \frac{q_1}{q} \frac{q_2}{q} e_3^{(\lambda)}(\mathbf{q}) \right]
\]

where \((\mathbf{q}, e^{(\lambda)}(\mathbf{q}))\) is the angle between wave vector \(\mathbf{q}\) and polarization vector \(e^{(\lambda)}(\mathbf{q})\).

Then we have important explanation of features for electron-phonon couplings when the effective deformation potential and the effective piezoelectric constant are considered. It is obvious that \(\Xi^{(t)}_{\text{eff}}(\mathbf{q}) = 0\) for transverse phonons and \(\Xi^{(l)}_{\text{eff}}(\mathbf{q}) = \Xi_h\) for longitudinal phonons in any direction. Therefore, the electron-phonon coupling via the deformation potential in 3D GaAs contributes only to longitudinal phonon emission. However, when a phonon with a wave vector \(\mathbf{q}\) is propagated in the direction \(<111>\), the effective piezoelectric constants are \(k^{(l)}_{\text{eff}}(\mathbf{q}) = 0\) for transverse phonons and \(k^{(l)}_{\text{eff}}(\mathbf{q}) = (\varepsilon_0/\varepsilon)(h_{14}/\sqrt{3})\) for longitudinal phonons, respectively. In addition, if the phonon is propagated in the direction \(<100>\), the effective piezoelectric constants are zero for both longitudinal and transverse phonons. Therefore, the study of phonon emission would be a more straightforward way to investigate electron-phonon couplings in low-dimensional systems.
CHAPTER 4

Electron-phonon Interaction in 2D- and 3D- Deformable Jellium

4.1 Introduction

general proofs of the deformation potential theorem (i.e., relation between the ma-
trix elements of the electron-phonon interaction and the shifts of the electronic
levels as a function of macroscopic strain) have been provided by Khan and Allen
(1984) for the rigid-ion model, by Kartheuser and Rodriguez (1986) [see also Ro-
driguez and Kartheuser (1985)] for both rigid-ion and deformable-ion models, and
by Resta (1991) within the framework of density-functional theory.

There have been some discussions lately on the deformable jellium model
et al (1990, 1992)]. In the ordinary jellium model of a homogeneous electron gas
the positive background is nonresponsive, providing local charge neutrality only in
equilibrium. In the case of low electron density, when the electronic part of the
system develops long-range order (e.g., charge-density waves or Wigner solid) [Das
and Mahanty (1988), Choudhury and Ghosh (1995)], it is instructive to consider a
deformable jellium in which the background shows its response by deforming itself
to preserve local charge neutrality, so that the long-range Coulomb interaction
is diminished. Therefore, there are no long-range electrostatic contributions to
deformation potentials in the deformable jellium. The evaluation of deformation
potentials is done from the change in electronic band parameters caused by strain
and the consequent change in the lattice constants of the crystal. When the strain is
due to acoustic waves of long wavelength, the background can be well approximated
by a continuum as in the deformable jellium model.

Deformation potentials play a major rôle in the properties of carrier mo-
bilities [Dumke (1956), Herring and Vogt (1956, 1957), Price (1985), Walukiewicz
cyclotron resonances [Hensel and Feher (1963), Murase et al (1970)], piezo-
electroreflectance [Pollak and Cardona (1968)], electron-phonon interaction [Khan
et al (1983a, 1983b), Hardy et al (1989)], band line-up in semiconductor heterojunc-
tions [Van de Walle (1989), Van de Walle and Martin (1989)], etc. There are several
different definitions of deformation potential depending on the kinds of strain ap-
4. **Electron-phonon Interaction in 2D- and 3D- Deformable Jellium**

applied to the system [Bardeen and Shockley (1950), Herring and Vogt (1956, 1957)] and the energy states compared before and after the deformation [Khan and Allen (1984), Kartheuser and Rodriguez (1986)]. Furthermore, there is some confusion in terminology [compare Dumke (1956) with Herring and Vogt (1956, 1957)], and the definition of deformation potentials [compare Bardeen and Shockley (1950) and Pikus (1958)].

This Chapter deals with deformation potentials in a deformable jellium where the density parameter \( r_s \) is less than that at the melting point of the Wigner crystal [Das and Mahanty (1988)], and also in a semiconductor heterostructure. We shall deal with the hydrostatic deformation potential associated with hydrostatic strains. Most calculations for low-dimensional systems of physical quantities that depend on the deformation potential have used the 3D results [Vinter (1984), Walukiewicz *et al* (1984), Sirenko and Mitin (1993), Senna and Das Sarma (1993), Stocker *et al* (1994)]. To our knowledge, *ab initio* estimates of the deformation potential of a 2D system have not been done before.

We compare the energy of 2D- and 3D- deformable jellium in Section 4.2. We shall give a brief discussion of the several definitions of deformation potentials and the relations between them and provide exact expressions of the hydrostatic deformation potentials in 2D- and 3D- deformable jellium within the Hartree-Fock (HF) approximation in Section 4.3. In Section 4.4 we discuss the deformation potentials in semiconductor heterostructures. Finally, Section 4.5 gives a brief summary.

### 4.2 Hamiltonian for a deformable jellium in Hartree-Fock approximation

The jellium model [Inkson (1984)] consists of a system of \( N \) electrons embedded in a homogeneous background of equal positive charge so that the system is electrically neutral. The jellium Hamiltonian \( \mathcal{H} \) may be written as

\[
\mathcal{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + V_{bb} + V_{eb},
\]
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where $V_{bb}$ and $V_{eb}$ are the background-background interaction and the electron-background interaction respectively. In the HF approximation, the Hamiltonian can be written as

$$\mathcal{H}_{HF} = T + V_d + V_{ex} + V_{bb} + V_{eb},$$

where $T$ is the kinetic energy, and $V_d$ and $V_{ex}$ are the direct and non-local exchange parts of electron-electron interaction respectively. The deformable jellium is defined by the condition [Barrera et al (1979)]

$$V_d + V_{bb} + V_{eb} = 0,$$

which means that the positive background deforms itself in order to locally neutralize the system. In this deformable jellium, the single-particle energy $\mathcal{E}(k)$ can be written in terms of the kinetic energy and exchange energy parts:

$$\mathcal{E}(k) = t(k) + v_{ex}(k) \quad (4.1)$$

where

$$t(k) = \left\langle \psi_k(r) \left| -\frac{\hbar^2}{2m} \nabla^2 \right| \psi_k(r) \right\rangle \quad (4.2)$$

$$v_{ex}(k) = -\sum_{k_1(occ)} \left\langle \psi_k(r_1) \psi_{k_1}(r_2) \left| \frac{e^2}{|r_1 - r_2|} \right| \psi_k(r_2) \psi_{k_1}(r_1) \right\rangle. \quad (4.3)$$

Let us consider a deformable jellium in which has the electron density parameter ($r_s$) is less than the melting point of the Wigner crystal [Das and Mahanty (1988)]. In this case, we use plane waves as solutions in an approximation [Méndez-Moreno et al (1989)]. In the 3D-deformable jellium, the plane wave function $\psi_k(r) = (1/\sqrt{\Omega_0}) e^{i k \cdot r}$, with normalization volume $\Omega_0$, gives the energy eigenvalue from equations (4.1), (4.2), (4.3) as [Madelung (1978)]:

$$\mathcal{E}^{3D}(\eta, r_s) = (9\pi/4)^{2/3}(\eta/r_s)^2 - (4/\pi)(9\pi/4)^{1/3}(1/r_s)F(\eta)$$

$$F(\eta) = \left[ \frac{1}{2} + [(1-\eta^2)/4\eta] \ln |(1 + \eta)/(1 - \eta)| \right]$$

$$r_0 = (3/4\pi \rho)^{1/3} = (9\pi/4)^{1/3}/k_F$$

$$r_s = r_0/a_0 \quad \eta = k/k_F,$$

where $\rho$ is the volume density of electrons, $k_F$ is the Fermi wave vector, $r_0$ is the Wigner-Seitz radius, $r_s$ is the density parameter, and $a_0$ is the Bohr radius.
In the 2D-deformable jellium, the wavefunction of the state with wave vector \( k \) is

\[
\psi_k(R) = \frac{1}{\sqrt{A_0}} e^{ik \cdot R}
\]

where \( R \) is the 2D position vector, \( k \) is the 2D wave vector, and \( A_0 \) is the area for normalization. The exchange energy of one-electron with wave vector \( k \) [Stern (1973, 1974)]* is

\[
\nu_{ex}^{2D}(k) = -e^2 \sum_{i} \int \left( \psi_k(R_i) \psi_{k_i}(R_2) \right) \frac{1}{|R_1 - R_2|} \left| \psi_k(R_2) \psi_{k_1}(R_1) \right| \delta(R_2 - R_1)
\]

\[
= -\frac{2e^2 k_F}{\pi} \mathcal{E} \left( \frac{k}{k_F} \right),
\]

where \( \mathcal{E}(x) = E(\pi/2, x) = \int_0^{\pi/2} \sqrt{1 - x^2 \sin^2 \theta} d\theta \) is a complete elliptic integral of the second kind. Therefore, the energy eigenvalue in 2D-deformable jellium is given by

\[
\mathcal{E}^{2D}(\eta, r_s) = 2(\eta/r_s)^2 - (4\sqrt{2}/\pi)(1/r_s) \mathcal{E}(\eta)
\]

\[
r_0 = (1/\pi n)^{1/2} = \sqrt{2}/k_F
\]

\[
r_s = r_0/a_0 \quad \eta = k/k_F
\]

(4.5)

where \( n \) is the areal density of electron and \( k_F \) is the Fermi wave vector in 2D.

Figure 4.1(a) shows the energy eigenvalues of an electron in 2D- and 3D-deformable jellium. There are big differences between the band structures for high density (small \( r_s \)), while there are slight differences between them for low density (large \( r_s \)). The energy eigenvalues of the quasiparticles (HF electrons [see Madelung (1978)]) in deformable jellium in 3D and 2D respectively are \( \mathcal{E}^{3D}(0, r_s) = -(4/\pi)(9\pi/4)^{3/2} (1/r_s) \) and \( \mathcal{E}^{2D}(0, r_s) = -2\sqrt{2} (1/r_s) \) at \( k = 0 \), and \( \mathcal{E}^{3D}(1, r_s) = (9\pi/4)^{3/2} (1/r_s)^2 - (2/\pi)(9\pi/4)^{1/2} (1/r_s) \) and \( \mathcal{E}^{2D}(1, r_s) = 2(1/r_s)^2 - (4\sqrt{2}/\pi) (1/r_s) \) at the Fermi surface(\( k = k_F \)). Therefore, the exchange energy effect for 2D at the band minimum is stronger than that for 3D. In the ground state, the quasiparticle energies are always negative for \( r_s > 3.015 \) in 3D and for \( r_s > 1.111 \) in 2D.

*The exchange energy of an electron with wave vector \( k \) in the extreme 2D limit of inversion layers was calculated by assuming no excited subbands exist. There are two types of definitions of complete elliptic integrals, differing in their arguments. Stern’s papers used the definition \( \mathcal{E}(x) = E(\pi/2, x) = \int_0^{\pi/2} \sqrt{1 - x \sin^2 \theta} d\theta \).
Figure 4.1: The comparisons of (a) the energy eigenvalues of an electron as a function of $\eta = k/k_F$ and (b) the average energy per electron in deformable jellium as a function of the electron density parameter $r_s$. 
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The total energy can now be calculated from

\[ E_{\text{total}} = 2 \sum_k t(k) + \sum_k u_{\text{ex}}(k). \] (4.6)

Therefore, the average energy of an electron in 2D- and in 3D- deformable jellium can be derived from equations, (4.4), (4.5), (4.6):

\[ \mathcal{E}^{2D}_{\text{ave}}(r_s) = \frac{1}{r_s^2} - \frac{8\sqrt{2}}{3\pi} \frac{1}{r_s}. \]

\[ \mathcal{E}^{3D}_{\text{ave}}(r_s) = \frac{3}{5} \left( \frac{9\pi}{4} \right)^{\frac{3}{2}} \frac{1}{r_s^2} - \frac{3}{2}\pi \left( \frac{9\pi}{4} \right)^{\frac{1}{2}} \frac{1}{r_s}. \]

As shown in Figure 4.1(b), while the average energy per electron in 2D differs significantly from that in 3D for high density, the average energy per electron for low density is similar for both dimensions. The minima of the average energy per electron with respect to \( r_s \) in 2D and 3D are -0.360 Ryd at \( r_s = 1.67 \) and -0.095 Ryd at \( r_s = 4.82 \) respectively. The average energy per electron in 2D is more sensitive than that in 3D as a function of the electron density parameter \( r_s \). The average energy per electron is always negative in the range of \( r_s > 0.83 \) in 2D and \( r_s > 2.41 \) in 3D.

4.3 Effect of strain on energy eigenvalues

Let us first consider the effect of a general external macroscopic strain, \( u_{ij} \), on the energy eigenvalues in deformable jellium. There are several definitions of deformation potentials [Khan and Allen (1984), Kartheuser and Rodriguez (1986)]. Before classifying the deformation potentials, we first consider the effect of a strain on energy eigenvalues in a deformable jellium. The Schrödinger equation for an electron in an unstrained deformable jellium is

\[ [H_0(r, \nabla, \psi_k)] \psi_k] = -\frac{\hbar^2}{2m} \nabla^2 \psi_k(r) - e^2 \sum_{k_1} \frac{\psi_{k_1}^*(r_1)\psi_k(r_1)}{|r - r_1|} dr_1 \psi_{k_1}(r) \]

\[ = \mathcal{E}^0(k) \psi_k(r), \]

with \( \mathcal{E}^0(k) = t^0(k) + u_{\text{ex}}^0(k) \) and \( \psi_k(r) = (1/\sqrt{\Omega_0})e^{ikr} \). The wave vector in the unstrained deformable jellium is given by

\[ k_i = \frac{2\pi n_i}{L_i^0}, \quad (i = x, y, z), \quad n_i = 0, \pm 1, \pm 2, \ldots, \]
where \( L_0^0 \) is the size of the unstrained system (\( \Omega_0 = L_x^0 L_y^0 L_z^0 \)). The Schrödinger equation for an electron in the strained deformable jellium can be written as

\[
[H(r, \nabla, \psi_{k_i\mathbf{u}})\psi_{k\mathbf{u}}] = -\frac{\hbar^2}{2m} \nabla^2 \psi_{k\mathbf{u}}(r) - e^2 \sum_{k_i\mathbf{u}} \frac{\psi_{k_i\mathbf{u}}(r_2)\psi_{k\mathbf{u}}(r_2)}{|r - r_2|} \, dr_2 \psi_{k_i\mathbf{u}}(r)
\]

\[= \mathcal{E}(k\mathbf{u})\psi_{k\mathbf{u}}(r),\]

where \( \mathcal{E}(k\mathbf{u}) = t(k\mathbf{u}) + v_{ex}(k\mathbf{u}) \) is the single electron energy and \( \psi_{k\mathbf{u}}(r) = (1/\Omega)e^{ik\mathbf{u}\cdot r} \) is the eigenfunction in the strained deformable jellium. If the eigenstate in the unstrained deformable jellium has a wave vector \( \mathbf{k} \), the corresponding eigenstate in the strained deformable jellium has the wave vector \( k\mathbf{u} = (\mathbf{I} - \mathbf{u}) \cdot \mathbf{k} \). The effect of a small strain \( \mathbf{u} \) may be treated as a perturbation. Using the inverse transformation of coordinates, equation (3.36), suggested by Pikus and Bir (1959), the Schrödinger equation in the new coordinates, to within the first order of strain \( \mathbf{u} \), can be written as

\[
[H'] = [H_0(r', \nabla', \psi'_{k_i\mathbf{u}})\psi'_{k\mathbf{u}}] + \sum_{ij} u_{ij} D_{ij}(r', \nabla', \psi'_{k\mathbf{u}}, \psi'_{k_i\mathbf{u}})
\]

\[= \mathcal{E}(\mathbf{I} - \mathbf{u}) \cdot k\mathbf{u})\psi_{k\mathbf{u}}(\mathbf{I} + \mathbf{u}) \cdot r')
\]

with

\[
[H_0(r', \nabla', \psi'_{k_i\mathbf{u}})] \psi'_{k\mathbf{u}}(\mathbf{I} + \mathbf{u}) \cdot r') = -\frac{\hbar^2}{2m} \nabla'^2 \psi'_{k\mathbf{u}}(\mathbf{I} + \mathbf{u}) \cdot r')
\]

\[-e^2 \sum_{k_i\mathbf{u}} \int_{\Omega_0} \frac{\psi'_{k_i\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r')\psi_{k\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r')}{|r' - r'_1|} \, dr'_1 \psi_{k_i\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r')
\]

and

\[
[D_{ij}(r', \nabla', \psi'_{k\mathbf{u}})] \psi'_{k\mathbf{u}} = -\frac{\hbar^2}{m} \nabla'_i \nabla'_j \psi'_{k\mathbf{u}}(\mathbf{I} + \mathbf{u}) \cdot r')
\]

\[+ e^2 \sum_{k_i\mathbf{u}} \int_{\Omega_0} \frac{\psi'_{k_i\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r'_1)(r' - r'_1)(r' - r'_1)_j \psi_{k\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r'_1)}{|r' - r'_1|^3} \, dr'_1 \psi_{k_i\mathbf{u}}((\mathbf{I} + \mathbf{u}) \cdot r').
\]

In other words, the energy eigenvalue of the strained deformable jellium in the new coordinates can be written as

\[
\mathcal{E}((\mathbf{I} - \mathbf{u}) \cdot k\mathbf{u}) = \mathcal{E}((\mathbf{I} - \mathbf{u}) \cdot k),
\]
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because we have \( k'_y = (I - \mathbf{u}) \cdot k \) from the coordinate transformation and \( k_y = (I - \mathbf{u}) \cdot k \) from the effect of the strain. Therefore, we have \( k'_y = k \). \([H]\) can now be regarded as a perturbation on \([H_0]\). The wavefunction of \([H_0(r', \nabla', \psi_{k_y})\psi_{k_y}']\) is just the plane wave form \((1/\sqrt{\Omega_0})e^{ik'r'}\). When it is written in terms of the original coordinates of the strained deformable jellium, the wave function is

\[
\psi_k(r') = \frac{1}{\sqrt{\Omega_0}}e^{ik(I-\mathbf{u})r}.
\]

Therefore, \( \psi_k \) belongs to the wave vector \( k_y = (I - \mathbf{u}) \cdot k \) and to energy \( E^0(k_y) \).

The energy eigenvalue of \([H']\) associated with the solution of

\[
[H_0(r', \nabla', \psi_k(r'))\psi_k(r')] \equiv E^0(k)\psi_k(r')
\]

is

\[
E((I - \mathbf{u}) \cdot k) = E^0(k) + \sum_{ij} u_{ij} < D_{ij} > , \quad < D_{ij} > = \int_{\Omega_0} \psi_k^*(r)[D_{ij}]dr
\]

Let us now consider the deformation potentials due to the kinds of strain applied to a 3D system. The hydrostatic deformation potential \( \Xi_h(k) \) [Vergés et al (1982)] due to a uniform hydrostatic strain \( \mathbf{u}_h = u_{xx}\hat{x}\hat{x} + u_{yy}\hat{y}\hat{y} + u_{zz}\hat{z}\hat{z} \) (\( d\ln \Omega_0 = \text{tr}(\mathbf{u}) = 3u_{xx}, u_{xx} = u_{yy} = u_{zz} = u_{uu} = \frac{\text{d}\Omega}{\Omega_0} \)) is defined by

\[
\Delta E(k) = \Xi_h(k)(u_{xx} + u_{yy} + u_{zz}) = \Xi_{xx}(k)u_{xx} + \Xi_{yy}(k)u_{yy} + \Xi_{zz}(k)u_{zz} . \quad (4.7)
\]

The deformation potential \( \Xi_d(k) \) [Herring (1955), Herring and Vogt (1956, 1957)] due to a dilatation* \( \mathbf{u}_d = u_{xx}\hat{x}\hat{x} + u_{yy}\hat{y}\hat{y} \) (\( d\ln A_0 = u_{xx} + u_{yy} = 2u_{uu}, u_{xx} = u_{yy} \)), which is a strain of two directions perpendicular to one axis (\( e.g. z\)-axis) without a strain in the axis, is given by

\[
\Delta E(k) = \Xi_d(k)(u_{xx} + u_{yy}) = \Xi_{xx}(k)u_{xx} + \Xi_{yy}(k)u_{yy} .
\]

And the deformation potential \( \Xi_u(k) \) [Herring and Vogt (1956, 1957)] due to a uniaxial strain \( \mathbf{u}_u = u_{xx}\hat{x}\hat{x} + u_{yy}\hat{y}\hat{y} + u_{zz}\hat{z}\hat{z} \) (\( u_{xx} = u_{yy} = -\frac{u_{zz}}{2} \)), which is a

* In some papers or books, the dilatation is used as the hydrostatic strain. Here we follow Herring and Vogt's definition of dilatation.
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combination of a tension along an axis (e.g. z-axis) and a compression in the two
directions perpendicular to the axis, is defined by

$$\Delta \varepsilon(k) = \Xi_u(k)u_{zz} = \Xi_{xx}(k)u_{xx} + \Xi_{yy}(k)u_{yy} + \Xi_{zz}(k)u_{zz}$$

$$= \left( -\frac{1}{2} \{\Xi_{xx}(k) + \Xi_{yy}(k)\} + \Xi_{zz}(k) \right) u_{zz}.$$

It is easy to handle the uniaxial deformation potentials from the viewpoint of experiments [Weinreich et al (1959), Murase et al (1970)].

In this Chapter, we shall use the band structure deformation potential as given in equation (3.37) and the hydrostatic deformation potential as defined by equation (4.7). Therefore, the hydrostatic deformation potential in 3D can be written as

$$\Xi^{3D}_h(k) = \frac{1}{3} \sum_{i=1}^{3} \Xi^b_{ii}(k) = \frac{1}{3} \sum_{i=1}^{3} < D_{ii} >$$

Let us define the hydrostatic deformation potential in 2D by

$$\Xi^{2D}_h(k) = \frac{1}{2} \sum_{i=1}^{2} \Xi^b_{ii}(k) = \frac{1}{2} \sum_{i=1}^{2} < D_{ii} >$$

Also, we can define a uniaxial deformation potential in 2D due to a strain $u_{us}^{2D} = u_{xx}\hat{x}\hat{x} + u_{yy}\hat{y}\hat{y}$ ($u_{xx} = -u_{yy}$), which is a combination of an expansion along an axis (e.g. y-axis) and a compression along the other axis (e.g. x-axis), by

$$\Delta \varepsilon(k) = \Xi^{2D}_u(k)u_{yy} = \Xi_{xx}(k)u_{xx} + \Xi_{yy}(k)u_{yy} = (-\Xi_{xx}(k) + \Xi_{yy}(k))u_{yy}.$$ 

The uniaxial deformation potential in both 2D and 3D should vanish for an isotropic band structure.

In the case of 2D-deformable jellium, the hydrostatic deformation potential due to a uniform strain associated with $d\ln \Omega_0 = u_{xx} + u_{yy} = 2u_{us}$ ($u_{us} = \frac{dr}{r_0}$) from equation (4.9) will be

$$\Xi^{2D}_h(r_s, \eta) = \frac{4\sqrt{2}}{\pi} \left( \frac{1}{r_s} \right) \mathcal{E}(\eta) - 2 \left( \frac{\eta}{r_s} \right)^2$$

In the 3D-deformable jellium, the hydrostatic deformation potential due to a uniform strain associated with $d\ln \Omega_0 = 3u_{us} = 3\frac{dr}{r_0}$ from equation (4.8) is

$$\Xi^{3D}_h(r_s, \eta) = \frac{4}{\pi} \left( \frac{9\pi}{4} \right)^{\frac{1}{3}} \frac{1}{r_s} \mathcal{F}(\eta) - 2 \left( \frac{9\pi}{4} \right)^{\frac{2}{3}} \left( \frac{\eta}{r_s} \right)^2.$$
Figure 4.2: The hydrostatic deformation potentials of a quasiparticle in (a) 2D-deformable jellium and in (b) 3D-deformable jellium.
As shown in Figure 4.2, the kinetic energy contribution to the deformation potential is larger in the case of high electron density (for small \( r_s \)) than for low electron density (for large \( r_s \)) in both 2D and 3D. The deformation potential in 2D is generally higher than that in 3D for the same value of \( r_s \) [see Figure 4.3]. At the band minima, the deformation potentials are given by \( \Xi^{2D}(r_s,0) = 2\sqrt{2}(1/r_s) \) in 2D and \( \Xi^{3D}(r_s,0) = (4/\pi)(9\pi/4)^{1/3}(1/r_s) \) in 3D. Therefore, for the higher electron density, the deformation potential at the band minimum will also be higher. The quasiparticle deformation potential at the Fermi surface changes over from negative
to positive value for increasing $r_s$ at $r_s=1.11$ for 2D and at $r_s=2.01$ for 3D, and has maximum values, 0.41 Ryd at $r_s=2.22$ for 2D, and 0.15 Ryd at $r_s=4.02$ for 3D [see Figure 4.3].

Let us now define the average deformation potential, which is the change of the average energy of an electron per uniform hydrostatic strain $d \ln S^{nD}(s^{2D} = A_0, s^{3D} = \Omega_0)$, by

$$
\Xi_{\text{ave}}^{nD} = \frac{\Delta \mathcal{E}_{\text{ave}}^{nD}}{d \ln S^{nD}} = \frac{1}{n} \frac{\partial \mathcal{E}_{\text{ave}}^{nD}}{\partial r_s},
$$

where $nD$ represents the dimension of the system and $\mathcal{E}_{\text{ave}}^{nD}$ is the average energy of an electron in dimension $nD$. Therefore, the average deformation potential in 2D-deformable jellium will be

$$
\Xi_{\text{ave}}^{2D} = 4\sqrt{2} \frac{1}{3\pi} \frac{1}{r_s} - \frac{1}{r_s^2},
$$

and the average deformation potential in 3D-deformable jellium will be given by

$$
\Xi_{\text{ave}}^{3D} = \frac{1}{2\pi} \left( \frac{9\pi}{4} \right)^{\frac{1}{2}} \frac{1}{r_s} - \frac{2}{5} \left( \frac{9\pi}{4} \right)^{\frac{3}{2}} \frac{1}{r_s^2}.
$$

The maximum of the average deformation potential is 0.090 Ryd at $r_s = 3.33$ in the 2D-deformable jellium and 0.016 Ryd at $r_s = 9.65$ in the 3D-deformable jellium [see Figure 4.3]. Neglecting the exchange part in 3D, while the average deformation potential $\Xi_{\text{ave}}^{3D}$ is $-\frac{2}{3} \mathcal{E}_F$, the deformation potential $\Xi_{h}^{3D}$ of a quasiparticle at the Fermi surface is given by $-\frac{2}{3} \mathcal{E}_F$, which was pointed out by Ziman (1960). In the 2D case, considering only the kinetic part, the average deformation potential $\Xi_{\text{ave}}^{2D}$ is $-\frac{1}{2} \mathcal{E}_F$ and the deformation potential $\Xi_{h}^{2D}$ of a quasiparticle at the Fermi surface is $-\mathcal{E}_F$.

In this section, we discussed the dimensional dependence of the deformation potential from the first principle. Since jellium description is successful for metallic systems, the above results are useful for understanding the electron mobilities and the phonon emission profiles.

4.4 Comments on semiconductor heterostructures

Low-dimensional electronic systems in semiconductor heterostructures are realised at surfaces or interfaces where an electronic band discontinuity occurs. The
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electronic band discontinuity causes the motion of the electrons to be restricted to lower dimensions, e.g. 2D, 1D, and 0D. In a semiconductor without electronic confinements i.e. a 3D system, free electrons at low temperatures will occupy states near the bottom of the conduction band of the semiconductor. Hence the electron-phonon interaction via deformation potential couplings can be determined from the shift of the conduction band minimum due to a strain associated with phonons. However, in semiconductor heterostructures, e.g., inversion layers, heterojunctions, or single quantum wells, where electrons are confined by an electronic band discontinuity, the electrons have subbands in one direction and are free to move in the plane perpendicular to that direction. In this section we are going to give a qualitative estimate of the deformation potential for modulation doped heterostructures, based on the energy band calculations of Section 2.5. From equation (2.36), the energy shift of an electron in a state \((n, k)\) due to a strain can be written

\[
\Delta E_n(k) = \Delta E_{n,k_0} + \Delta E_n + \Delta E_{K,E}^{2D}.
\]  

where \(\Delta E_{n,k_0}\) denotes the energy shift at the band extremum \(k_0\), \(\Delta E_n\) represents the subband energy shift, and \(\Delta E_{K,E}^{2D}\) is the kinetic energy shift in 2D due to a strain. The energy shift at the band extremum \(k_0\) is available from the 3D result of the semiconductor under consideration. The kinetic energy shift \(\Delta E_{K,E}^{2D}\) in 2D will be taken from the kinetic part of the 2D deformation potential which was given in the previous section. Let us consider a 2D uniform strain \((d\ln A_0 = u_{xx} + u_{yy}, u_{xx} = u_{yy} = u_{zz})\) which is an areal expansion. For a Si inversion layer, where the conduction band minimum is at \(X_1\)* when only the lowest band is occupied, the energy shift of an electron may be written

\[
\Delta E_0(k) = \Delta E_{X_1} + \Delta E_0 + \Delta E_{K,E}^{2D}.
\]  

Here \(\Delta E_{X_1}\) is the energy shift of the conduction band minimum \(X_1\) due to the strain and is given by

\[
\Delta E_{X_1} = \Xi_d(u_{xx} + u_{yy})
\]

where \(\Xi_d\) is the deformation potential at \(X_1\) due to the dilatation strain in 3D Si.

*The conduction band minimum of Si lies not at the point \(X_1\) but in near the \(<100>\) direction.
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In a GaAlAs/GaAs heterojunction where the electrons occupy only the lowest subband, the energy shift of an electron in the well side, whose band minimum is at \( k_0 = \Gamma_e \), can be expressed as

\[
\Delta E_0(k_{\parallel}) = \Delta E_{\Gamma_e} + \Delta E_0 + \Delta E_{K,E}^{2D}. \tag{4.13}
\]

where \( \Delta E_{\Gamma_e} \) is the energy shift of the conduction band minimum \( \Gamma_e \) due to the strain and is given by

\[
\Delta E_{\Gamma_e} = \Xi_h(u_{xx} + u_{yy}).
\]

Here \( \Xi_h \) is the deformation potential for 3D GaAs.

Now we need to evaluate the subband energy shift \( \Delta E_0 \) in equations (4.12) and (4.13). In order to have an analytic form for the deformation potential, we shall use the Airy wavefunction and the Fang-Howard wave function as discussed in Section 2.5. We also make the following reasonable assumptions: (1) the number of charges in each layer is conserved under the strain, and (2) the change of the dielectric constant is small enough to be neglected. The area \( A(u_{us}) \) under the uniform strain can be written

\[
A(u_{us}) = A_0(1 + u_{xx} + u_{yy}) = A_0(1 + 2u_{us})
\]

where \( A_0 \) is the area of the unstrained system. For the number density \( N \) of charges in the unstrained system, we obtain the following relation

\[
N = N^0(1 - [u_{xx} + u_{yy}]) = N^0(1 - 2u_{us})
\]

where \( N^0 \) is the areal number density in the unstrained system. From equations (2.41), (2.42), (2.43), (2.44), (2.45), and (2.46), we easily obtain the energy shift for the lowest subband for the three types of analytic solutions;

\[
\Delta E_0 = -\left(\frac{2}{3}E_0\right)(u_{xx} + u_{yy}) = -\left(\frac{4}{3}E_0\right)u_{us}. \tag{4.14}
\]

Now the hydrostatic deformation potential for an electron in the state \((n, k_{\parallel})\) in a heterostructure can be expressed as

\[
\Delta E_n(k_{\parallel}) = \Xi_h^{2D}(n, k_{\parallel})(u_{xx} + u_{yy}). \tag{4.15}
\]
Therefore, the hydrostatic deformation potential for the lowest subband in the heterostructure will be given by

\[
\Xi^2_{h}(0, k_{\parallel}) = \Xi^3_{k_{0}} - \frac{2}{3} E_0 - \frac{\hbar^2 k_{\parallel}^2}{2m^*}
\]  

(4.16)

where \(\Xi^3_{k_{0}}\) stands for the 3D deformation potential depending on the band minimum and the strain, and where the last term, which is given in equation (4.10), is the 2D kinetic energy contribution to the 2D hydrostatic deformation potential. The last term in equation (4.16) takes values from 0 to \(E_F\) depending on the wave vector \(k_{\parallel}\). The ranges of \(E_0\), which depend on the charge concentrations and the band offset in a heterostructure, run approximately from 10 meV to 200 meV for a Si-inversion layer and from 20 meV to 70 meV for a GaAlAs/GaAs heterojunction. The Fermi energies \(E_F\) depend on the charge concentrations and range up to approximately 20 meV for a Si-inversion layer and up to approximately 50 meV for a GaAlAs/GaAs heterojunction. Therefore, the last two terms in equation (4.16) contribute less than 200 meV for both the heterostructures in which just one subband is occupied. Hence their contributions to the deformation potential in a heterostructure, where charge carrier density is much smaller than that in a metallic material, can be neglected.

4.5 Discussion

We have established that the deformable jellium model provides a good description of the ground state properties of many-particle metallic systems in the low density regime. The model has been successfully applied [Méndez-Moreno et al (1989, 1990), Orozco et al (1990, 1992)] to electronically ordered states like charge density wave states [Aguilera-Navarro et al (1977)] and the Wigner solid. Unlike ordinary jellium, the deformable jellium includes the response of the background. The long range Coulomb interactions are effectively screened by this response. In this chapter we have used the deformable jellium model to calculate the energy spectrum of quasi-particles in the HF approximation. Since we are away from any electronically ordered phase, we have used a plane wave approximation to the electronic states. Calculations of the quasi-particle energies have been performed for
2D- and 3D- deformable jellium. The quasi-particle energies are used to calculate the deformation potentials. It has been found that the strength of the deformation potential in 2D-deformable jellium is higher than that in 3D case.

In particular, the dependence of the deformation potential on the dimensionality of the solid can be dramatic for materials with high charge carrier densities such as metals. However, it is not much different between the different dimensions for materials with low charge carrier densities as shown in Figure 4.3. From a envelope wavefunction point of view, the deformation potential in a semiconductor heterostructure is not much different from that for the corresponding bulk semiconductor. This is in conflict with the suggestion by several authors [Vinter (1986a, 1986b), Kawamura and Das Sarma (1990), Das Sarma (1991)] that the deformation potential in 2D systems for GaAs should be greater than that in 3D systems. It therefore seems that the electron-acoustic phonon coupling via deformation potential in a heterostructure should be reconsidered. In fact, the electrons in a semiconductor heterostructure are confined to lower dimensions but the lattices are still bulk-like structures except for interface effects on the lattice vibrations. When electrons in the semiconductor undergo transitions, the transitions will provide a source of force which causes the generation of acoustic fields (i.e. acoustic phonons). In this situation, the mechanism for electron-phonon coupling in low-dimensional systems may be different from that in bulk electronic systems. In the bulk electronic systems, the electronic transitions cause a strain field in any direction. But, for instance, in two-dimensional electronic systems, the electronic transitions first give a strain field in a direction parallel to the 2DEG plane. Furthermore, the strain field will cause a strain field in the direction perpendicular to the the 2DEG plane depending on the Poisson’s ratio because the lattices in the heterostructures are not 2D systems but bulk-like systems with interfaces and surfaces. The strain field in the perpendicular direction to the the 2DEG plane can decay or propagate depending on the interface and surface effects and the frequency of the strain field in the heterostructures. A detailed discussion of these matters will be given in Section 5.4.
CHAPTER 5

Phonon Emission from Semiconductor Heterostructures

5.1 Introduction

The problem of phonons interacting with a two-dimensional electron gas (2DEG) in a semiconductor heterostructure has received some attention lately in connection with experimental and theoretical studies of the absorption of heat pulses [Hensel et al (1982, 1983a, 1983b, 1984)], and also in connection with acoustic phonon emission, both in the presence of a magnetic field [Toombs et al (1987), Kent et al (1988), Challis et al (1989), Badalian and Levinson (1989, 1991), Benedict (1991, 1992)], and in its absence [Rothenfusser et al (1986), Vass (1987, 1993), Kitagawa and Tamura (1992), Hawker et al (1995), Vasko and Mitin (1995)]. The study of phonon emission from semiconductor heterostructures gives the most detailed information about the character and features of the electron-phonon interaction, as compared with studies of processes such as charge carrier mobility, which is more complicated. There always exist interfaces in real semiconductor heterostructures such as inversion layers and quantum wells. Features of the phonon emission from such structures can be determined from the form of the electron-phonon coupling and the interface effects. Phonon emission processes in heterostructures have recently been investigated theoretically by taking into account the effect of the reflection of phonons from various interfaces [Badalian and Levinson (1988, 1989, 1991, 1992)]. However, the strength of the electron-phonon couplings in low-dimensional systems has not been considered in detail satisfactorily. There have been some discussions about the deformation potentials in GaAs heterostructures.
5. Phonon Emission from Semiconductor Heterostructures

[Price (1985), Walukiewicz et al (1985), Vinter (1986a, 1986b), Hirakawa and Sakaki (1986), Kawamura and Das Sarma (1990), Das Sarma (1991)]. In such discussions it is suggested that the deformation potential in GaAs heterostructures is greater than that in the bulk GaAs. Hence the empirical value of the deformation potential $\Xi_h = 12$ eV is commonly used for GaAs heterostructures, while the deformation potential $\Xi_h = 7$ eV is used for bulk GaAs. The empirical value of the deformation potential has been obtained from the linear relation between the reciprocal of mobility and the temperature [Harris et al (1990), Kawamura and Das Sarma (1990), Das Sarma (1991), Gorczyca et al (1992)], and from the relation between energy-loss rate and 2D electron density [Hirakawa and Sakaki (1986)].

Recently, experimentalists have obtained LA and TA phonon signals by the time-of-flight method using a sensitive bolometer in a Si MOSFET [Rothenfusser et al (1986), Challis et al (1987)] and in GaAs heterostructures [Danilchenko et al (1994)]. Their data usually show that the intensity of TA modes is greater than that of LA modes. However, attempts to explain these effects on the basis of an isotropic deformation potential have been unsuccessful, even though the interface effects are taken into account [Badalian and Levinson (1991)].

One of theoretical methods used to evaluate the phonon intensity in a solid involves the elastic response functions (or elastic Green's functions) of the solid [Cottam and Maradudin (1984)]. The full dynamical elastic Green's functions for elastic media have been worked out for various geometries, such as a half space with a stress free boundary [Maradudin and Mills (1976)], an elastic slab with two stress free boundaries [Portz (1979), for review, Cottam and Maradudin (1984)], and at an interface between two different half spaces [Djafari-Rouhani and Dobrzynski (1976), Djafari-Rouhani et al (1977b, 1981)]. The dynamical elastic Green's functions for specific modes in layered media have been obtained, for example, for the transverse modes in periodically layered infinite and semi-infinite media [Camley et al (1983)], and the transverse modes in a elastic film with a semi-infinite substrate [Cottam and Maradudin (1984)].

In this Chapter, the theoretical aspects of the problem of phonon emission in heterostructures are examined in a framework that can readily be adapted to
a variety of systems and situations. The framework is based on the premise that electronic transitions in a 2DEG on a solid surface or interface create an electric field in the solid, and that the emitted phonons are basically the response of the solid to the impressed electric field. The isotropic approximation for elastic constants will be used.

5.2 Theory of phonon emission

First of all, we shall review the dynamics of acoustic waves in a cubic bulk semiconductor which lacks inversion symmetry. The equation of motion of the displacements in the cubic crystal when the electronic transition occurs is given by

\[\rho_m \frac{\partial^2 \mathbf{u}}{\partial t^2} - C^* \left( \frac{\partial^2 u_1}{\partial x_1^2} + \frac{\partial^2 u_2}{\partial x_2^2} + \frac{\partial^2 u_3}{\partial x_3^2} \right) - C_{44} \nabla^2 \mathbf{u} = (C_{12} + C_{44}) \nabla (\nabla \cdot \mathbf{u}) = \mathbf{F}^{(s)}(\mathbf{r}, t)\]

with \(C^* = C_{11} - C_{12} - 2C_{44}\), which is a measure of elastic anisotropy of the crystal, and where \(\mathbf{F}^{(s)}(\mathbf{r}, t)\) is the source force from the deformation potential coupling and the piezoelectric coupling [see Section 3.3]. Within the isotropic approximation for the elastic constants in the crystal, the constants may be averaged over all solid angles [see Section 5.3] and the equation of motion of the displacements may be expressed as

\[\rho_m \frac{\partial^2 \mathbf{u}}{\partial t^2} - (c_{12} + c_{44}) \nabla (\nabla \cdot \mathbf{u}) - C_{44} \nabla^2 \mathbf{u} = \mathbf{F}^{(s)}(\mathbf{r}, t)\]

where \(c_{12}\) and \(c_{44}\) correspond to the Lamé constants, \(\lambda\) and \(\mu\), respectively. The equations of motion of the displacements for longitudinal waves (\(u_l\)) and transverse waves (\(u_t\)) in the cubic crystal are given respectively by the Lagrangian equations:

\[\rho_m \frac{\partial^2 u_l}{\partial t^2} - C^* \left( \frac{\partial^2 u_{l1}}{\partial x_1^2} + \frac{\partial^2 u_{l2}}{\partial x_2^2} + \frac{\partial^2 u_{l3}}{\partial x_3^2} \right) - (C_{12} + 2C_{44}) \nabla^2 u_l = \mathbf{F}^{(s)}_l(\mathbf{r}, t)\]

\[\rho_m \frac{\partial^2 u_t}{\partial t^2} - C^* \left( \frac{\partial^2 u_{t1}}{\partial x_1^2} + \frac{\partial^2 u_{t2}}{\partial x_2^2} + \frac{\partial^2 u_{t3}}{\partial x_3^2} \right) - C_{44} \nabla^2 u_t = \mathbf{F}^{(s)}_t(\mathbf{r}, t)\]

The equation of motion for \(u\) in the isotropic crystal can then be obtained from the Lagrangian equation in the form (with the right hand side being the force term)

\[\frac{\partial^2 u_l}{\partial t^2} - v_l^2 \nabla^2 u_l = \mathbf{F}^{(s)}_l(\mathbf{r}, t)\]
5. Phonon Emission from Semiconductor Heterostructures

\[ v_{l}^2 = \frac{c_{12} + 2c_{44}}{\rho_m} = \frac{c_{11}}{\rho_m} \]  

(5.1)

\[ \frac{\partial^2 u_t}{\partial t^2} - v_t^2 \nabla^2 u_t = F_{l}^{(s)}(r, t) \]

(5.2)

where \( u_l \) corresponds to the longitudinal acoustic waves and \( u_t \) corresponds to the transverse acoustic waves. Once the source force is known, the equations (5.1) and (5.2) can be solved for \( u_l \) and \( u_t \) respectively, and thence the intensity of the emitted phonons is obtained [see equation (5.15)].

Let us now consider semiconductor heterostructures where surfaces and interfaces exist. The dynamic properties of lattice vibrations are specified by a Lagrangian density, \( \mathcal{L} \), which may be written as

\[ \mathcal{L} = \mathcal{L}(u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_j}). \]

From the Hamilton's principle, we can write the Lagrangian equations of motion as

\[ \frac{\partial}{\partial t} \left[ \frac{\partial \mathcal{L}}{\partial (\frac{\partial u}{\partial t})} \right] + \sum_{j=1}^{3} \frac{\partial}{\partial x_j} \left[ \frac{\partial \mathcal{L}}{\partial (\frac{\partial u}{\partial x_j})} \right] - \frac{\partial \mathcal{L}}{\partial u_i} = 0. \]

In principle, the equations of the forced vibrations of the lattice under the influence of a time-dependent distribution of applied force density \( F^{(o)}(r, t) \) can be written directly in the form

\[ \rho_m \frac{\partial^2 u(r, t)}{\partial t^2} - \nabla \cdot \mathbf{T}(r, t) = F^{(o)}(r, t) \]  

(5.3)

where the stress tensor \( \mathbf{T} \) is a second rank tensor with elements

\[ T_{ij} = \sum_{kl} C_{ijkl} \frac{\partial u_k}{\partial x_l} \]  

(5.4)

where \( C_{ijkl} \) are given by \( C_{ijkl}^{E} \) for a non-piezoelectric solid and \( C_{ijkl}^{P} \) for a piezoelectric solid, respectively, as discussed in Chapter 3. Introducing Voigt's notation for the stress tensor \( \mathbf{T} \), i.e., \( T_r, r=1, 2, \cdots, 6, (T_1=T_{11}, T_2=T_{22}, T_3=T_{33}, T_4=T_{23}=T_{32}, T_5=T_{31}=T_{13}, T_6=T_{12}=T_{21}) \) [see e.g., Chen et al (1992)], the equation of motion (5.3) may be written in matrix form (c.f. equation (3.28)) as

\[ \rho_m \frac{\partial^2 \mathbf{u}(r, t)}{\partial t^2} - \nabla \mathbf{T}(r, t) = \mathbf{F}^{(o)}(r, t). \]  

(5.5)
On introducing a matrix differential operator $\hat{L}(r,t)$, we can express equation (5.3) as

$$\hat{L}(r,t)u(r,t) = -\frac{F^{(1)}(r,t)}{\rho_m(r)} = F^{(0)}(r,t)$$

with

$$\hat{L}(r,t) = \hat{L}^{(0)}(r,t) + \hat{B}(r,t)$$

where $\hat{L}^{(0)}$ is the bulk matrix differential operator and $\hat{B}$ is the cleavage operator [Dobrzynski (1986), Dobrzynski et al (1989), Dobrzynski (1990)] for the system. The Green’s function associated with the matrix differential operator $\hat{L}$ is now defined by

$$\hat{L}^{(0)}(r,t)G(r,r';t-t') = I\delta(r-r')\delta(t-t')$$

and must satisfy the boundary conditions associated with the cleavage operator $\hat{B}$. These conditions depend on the structure of the system and will be given in details as required [see Appendix B].

The formal solution of equation (5.6) is

$$u(r,t) = \int dt' \int d^3r'G(r,r';t-t')F^{(0)}(r',t').$$

The formal properties of the Green’s function matrix $G$ for various lattice models (including surface effects, impurities and inhomogeneities) are well-known [Mahanty (1974), Cottam and Maradudin (1984)]. Thus equation (5.8) represents the solution to the problem of generation of the lattice waves when stimulus by a source force occurs in the system. When the stimulus has a harmonic time dependence $F^{(0)}(r,t) = F^{(0)}(r,\omega)e^{-i\omega t}$, the equation (5.3) may be written

$$\omega^2\mathbf{L} \cdot u(r,\omega) + \frac{1}{\rho_m(r)} \nabla \cdot [G(r) : \mathbf{u}(r,\omega)] = F^{(0)}(r,\omega),$$

or in a matrix form,

$$\hat{L}(r,\omega)u(r,\omega) = F^{(0)}(r,\omega)$$

with

$$\hat{L}(r,\omega) = \hat{L}^{(0)}(r,\omega) + \hat{B}(r,\omega),$$

and where the Green’s function satisfies

$$\hat{L}^{(0)}(r,\omega)G(r,r';\omega) = I\delta(r-r').$$
The solution of equation (5.10) can be written in the form

\[ u(r, \omega) = \int d^3r' G(r, r'; \omega) F^{(0)}(r', \omega). \]  

(5.12)

Let us now consider the Poynting vector which is the energy flux across unit area in unit time. The energy density \( \mathcal{E}_p \) for an elastic solid is the sum of the kinetic energy density and the potential energy density

\[ \mathcal{E}_p = \frac{1}{2} \rho_m \sum_i \dot{u}_i^2 + \frac{1}{2} \sum_{ijkl} C_{ijkl} \dot{u}_{ij} \dot{u}_{kl}. \]  

(5.13)

The Poynting vector \( \mathbf{S} \) is defined by

\[ \frac{\partial \mathcal{E}_p}{\partial t} + \nabla \cdot \mathbf{S} = 0. \]  

(5.14)

Differentiating the energy density \( \mathcal{E}_p \) with respect to time \( t \), we have the following relation

\[ \frac{\partial \mathcal{E}_p}{\partial t} = \rho_m \sum_i \dot{u}_i \ddot{u}_i + \sum_{ij} T_{ij} \left( \frac{\partial \dot{u}_i}{\partial x_j} \right) = \rho_m \sum_i \dot{u}_i \ddot{u}_i + \sum_{ij} \left( \frac{\partial}{\partial x_j} (T_{ij} \ddot{u}_i) - (\frac{\partial T_{ij}}{\partial x_j}) \dot{u}_i \right). \]

Rewriting, we can obtain the Poynting vector \( \mathbf{S} \);

\[ \frac{\partial \mathcal{E}_p}{\partial t} - \sum_j \left( \frac{\partial}{\partial x_j} \sum_i (T_{ij} \ddot{u}_i) \right) = \sum_i \dot{u}_i (\rho_m \ddot{u}_i - \sum_j \frac{\partial T_{ij}}{\partial x_j}) = 0, \]

\[ S_i = -\sum_j \dot{u}_j T_{ij} = -\sum_{jkl} C_{ijkl} \dot{u}_j \frac{\partial u_k}{\partial x_l}. \]

For time harmonic acoustic waves, the Poynting vector can be calculated conveniently using the complex exponential notation. The time-average value of the Poynting vector, which is a pulsating unidirectional power flow, is given by

\[ < S_i > = -\frac{1}{2} \text{Re} \left( \sum_j \dot{u}_j^* T_{ij} \right) = -\frac{1}{2} \sum_{jkl} C_{ijkl} \text{Re} \left( \dot{u}_j^* \frac{\partial u_k}{\partial x_l} \right). \]  

(5.15)

Then the spectral energy flux at frequency \( \omega \) is

\[ < S_i (r, \omega) > = -\frac{\omega}{2} \sum_{jkl} C_{ijkl} \text{Re} \left( u_j^* \frac{\partial u_k}{\partial x_l} \right) \omega. \]  

(5.16)

where \( u_j^* \) and \( u_k \) are the phonon field operators and \( < \cdots >_\omega \) is the Fourier component at frequency \( \omega \) [Badalian and Levinson (1991)].
5.3 Elastic and piezoelectric constants in heterostructures

Let us consider the relations between elastic and piezoelectric tensors in different coordinate systems. In a crystal, the elastic tensor and the piezoelectric tensor of the crystal in the crystallographic coordinates (X, Y, Z) [see Figure 5.1] are given by $C_{ijkl}$ and $h_{ijk}$. When the elastic tensor and the piezoelectric tensor are described using phonon coordinates $(x, y, z)$ [see Figure 5.1], they are given in the following form:

\[
C'_{ijkl} = a_{ii'}a_{jj'}a_{kk'}a_{ll'}C_{ij'kl'},
\]

(5.17)

Figure 5.1: The coordinate transformation for the elastic constant tensor and the piezoelectric tensor. $x'$-$z'$ and $x$-$z$ planes are in the same plane.
and

\[ h'_{ijk} = \sum_{i'j'k'} a_{ii'} a_{jj'} a_{kk'} h_{i'j'k'} \]  (5.18)

with

\[
a(q) = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = R(q_3, q||) U(q_1, q_2) = \begin{pmatrix} \cos \theta \cos \phi & \cos \theta \sin \phi & -\sin \theta \\ -\sin \phi & \cos \phi & 0 \\ \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \end{pmatrix} \]

\[
eq \begin{pmatrix} q_1 q_3 / q_\parallel & q_2 q_3 / q_\parallel & -q_\parallel / q \\ -q_2 / q_\parallel & q_1 / q_\parallel & 0 \\ q_1 / q & q_2 / q & q_3 / q \end{pmatrix}, \quad q_\parallel = \sqrt{q_1^2 + q_2^2}. \]  (5.19)

The transformation matrix \( a(q) \) is the composition of the rotation matrices \( R(\theta) \) and \( U(\phi) \):

\[
R(q_3, q||) = R(\theta) = \begin{pmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{pmatrix} = \frac{1}{q} \begin{pmatrix} q_3 & 0 & -q_\parallel \\ 0 & q & 0 \\ q_\parallel & 0 & q_3 \end{pmatrix} \]  (5.20)

and

\[
U(q_1, q_2) = U(\phi) = \begin{pmatrix} \cos \phi & \sin \phi & 0 \\ -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} = \frac{1}{q_\parallel} \begin{pmatrix} q_1 & q_2 & 0 \\ -q_2 & q_1 & 0 \\ 0 & 0 & q_\parallel \end{pmatrix} \]  (5.21)

where the \( z \)-axis is chosen to be along the \( q \)-direction of propagation of the phonon, and the \( y \)-axis is chosen to be in the \((X, Y)\) plane. When the elastic anisotropy of a crystal is not too large, the normal modes lie approximately along the axes of the phonon coordinates. For cubic crystals without inversion symmetry, the elastic constants and the piezoelectric constants in the phonon coordinates can be written as

\[
C'_{3333} = C_{11} - 2C^* \Gamma(q) \\
\frac{1}{2}(C'_{1313} + C'_{2323}) = C_{44} + C^* \Gamma(q) \\
C^* = C_{11} - C_{12} - 2C_{44} \]  (5.22)

with

\[
\Gamma(q) = (\sin^4 \theta \cos^2 \phi \sin^2 \phi + \sin^2 \theta \cos^2 \phi \sin^2 \phi + \sin^2 \theta \cos^2 \theta \cos^2 \phi) \\
= (q_1^2 q_2^2 + q_2^2 q_3^2 + q_3^2 q_1^2) / q^4, \]  (5.23)
and
\[ h'_{333} = 6 h_{14} \Gamma_1(q), \quad h'_{323} = 2 h_{14} \Gamma_2(q), \quad h'_{313} = 2 h_{14} \Gamma_3(q), \]
with
\[ \Gamma_1(q) = \sin^2 \theta \cos \phi \sin \phi = \left( q_1 q_2 q_3 / q^3 \right), \]
\[ \Gamma_2(q) = \sin \theta \cos \phi (2 \cos^2 \phi - 1) = \frac{[q_3 (q_1^2 - q_2^2)](q^2 q_3)}{[q_1 (q_2^2 - q_3^2)]}, \]
\[ \Gamma_3(q) = \sin \theta (3 \cos^2 \theta - 1) \cos \phi \sin \phi = \frac{[q_1 q_2 (2q_3^2 - q_2^2)](q^2 q_3)}{[q_1 (q_2^2 - q_3^2)]}, \]
where we consider just the piezoelectric components associated with the longitudinal electric field which are much larger than the transverse fields.

From now on, we shall consider GaAlAs-GaAs heterostructures. For both GaAs and AlAs, the elastic constant \( C^E_{ijkl} \) measured at constant electric field is almost the same as the stiffened elastic constant \( C^D_{ijkl} \) measured at constant electric displacement field. In other words, the electromechanical coupling constants \( K_{14} = h_{14}^2 / (\varepsilon C_{44}) \) are small, i.e., 0.0617 for GaAs and 0.094 for AlAs, respectively [Adachi (1985)]. Therefore, for convenience, we shall henceforth omit the superscripts on the elastic constants.

### 5.3.1 Elastic constants

In this Section, an approximation for the elastic constants in heterostructures will be discussed. We assume that each layer in the heterostructures has the same elastic properties as in the corresponding bulk semiconductor. Furthermore, each layer will be approximated in the same method. The simplest possible approximation is the isotropic approximation and it has been used for theoretical calculations of phonon intensity in semiconductor heterostructures by many authors [Hensel et al (1983b), Badalian and Levinson (1991), Kitagawa and Tamura (1992), Bannov et al (1994)]. In the usual experimental environments for phonon generations in semiconductor heterostructures, a sensitive bolometer has been used as a detector. Such a detector allows measurements of the angular distribution of the phonon intensity (i.e. the \( \theta \)-dependence of the phonon intensity) and to distinguish between

---

**There are misprints in equation (22) in the reference [Zook (1964)]. The equation should read\[ h'_{323} = 2 h_{14} [q_3 (q_1^2 - q_2^2)](q^2 q_3)/(q_1^2 q_3), \quad h'_{313} = 2 h_{14} [q_1 q_2 (2q_3^2 - q_2^2)](q^2 q_3)/q_3 \].**
LA modes and TA modes of phonons. In the isotropic approximation for the elastic constants, the spherical average of the elastic constants is given by

\[ c_{11} = \frac{1}{4\pi} \int C'_{3333} d\Omega_q = C_{11} - \frac{2}{5} C^* \]

\[ c_{44} = \frac{1}{4\pi} \int \left[ \frac{1}{2} (C'_{1313} + C'_{2323}) \right] d\Omega_q = C_{44} + \frac{1}{5} C^* \]

where \( d\Omega_q \) is the solid angle in the phonon coordinates.

Let us first consider a semiconductor single heterojunction as in Figure 5.2. The elastic constant tensor and material density in the heterojunction can be expressed in the form

\[ C_{ijkl}(r) = C^A_{ijkl} \Theta(x_3) + (C^B_{ijkl} - C^A_{ijkl}) \Theta(x_3 - z_0) \]

\[ \rho_m(r) = \rho^A_m \Theta(x_3) + (\rho^B_m - \rho^A_m) \Theta(x_3 - z_0) \]

Here \( z_0 \) is the thickness of the A-material inversion layer, and \( \Theta(x_3) \) is the Heaveside step function:

\[ \Theta(f(x)) = \begin{cases} 0 & \text{if } f(x) < 0 \\ 1 & \text{if } f(x) > 0 \end{cases} \]

In a semiconductor single quantum well with a substrate as in Figure 5.3, the elastic constant tensor and material density can be written as follows:

\[ C_{ijkl}(r) = C^A_{ijkl} \Theta(x_3) + (C^B_{ijkl} - C^A_{ijkl}) \]

\[ \times \left[ \Theta(x_3 - z_1) - \Theta(x_3 - (z_1 + L)) + \Theta(x_3 - (2z_1 + L)) \right] \]

\[ \rho_m(r) = \rho^A_m \Theta(x_3) + (\rho^B_m - \rho^A_m) \]

\[ \times \left[ \Theta(x_3 - z_1) - \Theta(x_3 - (z_1 + L)) + \Theta(x_3 - (2z_1 + L)) \right] \]

where \( L \) is the width of the quantum well (B-material) and \( z_1 \) is the thickness of the barrier layer (A-material).

Consider now the matrix representation of the elastic constant tensor. In GaAs/GaAlAs heterojunction, the elastic constants are given by

\[ C_{rs}(r) = C^\text{GaAlAs}_{rs} \Theta(x_3) + (C^\text{GaAs}_{rs} - C^\text{GaAlAs}_{rs}) \Theta(x_3 - z_0) \]
5. Phonon Emission from Semiconductor Heterostructures

Figure 5.2: Schematic of a single semiconductor heterojunction and the elastic constant tensor as a function of $x_3$. 

Figure 5.3: Schematic of a single semiconductor quantum well with a substrate and the elastic constant tensor as a function of $x_3$. 

5. Phonon Emission from Semiconductor Heterostructures

For GaAlAs/GaAs/GaAlAs single quantum wells with a semi-insulated GaAs substrate, the elastic constants can be written in the form

\[ C_{rs}(r) = C_{rs}^{GaAlAs} \Theta(x_3) + (C_{rs}^{GaAs} - C_{rs}^{GaAlAs}) \times \left[ \Theta(x_3 - z_1) - \Theta(x_3 - (z_1 + L)) + \Theta(x_3 - (2z_1 + L)) \right]. \]  (5.29)

In a GaAlAs [i.e. Ga\(_x\)Al\(_{1-x}\)As] layer, any material parameters \( f_m \) can be approximated by the relation [Adachi (1985)]:

\[ f_m^{GaAlAs} = x f_m^{GaAs} + (1 - x) f_m^{AlAs} \]  (5.30)

where \( x \) is the mole fraction of GaAs and \( f_m^{GaAs} \) and \( f_m^{AlAs} \) are the material parameters in GaAs and AlAs, respectively. For instance, the elastic constant can be written in the form

\[ C_{rs}^{GaAlAs} = x C_{rs}^{GaAs} + (1 - x) C_{rs}^{AlAs}. \]  (5.31)

5.3.2 Piezoelectric constants

The piezoelectric constants in heterostructures can be described in a manner similar to that of the elastic constants when the materials in the heterostructures lack inversion symmetry. In a GaAs/GaAlAs heterojunction, the piezoelectric constants may be written

\[ h_{js}(r) = h_{js}^{GaAlAs} \Theta(x_3) + (h_{js}^{GaAs} - h_{js}^{GaAlAs}) \Theta(x_3 - z_0). \]  (5.32)

In a semiconductor single quantum well with a substrate as in Figure 5.3, we can express the piezoelectric constants as

\[ h_{js}(r) = h_{js}^{GaAlAs} \Theta(x_3) + (h_{js}^{GaAs} - h_{js}^{GaAlAs}) \times \left[ \Theta(x_3 - z_1) - \Theta(x_3 - (z_1 + L)) + \Theta(x_3 - (2z_1 + L)) \right] \]  (5.33)

where

\[ h_{js}^{GaAlAs} = x h_{js}^{GaAs} + (1 - x) h_{js}^{AlAs}. \]
5.4 Source force density due to electronic transitions

The general features of the source force density due to deformation potential coupling and piezoelectric coupling were discussed in Section 3.3. In this Section, the source force density in heterostructures will be considered. From the view point of the source force due to electronic transitions in heterostructures, the following differences from the situation in bulk semiconductors give the characteristics of the source force density in the heterostructures: (1) the spatial electron distribution (i.e., quantum confinement effects of electrons) and (2) the mechanism for electron-phonon coupling. As mentioned in Section 4.4, the deformation potential itself in a 2D system is not much different from that in a 3D system in a semiconductor.

Generally the charge density due to an electron undergoing an electronic transition from a higher state \((n, k_i)\) to a lower state \((m, k_f)\) and reverse transition can be expressed [Mott and Sneddon (1963)] as

\[
\rho_e(r, t) = -e \left( \psi_{nk_i}(r) \psi_{mk_f}^*(r) e^{-i\omega_{mn}(q)t} + \psi_{mk_f}^*(r) \psi_{nk_i}(r) e^{i\omega_{mn}(q)t} \right)
\]  

(5.34)

where

\[
\omega_{mn}(q) = \frac{E_n(k_i) - E_m(k_f)}{\hbar}, \quad q = k_i - k_f.
\]

When the electronic transitions are related to electron-phonon interactions, the electron densities in the first and second terms on the right hand side of equation (5.34) correspond to phonon emission and phonon absorption, respectively, and \(\omega_{mn}(q)\) and \(q\) are the frequency and wave vector of the phonon. There is also a similar current density associated with the electronic transitions. But our interest is in the near region in the non-retarded limit. From now on, the electron-phonon interaction via deformation coupling in a 2DEG with one occupied subband only will be considered. In this case only intraband transitions play a role in the source force of acoustic waves. Also, the charge density operator for electrons in the 2DEG undergoing the transition associated with the emitted phonon whose wave vector and frequency are \(q_\parallel\) and \(\omega(q_\parallel)\) may be written

\[
\hat{\rho}_e(r_\parallel, x_3, t) = -e \hat{n}_e(r_\parallel, x_3, t).
\]  

(5.35)
Here the number density operator of electrons $\hat{n}_e(r_\parallel, x_3, t)$ undergoing the transition can be obtained from the electron field operators

$$\hat{n}_e(r_\parallel, x_3, t) = \hat{\Psi}^\dagger(r_\parallel, x_3, t)\hat{\Psi}(r_\parallel, x_3, t)$$

where

$$\hat{\Psi}(r_\parallel, x_3, t) = \sum_{k\parallel} c_{k\parallel} \psi_{k\parallel}(r_\parallel, x_3) e^{-iE(k_\parallel)t/\hbar},$$

$$\hat{\Psi}^\dagger(r_\parallel, x_3, t) = \sum_{k\parallel} c_{k\parallel}^* \psi_{k\parallel}^*(r_\parallel, x_3) e^{iE(k_\parallel)t/\hbar}$$

with

$$\psi_{k\parallel}(r_\parallel, x_3) = \frac{1}{\sqrt{A_0}} \zeta(x_3) e^{ik_\parallel \cdot r_\parallel}.$$

In other word, we have

$$\hat{n}_e(r_\parallel, x_3, t) = |\zeta(x_3)|^2 \hat{n}_2(q_\parallel, \omega(q_\parallel)) e^{iq_\parallel \cdot r_\parallel - \omega(q_\parallel)t}$$

with

$$\hat{n}_2(q_\parallel, \omega(q_\parallel)) = \frac{1}{A_0} \sum_{k\parallel} c_{k\parallel}^* - c_{q\parallel} \delta \left[ \omega(q_\parallel) - \frac{E(k\parallel) - E(k\parallel - q_\parallel)}{\hbar} \right]$$

where $(k\parallel, E(k\parallel))$ is the initial state of the electron undergoing the transition associated with the emitted phonon $(q_\parallel, \omega(q_\parallel))$. From equation (5.37), we obtain a useful expression when we evaluate the intensity of the emitted phonons from a 2DEG:

$$\langle \hat{n}_2^\dagger(q_\parallel', \omega'(q_\parallel'))\hat{n}_2(q_\parallel, \omega(q_\parallel)) \rangle = \frac{1}{A_0^2} \sum_{k\parallel} n_{k\parallel}^2 (1 - n_{k\parallel}) \delta_{q\parallel q\parallel'} \delta(\omega' - \omega)$$

$$\times \delta \left( \omega(q_\parallel) - \frac{E(k\parallel) - E(k\parallel - q_\parallel)}{\hbar} \right).$$

Note that it is possible for a 2DEG to generate phonons with wave vectors in the plane of the gas, since such generation can satisfy momentum conservation (i.e., $k_\parallel = q_\parallel + k_\parallel'$ where $k_\parallel'$ is the electron wave vector for the final electronic state). However, experimental results make it clear that phonon emissions from a 2DEG in a heterostructure have a solid angle dependence, i.e., phonon can be emitted in the direction perpendicular to the 2DEG plane, and this seems to violate
the momentum conservation law. The perpendicular component of the momentum of the emitted phonons from the electronic transitions in the 2DEG can be understood using Heisenberg’s uncertainty principle. From the point of view of the uncertainty principle, the perpendicular component of the momentum of emitted phonons should depend only on the thickness $L$ of the confinement of the potentials (i.e. $|q_3| < 1/L$). In other words, according to the uncertainty principle the perpendicular momentum should not depend on the elastic properties or interface effects of the heterostructure at all.

![Figure 5.4: The momentum conservation law in the process of phonon emissions from a 2DEG.](image)

The existence of the perpendicular component of the momentum can however be explained in another way. First note that once a strain in the plane at a 2DEG has occurred due to electronic transitions, the strain may cause another strain in the perpendicular direction with a magnitude depending on Poisson’s ratio. This is because the lattice itself is not a 2D system but a bulk system with specified boundary conditions. Now note that the induced strain may propagate both upward
and downward from the 2DEG plane. In fact, the usual experimental environment for measuring phonon generation from a 2DEG involves a substrate with a 2DEG system (e.g., single quantum well) and with a detector (e.g., bolometer), attached to the bottom of the substrate rather than the side. In this case, we can explain the momentum conservation as in the schematic description in Figure 5.4. In Figure 5.4, \( \mathbf{q} \) is the wave vector of the phonon observed at an angle \( \theta \) in the detector. The wave vector of the observed phonon is related to the 2D phonon wave vector \( \mathbf{q}_\parallel \) which is directly associated with the electronic transition from \( \mathbf{k}_\parallel \) to \( \mathbf{k}_\parallel' \). From Figure 5.4 we obtain

\[
\mathbf{q}_\parallel = \mathbf{q} + \mathbf{q}' = \mathbf{k}_\parallel - \mathbf{k}_\parallel'
\]

with

\[
| \mathbf{q} | = | \mathbf{q}' |, \quad q_3 = -q'_3.
\]

Therefore, the direction of the emitted phonon should depend on the elastic properties of the heterostructure and the 2D electron wave vector associated with the electronic transition.

Following the above discussion, we propose a model deformation tensor for GaAlAs-GaAs heterostructures:

\[
\mathbf{\tilde{\Xi}} = \Xi_h(1,1,-\sigma,0,0,0) \tag{5.39}
\]

where \( \sigma \) denotes Poisson's ratio. The electron number density for electrons undergoing the transitions can be obtained from equation (5.36):

\[
n_e(q,\omega(q),x_3) = n_2(q,\omega(q))n_e(x_3), \quad n_e(x_3) = |\zeta(x_3)|^2 \tag{5.40}
\]

or

\[
n_e(q,\omega(q),q_3) = n_2(q,\omega(q))n_e(q_3) \tag{5.41}
\]

with

\[
n_e(q_3) = \int |\zeta(x_3)|^2 e^{-iq_3x_3} dx_3. \tag{5.42}
\]

From equations (3.30), (5.39), and (5.40), the source force density due to the deformation potential coupling can be written

\[
F^{(d)}(q,\omega(q),x_3) = \Xi_h n_2(q,\omega(q)) \begin{pmatrix} iq_1n_e(x_3) \\ iq_2n_e(x_3) \\ -\sigma(\partial n_e(x_3)/\partial x_3) \end{pmatrix}. \tag{5.43}
\]
As for piezoelectric couplings in heterostructures, there has not been much work done on the effect of interfaces on the piezoelectric constants in heterostructures. We shall use the 3D results for the piezoelectric coupling constants in heterostructures. The source force density due to piezoelectric coupling can be obtained from equations (3.23), (3.24), and (3.30);

\[
F^{(p)}(q_{\parallel}, \omega(q_{\parallel}), x_3) = \frac{2\varepsilon_{14142}(q_{\parallel}, \omega(q_{\parallel}))}{\varepsilon} \left( \begin{array}{c} q_2 f_1(q_{\parallel}, x_3) \\ q_1 f_1(q_{\parallel}, x_3) \\ q_1 q_2 f_2(q_{\parallel}, x_3) \end{array} \right)
\]  

(5.44)

with

\[
f_1(q_{\parallel}, x_3) = \int \frac{n_{1e}(q_3)}{q_{\parallel}^2 + q_3^2} e^{iq_3 x_3} dq_3
\]

(5.45)

\[
f_2(q_{\parallel}, x_3) = \int \frac{n_{1e}(q_3)}{q_{\parallel}^2 + q_3^2} e^{iq_3 x_3} dq_3.
\]

(5.46)

Now we can evaluate the emitted phonon intensity from a 2DEG in a semiconductor heterostructure by using the source force densities and the Green's functions of the semiconductor heterostructure.

5.5 Phonon emissions in GaAs/GaAlAs heterostructures

In this Section, we shall consider GaAs/GaAlAs heterostructures (i.e. a single heterojunction and a single quantum well) as shown in Figures 5.2 and 5.3. A single quantum well with a substrate may be approximated, as far as elastic properties are concerned, by a single heterojunction provided the thickness of the well is small enough [see Figures 5.2 and 5.3]. Hence we shall treat both the heterostructures as the same elastic structure, which is an overlayer with a semi-infinite substrate.

When the source force of the form \( F^{(s)}(r, t) = F^{(s)}(r) e^{i\omega t} \) as discussed in the previous Section, the equation of motion (5.3) in the heterostructures may be written

\[
\rho_m(\mathbf{r}) \ddot{u}_i - \sum_j \frac{\partial T_{ij}(r, t)}{\partial x_j} = F_i^{(s)}(r) e^{i\omega t}.
\]

(5.47)

Using equations (5.4), (5.24) and (5.25), equation (5.47) becomes

\[
-\{\rho_m^A \Theta(x_3) + (\rho_m^B - \rho_m^A) \Theta(x_3 - z_0)\} \omega^2 u_i(r)
\]

\[
- \sum_{jkl} \{\delta(x_3) C_{ijkl}^A + \delta(x_3 - z_0)(C_{ijkl}^B - C_{ijkl}^A)\} u_{ij}(r)
\]
The elastic Green's functions for the above equation satisfy the following differential equations:

\[
\sum_k (\delta_{ik}\omega^2 + \frac{1}{\rho_m} \sum_{jl} C^A_{ijkl} \frac{\partial^2}{\partial x_j \partial x_l}) G_{km}(\mathbf{r}, \mathbf{r}'; \omega) = \delta_{im} \delta(\mathbf{r} - \mathbf{r}') \quad \text{for } 0 < x_3 < z_0
\]

\[
\sum_k (\delta_{ik}\omega^2 + \frac{1}{\rho_m} \sum_{jl} C^B_{ijkl} \frac{\partial^2}{\partial x_j \partial x_l}) G_{km}(\mathbf{r}, \mathbf{r}'; \omega) = \delta_{im} \delta(\mathbf{r} - \mathbf{r}') \quad \text{for } z_0 < x_3 < \infty
\]

and with boundary conditions taken from the coefficients of the \( \delta \) functions in equation (5.48);

\[
\sum_{kl} C^A_{ijkl} \frac{\partial}{\partial x_l} G_{km}(\mathbf{r}, \mathbf{r}'; \omega) \bigg|_{x_3 = 0} = 0
\]

\[
\sum_{kl} C^A_{ijkl} \frac{\partial}{\partial x_l} G_{km}(\mathbf{r}, \mathbf{r}'; \omega) \bigg|_{x_3 = z_0 - 0} = \sum_{kl} C^B_{ijkl} \frac{\partial}{\partial x_l} G_{km}(\mathbf{r}, \mathbf{r}'; \omega) \bigg|_{x_3 = z_0 + 0}
\]

Since the elastic properties are translationally symmetric in the \( x-y \) plane, the Green's function can be Fourier transformed to give

\[
G_{ij}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{1}{(2\pi)^2} \int dk^2 G_{ij}(k^\parallel, x_3, x_3'; \omega) e^{ik^\parallel \cdot (\mathbf{r} - \mathbf{r}')}
\]

In general, we have a set of nine components for \( G_{ij}(k^\parallel, x_3, x_3'; \omega) \). The set of the components can however be simplified by rotating the coordinate axis about the \( x_3 \)-direction to a new set with \( x_1 \)-direction (i.e. \( x^\prime \)-direction in Figure 5.1) aligned along the direction of \( k^\parallel \) using the transformation \( U \) as in equation (5.21). The transformation gives the simplified Green's function matrix in the form

\[
g(k^\parallel, \omega; x_3, x_3') = U G(k^\parallel, \omega; x_3, x_3') U^{-1}
\]

The Green's function for an isotropic half-space is given in Appendix B.1 and the Green's function for an overlayer with a semi-infinite substrate is obtained exactly in Appendix B.2. In order to evaluate the emitted phonon intensity in GaAlAs/GaAs heterostructures, we may, as an approximation, use the Green's function for an isotropic half-space given in Appendix B.1, where only the free surface effect is taken
into account. A better approximation for the Green’s function in the heterojunction to use the Green’s function given in Appendix B.2, since both the free surface and interface effects are taken into account.

The simplified Green’s function \( g_{ij}(k, \omega; x, x') \) can easily be decoupled into longitudinal and transverse parts. Once we know the effective longitudinal and transverse force densities, we can calculate the displacement vector in \((x', y', z')\) coordinates [see Figure 5.1]:

\[
\mathbf{u}^{(m)}(k, \omega; x_3) = \frac{1}{(2\pi)^2} \int dx'_3 \mathbf{g}^{(m)}(k, \omega; x, x'_3) \mathbf{F}_{eff}^{(m,0)}(k, \omega; x'_3)
\]

(5.56)

where superscript \( m \) indicates the mode of phonons, i.e. LA and TA(TA1, TA2) phonons, and \( \mathbf{F}_{eff}^{(m,0)} \) is the effective source force density for the \( m \)-mode phonon. The effective force density for LA phonons is obtained using the transformation matrices \( \mathbf{U} \) and \( \mathbf{R} \) [see Appendix C]:

\[
\mathbf{F}_{eff}^{(LA,0)}(k, \omega; x'_3) = \frac{\Xi_n n_2(k, \omega)k}{\rho_m} \begin{pmatrix}
    i \sin^2 \theta n_e(x'_3) - \frac{\sigma}{k} \cos \theta \sin \theta \frac{\partial n_e(x'_3)}{\partial x_3} \\
    0 \\
    i \sin \theta \cos \theta n_e(x'_3) - \frac{\sigma}{k} \cos^2 \theta \frac{\partial n_e(x'_3)}{\partial x_3}
\end{pmatrix}
\]

\[
+ \frac{2\epsilon h_{14} n_2(k, \omega)k \cos \phi \sin \phi}{\epsilon \rho_m} \begin{pmatrix}
    2 \sin^2 \theta f_1 + \cos \theta \sin \theta k_1 f_2 \\
    0 \\
    2 \sin \theta \cos \theta f_1 + \cos^2 \theta k_1 f_2
\end{pmatrix}
\]

(5.57)

where the first and second terms are due to the deformation potential and piezoelectric couplings, respectively. The effective force densities for the TA modes (i.e. TA1-, TA2- modes) are given by

\[
\mathbf{F}_{eff}^{(TA1,0)}(k, \omega; x'_3) = \frac{\Xi_n n_2(k, \omega)k}{\rho_m} \begin{pmatrix}
    i \cos^2 \theta n_e(x'_3) + \frac{\sigma}{k} \cos \theta \sin \theta \frac{\partial n_e(x'_3)}{\partial x_3} \\
    0 \\
    -i \sin \theta \cos \theta n_e(x'_3) - \frac{\sigma}{k} \sin^2 \theta \frac{\partial n_e(x'_3)}{\partial x_3}
\end{pmatrix}
\]

\[
+ \frac{2\epsilon h_{14} n_2(k, \omega)k \cos \phi \sin \phi}{\epsilon \rho_m} \begin{pmatrix}
    2 \cos^2 \theta f_1 - \cos \theta \sin \theta k_1 f_2 \\
    0 \\
    -2 \sin \theta \cos \theta f_1 + \sin^2 \theta k_1 f_2
\end{pmatrix}
\]

(5.58)

and

\[
\mathbf{F}_{eff}^{(TA2,0)}(k, \omega; x'_3) = \frac{2\epsilon h_{14} n_2(k, \omega)k}{\epsilon \rho_m} \begin{pmatrix}
    0 \\
    (\cos^2 \phi - \sin^2 \phi)f_1 \\
    0
\end{pmatrix}
\]

(5.59)

where the first and second terms for the TA1-mode are also due to the deformation potential and piezoelectric couplings, respectively, and the source force density for
the TA₂-mode is due to only piezoelectric coupling. For the numerical calculations in this Section, we use the basic material parameters shown in Table 5.1 for GaAlAs/GaAs heterostructures. The material parameters in the barrier layers (i.e. GaAlAs layers) of the heterostructures are obtained from equation (5.30).

Table 5.1: Material parameters which are used in this thesis [see Adachi (1985)].

<table>
<thead>
<tr>
<th></th>
<th>( \rho_m ) (g/cm³)</th>
<th>( C_{11} ) ( \times 10^{11} \text{dynes/cm}^2 )</th>
<th>( C_{12} ) ( \times 10^{11} \text{dynes/cm}^2 )</th>
<th>( C_{44} ) ( \times 10^{11} \text{dynes/cm}^2 )</th>
<th>Poisson’s ratio (( \sigma ))</th>
<th>( h_{14} ) (Coul/m²)</th>
<th>( \varepsilon ) (static)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaAs</td>
<td>5.360</td>
<td>11.88</td>
<td>5.38</td>
<td>5.94</td>
<td>0.31</td>
<td>-0.160</td>
<td>13.18( \varepsilon_0 )</td>
</tr>
<tr>
<td>AlAs</td>
<td>3.760</td>
<td>12.02</td>
<td>5.70</td>
<td>5.89</td>
<td>0.32</td>
<td>-0.225</td>
<td>10.06( \varepsilon_0 )</td>
</tr>
</tbody>
</table>

5.5.1 Phonon emissions in a GaAs/GaAlAs single heterojunction

In a GaAlAs/GaAs single heterojunction as shown in Figure 5.2, the Fang-Howard type trial function for the electronic wave function may be used as an approximate solution as discussed Section 2.5. This has the form

\[
\zeta(x_3) = \begin{cases} 
0 & \text{for } x_3 \leq z_0 \\
(b^3/2)^{1/2}(x_3 - z_0) \exp[-b(x_3 - z_0)/2] & \text{for } x_3 > z_0
\end{cases}
\]  

(5.60)

The electron density and its Fourier transformation may now be obtained from equations (5.40) and (5.42):

\[
n_e(x_3) = \begin{cases} 
0 & \text{for } x_3 \leq z_0 \\
(b^3/2)(x_3 - z_0)^2 \exp[-b(x_3 - z_0)] & \text{for } x_3 > z_0
\end{cases}
\]  

(5.61)

\[
n_e(q_3) = \left( \frac{b}{b + iq_3} \right)^3 e^{iq_3 z_0}.
\]  

(5.62)

Using equations (5.16), and (5.56) through (5.59), numerical calculations have been carried out for a GaAs/GaAlAs heterojunction with the following sample parameters: the thickness of GaAlAs layer \( z_0 = 1000 \text{Å} \), the areal electron concentration \( N_s = 6.0 \times 10^{11} \text{ cm}^{-2} \), the depletion charge density \( N_{\text{depl}} = 1.5 \times 10^{11} \text{ cm}^{-2} \), the electron temperature \( T_e = 15^\circ \text{K} \). In Figures 5.5 (a) and (b) the angular distributions of phonon intensities at frequency \( \omega = 1.2 \text{ THz} (\sim 0.8 \text{meV}) \) are shown for LA and TA phonons arriving at a detector. As shown in equations (5.57), (5.58) and (5.59), the \( \phi \)-angle dependence of the phonon intensity is due to piezoelectric coupling.
Figure 5.5: Angular distribution of phonon intensity for (a) LA phonons and (b) TA₁ phonons.
5. Phonon Emission from Semiconductor Heterostructures

Figure 5.6: (a) LA and (b) TA₁ phonon intensities as a function of frequency $\omega$. 
The contribution of the piezoelectric coupling to the phonon intensity is much smaller than that of the deformation potential coupling in the region of 1 THz. The $\phi$-angle dependence can therefore not be observed in this region. LA phonon intensity is much weaker than TA phonon intensity at most angles except near 90°. The total intensity of phonons at frequency $\omega=1.2$ THz arriving at a detector has strong peaks around 20-35°, weak peaks at angles 45-75°, and a peak near 90°. In Figures 5.6 (a) and (b), the frequency dependences of the phonon intensities are plotted at an angle $\theta=30°$. In most of the frequency region, TA phonons are more intense than LA phonons. Only in the region of frequencies less than approximately 20 GHz and more than approximately 1550 GHz are TA phonons weaker than LA phonons. Hence TA phonon intensity is greater than LA phonon intensity in the region of bolometer measurements (e.g. Pb bolometer [650-800 GHz], Al bolometer [100-800 GHz]) [Rothenfusser et al (1986)]. It is found that deformation potential coupling processes provide the main contribution to both LA and TA phonons in this region. This could explain the usual experimental results in a heterojunction [Chin et al (1984), Hawker et al (1989)]

5.5.2 Phonon emissions in a GaAs/GaAlAs single quantum well

For a GaAlAs/GaAs single quantum well with a semi-insulated GaAs substrate as shown in Figure 5.3, we shall use a simple infinite potential well model for the electronic wave functions. Then the lowest subband wave function is given in the form

$$\zeta(x_3) = \begin{cases} \sqrt{2/L} \sin[\pi(x_3 - z_1)/L] & \text{for } z_1 \leq x_3 \leq z_1 + L \\ 0 & \text{elsewhere} \end{cases} \quad (5.63)$$

The electron density and its Fourier transformation for the lowest subband are obtained in the forms

$$n_e(x_3) = \begin{cases} (2/L) \sin^2[\pi(x_3 - z_1)/L] & \text{for } z_1 \leq x_3 \leq z_1 + L \\ 0 & \text{elsewhere} \end{cases} \quad (5.64)$$

$$n_e(q_3) = \left( \frac{8\pi^2 \sin[q_3 z_1/L]}{Lq_3(4\pi^2 - L^2 q_3^2)} \right) e^{i q_3 (z_1 + L/2)} \quad (5.65)$$
Figure 5.7: Angular distribution of phonon intensity for (a) LA phonons and (b) TA\textsubscript{1} phonons.
Figure 5.8: (a) LA and (b) TA₁ phonon intensities as a function of frequency $\omega$. 

- (a) LA Phonon Intensity (Quantum well)
- (b) TA₁ Phonon Intensity (Quantum well)
Following the same procedure as in the previous Section, numerical calculations have been performed for a single quantum well with the following sample parameters: the width of well \( L = 140 \, \text{Å} \), the thickness of GaAlAs layer \( z_1 = 830 \, \text{Å} \) [see Figure 5.3], the areal electron concentration \( N_a = 6.0 \times 10^{11} \, \text{cm}^{-2} \), the electron temperature \( T_e = 15^\circ\text{K} \). Figures 5.7 (a) and (b) show the angular dependence of the phonon intensity for LA and TA phonons at frequency \( \omega = 1.2 \, \text{THz} \). Unlike a heterojunction [see Section 5.5.1], relative LA phonon peaks at angles 45-65° are greater than TA phonon peaks at angles 15-35°, and there are no peaks near 90°. In Figures 5.8 (a) and (b), the frequency dependences of the phonon intensities are plotted for LA and TA phonons at an angle \( \theta = 30^\circ \). In the region of frequencies less than approximately 1.4 THz, TA phonons are dominant compared with LA phonons. However the LA phonon intensity is stronger than the TA phonon intensity at frequencies 1.4-2.5 THz. The LA and TA phonons arriving at a detector are mainly due to deformation potential processes at frequencies more than approximately 90 GHz and 50 GHz, respectively. Only at low frequencies (e.g. less than 90 GHz for LA phonons and less than 50 GHz for TA phonons) can piezoelectric processes dominate the contribution to the phonons arriving at a detector.

### 5.6 Discussion

As discussed in Section 4.4, the magnitude of the deformation potential in a 2D system is not much different from that in a 3D system in a semiconductor. Note that when a deformation potential for a spherically symmetric band structure (e.g. \( \Gamma \) conduction band in GaAs) is taken, the deformation potential describes the interaction of electrons with LA phonons only. Within this context, the TA phonons emitted from a 2DEG in a GaAs/GaAlAs heterostructure should be due only to (1) piezoelectric couplings, as in a theoretical work based on the electron-phonon scattering rate method [Xu and Mahanty (1994b)], or (2) to reflection effects at an interface, as in an investigation using the elastic Green's functions with deformation potential coupling only [Badalian and Levinson (1991)]. However, both of these processes could not explain the experimental result that the TA phonons reaching a detector are more intense than the LA phonons [Chin et al (1984), Wigmore et al (1984)].
The square of the electron-acoustic phonon interaction matrix element is proportional to the phonon frequency $\omega$ for deformation potential coupling, and is inversely proportional to $\omega$ for piezoelectric coupling. The crossover of the electron-acoustic phonon scattering rates between the two processes occurs at around 140 GHz in GaAs [Hawker et al (1995)]. This implies that the electron-acoustic phonon scattering rate at frequencies much greater than 140 GHz is due mainly to deformation potential coupling and that the piezoelectric processes can be ignored in the region of the sensitivity of a Pb bolometer. A Pb bolometer acts as a narrow-band detector (approximately 650-800 GHz) and an Al bolometer behaves as a broad-band detector (approximately 100-800 GHz) [Rothenfusser et al (1986)]. Hence deformation potential processes contribute more than piezoelectric processes to the electron-acoustic phonon scattering rate for GaAs within the regime of the two bolometers, except for 100-140 GHz. Therefore, it is difficult to explain the experimental results using the electron-phonon scattering rate method. On the other hand, we can estimate the TA phonon intensity using only deformation couplings and taking into account interface effects as in Badalian and Levinson’s work [Badalian and Levinson (1991)]. In this case, the deformation coupling produces only LA phonons and the reflected LA and TA phonons at the interface are excited. Hence the reflected TA phonons can not be stronger than the LA phonons emitted directly from a 2DEG.

Experimentally, the data of phonon intensity are collected as a function of time in order to have the intensities for LA and TA phonons separately. This means that the collected data involve only phonons in the limited range of frequencies depending on a detector. Therefore, the periodic peaks, which are related with the interface effects (i.e. interference, reflection, refraction, etc.), can not be detected directly.

In Section 5.4 we proposed a model for a 2D electron-bulk phonon interaction mechanism via deformation potential couplings. Using the modified deformation potential, we calculated the intensities for LA and TA phonons in both a heterojunction and a single quantum well. We also took into account the interface effects
using the elastic Green’s functions which are derived in detail in Appendix B.2. As shown in Figures 5.6 and 5.8, at $\theta=30^\circ$ TA phonon intensity is greater than LA phonon intensity in both the two heterostructures in the region of bolometer sensitivity. According to the calculations of phonon intensities at $\theta=30^\circ$ in the previous Section, the phonon intensity crossovers between the deformation potential and piezoelectric processes occur at around 110 GHz for LA phonons in both the two heterostructures, and at 70 GHz and 50 GHz approximately for TA phonons in the heterojunction and in the quantum well, respectively. Furthermore, it is found that TA phonons are dominant at $\theta$-angles 20-35° approximately and that LA phonons are dominant at angles more than approximately 45° at 1.2 THz. In these cases, both the LA and TA phonons are due to deformation potential coupling unlike the usual mechanism for electron-acoustic phonon interaction where TA phonons are mainly due to piezoelectric couplings or due to reflection effects at an interface. Hence the model for the mechanism of deformation potential coupling can explain the experimental results discussed above.
An attempt to construct a feasible theoretical model for calculations of phonon intensity has been made in this thesis. In general, the detected phonon intensity from phonons, emitted from a 2DEG due to electronic transitions in a semiconductor heterostructure, may be determined from the following physical factors of the semiconductor heterostructure: (1) electron distribution undergoing the transitions, (2) elastic response functions (i.e. elastic Green's functions), and (3) electron-phonon coupling constants.

There are two main methods for the study of phonon emissions: (1) phonon emission rate (or energy loss rate of charge carriers) calculations based on electron-phonon scattering rate [Rothenfusser et al (1986), Toombs et al (1987), Vass (1987, 1993), Xu and Mahanty (1994b), Vasko and Mitin (1995)] (2) phonon intensity (or Poynting vector) calculations based on elastic response functions (i.e. elastic Green's functions) [Badalian and Levinson (1989, 1991), Kitagawa and Tamura (1992)]. The first method is based on the electron distribution undergoing the transitions and the electron-phonon coupling constants in a system. This method can not take into account interface effects of the system. Hence we choose the second method, which may explain the interface effects of the system, based on the three main factors as given in the previous paragraph. This is because practical experimental environments have always surfaces or interfaces.

First, an attempt to make ab initio estimates of deformation potentials has been made in 2D systems. We prove that the deformation potential in 2D deformable jellium can be drastically enhanced in the high electron density region compared with its 3D system, and that the deformation potentials of a 2D system...
6. Concluding Remarks

in a semiconductor heterostructure are not much different from that in its bulk semiconductor. This contradicts the suggestion that the 2D deformation potential in a GaAs heterostructure should be greater than that in bulk GaAs, which was suggested by several authors [Hirakawa and Sakai (1986), Harris et al (1990), Kawamura and Das Sarma (1990), Das Sarma (1991), Gorczyca et al (1992)]. This suggestion is based on electron mobility calculations which can be extracted from the integrated information of the several scattering mechanisms. In that sense, phonon intensity calculations may provide better information on electron-phonon couplings than other methods. This is because phonon emissions from a 2DEG are due only to electron-phonon couplings and it is possible to collect each mode of phonon intensities separately using time-of-flight measurements. Therefore we have tried to construct a feasible model for electron-phonon interactions by estimates of intensity of the phonons arriving at a detector.

Secondly, we provide a mechanism for deformation potential couplings in a heterostructure. As discussed in Sections 5.5.1, 5.5.2 and 5.6, deformation potential coupling processes of GaAs in the electron-acoustic scattering rate are dominant compared with piezoelectric coupling processes in the region of the sensitivity of Al and Pb bolometers [see Section 5.6]. These two bolometers have mainly been used for a detector [Chin et al (1984), Rothenfusser et al (1986), Wigmore et al (1991, 1993), Danilchenko et al (1994), Hawker et al (1995)]. From our calculations, it is found that the deformation potential processes contribute more than piezoelectric processes to the intensity of phonons arriving at a detector at frequencies of the bolometer sensitivity and that the TA phonon intensity is more intense than the LA phonon intensity in the frequency region. For the calculations, we have taken a modified deformation potential as discussed in Section 5.4, and have taken into account interface effects using elastic Green's functions as derived in Appendix B.2. We can explain experimental measurements using our calculations [see Sections 5.5.1, 5.5.2 and 5.6]. Our model for electron-phonon interactions via deformation potentials can be extended to calculate electron mobility in a 2D heterostructure.
APPENDIX A

Integration Associated Energy-momentum Conservation in 2D

Let us consider a function $F(k_i, k_f, \omega)$ depending on electronic momenta $k_i$ and $k_f$ and frequency $\omega$ of a 2DEG when a bulk-like phonon with wave vector $Q=q+2q_z$ and frequency $\omega_Q$ is emitted in a certain process. We can evaluate the summation of $F(k_i, k_f, \omega)$ over the momenta $k_i$ and $k_f$ with energy-momentum conservation as follows:

$$F_i(q, \omega_Q) = \sum_{k_i, k_f} n_{k_i}^e (1 - n_{k_f}^e) F(k_i, k_f, \omega) \delta \left( \frac{E_{k_i} - E_{k_f} - \omega}{\hbar} \right) \delta(k_i - k_f - q)$$

$$= \frac{A_0}{(2\pi)^2} \int d^2 k_f \sum_{k_i} n_{k_i}^e (1 - n_{k_f}^e) F(k_i, k_f, \omega) \delta \left( \frac{E_{k_i} - E_{k_f} - \omega_Q}{\hbar} \right) \delta(k_i - k_f - q)$$

$$= \frac{A_0}{(2\pi)^2} \sum_{k_i} n_{k_i}^e (1 - n_{k_i,q}^e) F(k_i, q, \omega) \delta \left( \frac{E_{k_i} - E_{k_i,q} - \omega}{\hbar} \right)$$

$$= \frac{A_0}{(2\pi)^4} \int d^2 k_i n_{k_i}^e (1 - n_{k_i,q}^e) F(k_i, q, \omega) \delta \left( E_{k_i} - E_{k_i,q} - \hbar\omega_Q \right)$$

(A.1)

We may write the momentum conservation as

$$k_f = k_i - q, \quad k_f^2 = k_i^2 + q^2 - 2k_i q \cos \theta$$

(A.2)

and the energy conservation as

$$E_{k_i} = E_{k_f} + \hbar\omega_Q, \quad \frac{\hbar^2 k_i^2}{2m^*} = \frac{\hbar^2 k_f^2}{2m^*} + \hbar\omega_Q.$$  

(A.3)
A. Integration Associated Energy-momentum Conservation in 2D

From equations (A.2) and (A.3), we have energy-momentum conservation in the form

\[ k_i \cos \theta = \frac{q}{2} + \frac{m^* \omega Q}{\hbar q} = \alpha(q) \]  

(A.4)

Let us introduce new coordinates [see Figure (A.1)] such that

\[
\begin{pmatrix}
  k'_{ix} \\
  k'_{iy}
\end{pmatrix} =
\begin{pmatrix}
  \cos \phi & \sin \phi \\
  -\sin \phi & \cos \phi
\end{pmatrix}
\begin{pmatrix}
  k_{ix} \\
  k_{iy}
\end{pmatrix} -
\begin{pmatrix}
  \alpha(q) \\
  0
\end{pmatrix}
\]  

(A.5)

and

\[
\begin{pmatrix}
  q'_{ix} \\
  q'_{iy}
\end{pmatrix} =
\begin{pmatrix}
  \cos \phi & \sin \phi \\
  -\sin \phi & \cos \phi
\end{pmatrix}
\begin{pmatrix}
  q_x \\
  q_y
\end{pmatrix} -
\begin{pmatrix}
  \alpha(q) \\
  0
\end{pmatrix}
\]  

(A.6)

Figure A.1: The coordinate transformation for the wave vector.

where

\[ k_{ix} = k_i \cos(\theta + \phi), \quad k_{iy} = k_i \sin(\theta + \phi), \quad q_x = q \cos \phi, \quad q_y = q \sin \phi. \]
It is straightforward to get the inverse transformations of equations (A.5) and (A.6). Setting $\phi=0$ for convenience, we have the following transformation relations

\[
\begin{align*}
k'_ix &= k_i \cos \theta - \alpha(q), & k'_iy &= k_i \sin \theta, & q'_x &= q - \alpha(q), & q'_y &= 0, \quad (A.7) \\
k_{ix} &= k'_{ix} + \alpha(q), & k_{iy} &= k'_{iy}, & q_x &= q'_x + \alpha(q) = q, & q_y &= 0. \quad (A.8)
\end{align*}
\]

Using the transformation relations (A.7) and (A.8), the $\delta$ function part of the integrand can be written as

\[
\delta(E_{ki} - E_{ki-q} - \hbar \omega_Q) = \delta\left(\frac{\hbar^2}{m^*}(k_{ix}q_x + k_{iy}q_y - \frac{q^2}{2}) - \hbar \omega_Q\right) = \delta\left(\frac{\hbar^2}{m^*}[k_{ix}'q_x + k_{iy}'q_y - \frac{q^2}{2}] - \hbar \omega_Q\right) = \delta\left(\frac{\hbar^2}{m^*}[k_{ix}'q_x + k_{iy}'q_y - \frac{q^2}{2}] - \hbar \omega_Q\right) = \delta\left(\frac{\hbar^2}{m^*}[k_{ix}'q_x + k_{iy}'q_y - \frac{q^2}{2}] - \hbar \omega_Q\right) = \frac{m^*}{\hbar^2 q} \delta(k_{ix}')
\]

Therefore the integral for $F_1(q, \omega_Q)$ in equation (A.1) is given by

\[
F_1(q, \omega_Q) = \frac{A_0^2 \hbar}{(2\pi)^4} \int d^2k_i n_{k_i}^e (1 - n_{k_i-q}^e) F(k_i, q, \omega) \delta(E_{ki} - E_{ki-q} - \hbar \omega_Q)
\]

\[
= \frac{A_0^2 \hbar}{(2\pi)^4} \int dk'_{ix} \int dk'_{iy} n_{k_i'}^e (1 - n_{k_i'-q'}^e) F(k_i', q', \omega) \frac{m^*}{\hbar^2 q} \delta(k_{ix}')
\]

with

\[
n_{k_i'}^e = \frac{1}{1 + e^{\frac{\hbar^2}{2m^*}[k_{ix}'(q + \alpha^2(q) + k_{iy}' - E_F)/k_B T_e]}}
\]

\[
(1 - n_{k_i'-q'}^e) = \frac{1}{1 + e^{-\frac{\hbar^2}{2m^*}[k_{ix}'(q + \alpha^2(q) + k_{iy}' - 2k_{iy}' - 2\hbar \omega_Q - E_F)/k_B T_e]}}
\]

where $E_F$ denotes the Fermi energy of the electrons, $k_B$ is Boltzmann constant, and $T_e$ is the electron temperature. In what follows, we remove the prime from the transformed coordinates. Integrating first over $k_{ix}$, the integral $F_1(q, \omega_Q)$ in equation (A.9) becomes

\[
F_1(q, \omega_Q) = \frac{A_0^2 m^*}{\hbar q(2\pi)^4} \int_{-\infty}^{\infty} dk'_{iy} F(k_{iy}, q, \omega) \left(\frac{1}{1 + e^{\frac{\hbar^2}{2m^*}[\alpha^2(q) + k_{iy}'^2 - E_F]/k_B T_e}}\right)
\]

\[
\times \left(\frac{1}{1 + e^{-\frac{\hbar^2}{2m^*}[\alpha^2(q) + k_{iy}'^2 - 2\hbar \omega_Q - E_F]/k_B T_e}}\right)
\]

(A.10)
Elastic Green's Function

The equations of the forced vibrations of a solid lattice under the influence of time-dependent distributions of applied force density \( F^s(r, t) \) per unit volume can be written directly in the form

\[ \rho_m \frac{\partial^2 u(r, t)}{\partial t^2} - \nabla \cdot T(r, t) = F^s(r, t) \]  

(B.1)

where the stress tensor \( T \) is a second rank tensor with elements

\[ T_{ij} = -\frac{\partial L_0}{\partial (\partial u_i/\partial x_j)} = \sum_{kl} C_{ijkl} \frac{\partial u_k}{\partial x_l} . \]  

(B.2)

On introducing a matrix differential operator \( \hat{L}(r, t) \), we can express equation (B.1) as

\[ \hat{L}(r, t) u(r, t) = -\frac{F^s(r, t)}{\rho_m(r)} = F^0(r, t) \]  

(B.3)

with

\[ \hat{L}(r, t) = \hat{L}^{(b)}(r, t) + \hat{B}(r, t) \]

where \( \hat{L}^{(b)} \) is the bulk matrix differential operator and \( \hat{B} \) is the cleavage operator [Dobrzynski (1986), Dobrzynski et al (1989), Dobrzynski (1990)] for the system. Then the Green's function associated with the matrix differential operator \( \hat{L} \) is defined by

\[ \hat{L}^{(b)}(r, t) G(r, r'; t - t') = \delta(r - r') \delta(t - t') \]  

(B.4)

and satisfies the boundary conditions associated with the cleavage operator \( \hat{B} \) which depends on the structure of the interfaces in the system. When the stimulus has a harmonic time dependence \( F^0(r, t) = F^0(r, \omega) e^{-i\omega t} \), equation (B.1) may be
B. Elastic Green's Function

written

\[ \omega^2 \mathbf{J} \cdot \mathbf{u}(r, \omega) + \frac{1}{\rho_m(r)} \nabla \cdot \left[ \mathbf{G}(r) : \mathbf{u}(r, \omega) \right] = \hat{\mathbf{L}}(r, \omega) \mathbf{u}(r, \omega) = F^{(0)}(r, \omega) \]  

with

\[ \hat{\mathbf{L}}(r, \omega) = \hat{\mathbf{L}}^{(b)}(r, \omega) + \hat{\mathbf{B}}(r, \omega) , \]

and the Green's function satisfies

\[ \hat{\mathbf{L}}^{(b)}(r, \omega) \mathbf{G}(r, r'; \omega) = \mathbf{I} \delta(r - r') \]  

and satisfies the boundary conditions associated with the cleavage operator \( \hat{\mathbf{B}} \).

When the elastic properties are translationally symmetric in the \( x-y \) plane, the Green's function can be Fourier transformed to give

\[ G_{ij}(r, r'; \omega) = \frac{1}{(2\pi)^2} \int d^3k_i G_{ij}(k_{||} \omega | x_3, x'_3) e^{{\mathbf{k}_{||}}(r - r'_||)} \]  

Generally, we have a set of nine components for \( G_{ij}(k_{||} \omega | x_3, x'_3) \). The set of the components can be simplified by rotating the coordinate axes about the \( x_3 \)-direction so that the \( x_1 \)-direction is aligned along the direction of \( k_{||} \). The rotation and its inverse are described by the transformations

\[
\begin{align*}
U(k_{||}) &= \frac{1}{k_{||}} \begin{pmatrix}
k_{1} & k_{2} & 0 \\
-k_{2} & k_{1} & 0 \\
0 & 0 & k_{||}
\end{pmatrix}, \\
U^{-1}(k_{||}) &= \frac{1}{k_{||}} \begin{pmatrix}
k_{1} & -k_{2} & 0 \\
k_{2} & k_{1} & 0 \\
0 & 0 & k_{||}
\end{pmatrix}
\end{align*}
\]

and give the simplified Green's function matrix in the form

\[ g(k_{||} \omega | x_3, x'_3) = U(k_{||}) G(k_{||} \omega | x_3, x'_3) U^{-1}(k_{||}) . \]

\( g(k_{||} \omega | x_3, x'_3) \) satisfies the differential equation

\[ \hat{\mathbf{L}}^{(0)}(k_{||} \omega | x_3) g(k_{||} \omega | x_3, x'_3) = \mathbf{I} \delta(x_3 - x'_3) \]  

and satisfies the boundary conditions associated with the cleavage operator \( \hat{\mathbf{B}}^{(0)} \).

Here

\[ \hat{\mathbf{L}}^{(0)}(k_{||} \omega | x_3) = U \hat{\mathbf{L}}^{(b)} U^{-1} , \\
\hat{\mathbf{B}}^{(0)}(k_{||} \omega | x_3) = U \hat{\mathbf{B}} U^{-1} . \]
B. Elastic Green’s Function

B.1 The elastic Green’s function for an isotropic half-space

In the simplest approximation, an isotropic half-space can be used for heterostructures such as a single heterojunction and a quantum well with a semi-insulated substrate. The elastic constant tensor and material density for the heterostructures within this approximation can be described in the form

\[ C_{ijkl}(r) = C_{ijkl} \Theta(x_3) , \]  
\[ \rho_m(r) = \rho_m \Theta(x_3) . \]  

Here \( \Theta(x_3) \) is the Heaveside step function which has the property;

\[ \Theta(f(x)) = \begin{cases} 0 & \text{if } f(x) < 0 \\ 1 & \text{if } f(x) > 0 \end{cases} \]

In an isotropic solid, the elastic properties of the solid are described by only two independent elastic constants \( (c_{11} \text{ and } c_{12}=c_{11}-2c_{44}) \). Therefore, we have the following differential operators for an isotropic half-space:

\[ \textbf{L}^{(0)}(k_\parallel | x_3) = \Theta(x_3) \begin{pmatrix} \omega^2 - v_1^2 k_\parallel^2 + v_1^2 \frac{d^2}{dx_3^2} & 0 & i k_\parallel (v_1^2 - v_2^2) \frac{d}{dx_3} \\ 0 & \omega^2 - v_2^2 k_\parallel^2 + v_1^2 \frac{d^2}{dx_3^2} & 0 \\ i k_\parallel (v_1^2 - v_2^2) \frac{d}{dx_3} & 0 & \omega^2 - v_1^2 k_\parallel^2 - v_2^2 \frac{d^2}{dx_3^2} \end{pmatrix} \]  
\[ \textbf{B}^{(0)}(k_\parallel | x_3) = \delta(x_3) \begin{pmatrix} v_1^2 \frac{d}{dx_3} & 0 & i v_1^2 k_\parallel \\ 0 & v_1^2 \frac{d}{dx_3} & 0 \\ i(v_1^2 - 2v_2^2)k_\parallel & 0 & v_1^2 \frac{d}{dx_3} \end{pmatrix} \]  

where

\[ v_1^2 = \frac{c_{11}}{\rho_m} , \quad v_2^2 = \frac{c_{44}}{\rho_m} . \]

From the equations (B.10) and the boundary condition operator (B.14), we can obtain the Green’s function as in reference [Maradudin and Mills (1976)]:

\[ g_{11}(k_\parallel, \omega | x_3, x'_3) = -\left( \frac{k_\parallel^2}{2\alpha_i \omega^2} \right) \left[ e^{-\alpha_i |x_3-x'_3|} - \xi e^{-\alpha_i |x_3-x'_3|} \right] \]

\[ -\left( \frac{k_\parallel^2}{2\alpha_i \omega^2 r'} \right) \left[ r e^{-\alpha_i (x_3+x'_3)} + e^{-\alpha_i x_3-x'_3} + e^{-\alpha_i x'_3-x_3} + \xi r e^{-\alpha_i (x_3+x'_3)} \right] \]  
\[ g_{13}(k_\parallel, \omega | x_3, x'_3) = -\left( \frac{i k_\parallel}{2\omega^2} \right) \left[ e^{-\alpha_i |x_3-x'_3|} - e^{-\alpha_i |x_3-x'_3|} \right] \text{sgn}(x_3 - x'_3) \]
B. Elastic Green’s Function

\[ g_{22}(k_{\parallel}, \omega | x_3, x_3') = -\left( \frac{1}{2}\xi \right) \left[ e^{-\alpha_t (x_3 - x_3')} + e^{-\alpha_t (x_3 + x_3')} \right] \]  
(B.16)

\[ g_{31}(k_{\parallel}, \omega | x_3, x_3') = -\left( \frac{1}{2}\xi \right) \left[ e^{-\alpha_t (x_3 - x_3')} - e^{-\alpha_t (x_3 + x_3')} \right] \text{sgn}(x_3 - x_3') \]  
(B.17)

\[ g_{32}(k_{\parallel}, \omega | x_3, x_3') = -\left( \frac{k_{\parallel}^2}{2}\xi \right) \left[ e^{-\alpha_t (x_3 - x_3')} - \xi e^{-\alpha_t (x_3 + x_3')} \right] \]  
(B.18)

\[ g_{33}(k_{\parallel}, \omega | x_3, x_3') = -\left( \frac{k_{\parallel}^2}{2}\xi \right) \left[ \xi e^{-\alpha_t (x_3 + x_3')} + e^{-\alpha_t (x_3 - x_3')} + e^{-\alpha_t (x_3 - x_3')} + e^{-\alpha_t (x_3 + x_3')} \right] \]  
(B.19)

\[ g_{12}(k_{\parallel}, \omega | x_3, x_3') = g_{21}(k_{\parallel}, \omega | x_3, x_3') = g_{23}(k_{\parallel}, \omega | x_3, x_3') = g_{32}(k_{\parallel}, \omega | x_3, x_3') = 0 \]  
(B.20)

where

\[ \alpha_t(k_{\parallel} \omega) = \begin{cases} 
(k_{\parallel}^2 - \omega^2/v_t^2)^{1/2} & \text{if } k_{\parallel}^2 > \omega^2/v_t^2 \\
-i(\omega^2/v_t^2 - k_{\parallel}^2)^{1/2} & \text{if } k_{\parallel}^2 < \omega^2/v_t^2 
\end{cases} \]  
(B.21)

\[ \alpha_t(k_{\parallel} \omega) = \begin{cases} 
(k_{\parallel}^2 - \omega^2/v_t^2)^{1/2} & \text{if } k_{\parallel}^2 > \omega^2/v_t^2 \\
-i(\omega^2/v_t^2 - k_{\parallel}^2)^{1/2} & \text{if } k_{\parallel}^2 < \omega^2/v_t^2 
\end{cases} \]  
(B.22)

\[ r_{\pm} = \frac{-4\alpha_t \alpha_t k_{\parallel}^2 \pm (\alpha_t^2 + k_{\parallel}^2)^{1/2}}{4\alpha_t \alpha_t (\alpha_t^2 + k_{\parallel}^2)^{1/2}} \]  
(B.23)

\[ \xi(k_{\parallel} \omega) = \frac{\alpha_t(k_{\parallel} \omega) \alpha_t(k_{\parallel} \omega)}{k_{\parallel}^2} \]  
(B.24)

*There is a misprint at pl52 in reference [Maradudin et al (1980)]; \( r_{\pm} \) should read \(-\frac{4\alpha_t \alpha_t k_{\parallel}^2 \pm (\alpha_t^2 + k_{\parallel}^2)^{1/2}}{4\alpha_t \alpha_t (\alpha_t^2 + k_{\parallel}^2)^{1/2}}\).
B.2 The elastic Green’s function for an overlayer with a semi-infinite substrate

Heterostructures such as single heterojunctions and quantum wells with semi-insulated substrates may be approximated by an overlayer with a semi-infinite substrate. In this case the elastic constant tensor and material density of the heterostructures can be described in the form

\[
C_{ijkl}(r) = C^A_{ijkl} \Theta(x_3) + (C^B_{ijkl} - C^A_{ijkl}) \Theta(x_3 - z_0) \quad (B.25)
\]

\[
\rho_m(r) = \rho^A_m \Theta(x_3) + (\rho^B_m - \rho^A_m) \Theta(x_3 - z_0) . \quad (B.26)
\]

Now the differential operators can be expressed as follows;

\[
\hat{\mathbf{L}}^{(0)}(k_\| \omega |x_3) = \Theta(x_3)\hat{\mathbf{L}}^{(A)} + \Theta(x_3 - z_0)(\hat{\mathbf{L}}^{(B)} - \hat{\mathbf{L}}^{(A)}) \quad (B.27)
\]

where

\[
\hat{\mathbf{L}}^{(A)} = \begin{pmatrix}
\omega^2 - v_t^2 k^2_\| + v_t^2 \frac{d^2}{dx_3^2} & 0 & ik_k(v_t^2 - v^2_\|) \frac{d}{dx_3} \\
0 & \omega^2 - v_t^2 k^2_\| + v_t^2 \frac{d^2}{dx_3^2} & 0 \\
0 & 0 & \omega^2 - v_t^2 k^2_\| - v_t^2 \frac{d^2}{dx_3^2}
\end{pmatrix}
\]

\[
\hat{\mathbf{L}}^{(B)} = \begin{pmatrix}
\omega^2 - v_t^2 k^2_\| + v_t^2 \frac{d^2}{dx_3^2} & 0 & ik_k(v_t^2 - v^2_\|) \frac{d}{dx_3} \\
0 & \omega^2 - v_t^2 k^2_\| + v_t^2 \frac{d^2}{dx_3^2} & 0 \\
0 & 0 & \omega^2 - v_t^2 k^2_\| - v_t^2 \frac{d^2}{dx_3^2}
\end{pmatrix}
\]

and

\[
\hat{\mathbf{B}}^{(0)}(k_\| \omega |x_3) = \delta(x_3)\hat{\mathbf{B}}^{(A)} + \delta(x_3 - z_0)(\hat{\mathbf{B}}^{(B)} - \hat{\mathbf{B}}^{(A)}) \quad (B.28)
\]

where

\[
\hat{\mathbf{B}}^{(A)} = \begin{pmatrix}
v_t^2 \frac{d}{dx_3} & 0 & iv_t^2 k_\|
0 & v_t^2 \frac{d}{dx_3} & 0 \\
i(v_t^2 - 2v^2_\|)k_\| & 0 & v_t^2 \frac{d}{dx_3}
\end{pmatrix}
\]

\[
\hat{\mathbf{B}}^{(B)} = \begin{pmatrix}
v_t^2 \frac{d}{dx_3} & 0 & iv_t^2 k_\|
0 & v_t^2 \frac{d}{dx_3} & 0 \\
i(v_t^2 - 2v^2_\|)k_\| & 0 & v_t^2 \frac{d}{dx_3}
\end{pmatrix}
\]

with

\[
v_t^2 = \frac{c_{11}^A}{\rho_m^A}, \quad v_\|^2 = \frac{c_{44}^A}{\rho_m^A}, \quad v_t^2 = \frac{c_{11}^B}{\rho_m^B}, \quad v_\|^2 = \frac{c_{44}^B}{\rho_m^B}.
\]
B. Elastic Green's Function

From the equations (B.10) and the boundary condition operator (B.28), we can obtain the Green's function as follows

(1) \(0 < x_3 < z_0, \quad 0 < x'_3 < z_0\)

\[g_{11}(k_\parallel, \omega \mid x_3, x'_3) = g^{(A)}_{11}(k_\parallel, \omega \mid x_3, x'_3)\]

\[+ A_t e^{-\alpha_1 x_3} + B_t e^{\alpha_1 x_3} + A_t e^{-\alpha_1 x'_3} + B_t e^{\alpha_1 x'_3}\]  
(B.29)

\[g_{13}(k_\parallel, \omega \mid x_3, x'_3) = g^{(A)}_{13}(k_\parallel, \omega \mid x_3, x'_3)\]

\[+ G_t e^{-\alpha_3 x_3} + H_t e^{\alpha_3 x_3} + G_t e^{-\alpha_3 x'_3} + H_t e^{\alpha_3 x'_3}\]  
(B.30)

\[g_{22}(k_\parallel, \omega \mid x_3, x'_3) = g^{(A)}_{22}(k_\parallel, \omega \mid x_3, x'_3)\]

\[+ E_t e^{-\alpha_3 x_3} + F_t e^{\alpha_3 x_3}\]  
(B.31)

\[g_{31}(k_\parallel, \omega \mid x_3, x'_3) = g^{(A)}_{31}(k_\parallel, \omega \mid x_3, x'_3)\]

\[- \Gamma_t (A_t e^{-\alpha_1 x_3} - B_t e^{\alpha_1 x_3}) - \Gamma_t (A_t e^{-\alpha_1 x'_3} - B_t e^{\alpha_1 x'_3})\]  
(B.32)

\[g_{33}(k_\parallel, \omega \mid x_3, x'_3) = g^{(A)}_{33}(k_\parallel, \omega \mid x_3, x'_3)\]

\[- \Gamma_t (G_t e^{-\alpha_3 x_3} - H_t e^{\alpha_3 x_3}) - \Gamma_t (G_t e^{-\alpha_3 x'_3} - H_t e^{\alpha_3 x'_3})\]  
(B.33)

(2) \(0 < x_3 < z_0, \quad x'_3 > z_0\)

\[g_{11}(k_\parallel, \omega \mid x_3, x'_3) = R_t (e^{-\alpha_3 x_3} - \Lambda_2 e^{-\alpha_3 x'_3} + \Lambda_1 e^{\alpha_3 x'_3})\]

\[+ S_t (e^{\alpha_3 x_3} + \Lambda_1 e^{-\alpha_3 x'_3} - \Lambda_2 e^{\alpha_3 x'_3})\]  
(B.34)

\[g_{13}(k_\parallel, \omega \mid x_3, x'_3) = X_t (e^{-\alpha_3 x_3} - \Lambda_2 e^{-\alpha_3 x'_3} + \Lambda_1 e^{\alpha_3 x'_3})\]

\[+ Y_t (e^{\alpha_3 x_3} + \Lambda_1 e^{-\alpha_3 x'_3} - \Lambda_2 e^{\alpha_3 x'_3})\]  
(B.35)

\[g_{22}(k_\parallel, \omega \mid x_3, x'_3) = V_t (e^{-\alpha_3 x_3} + e^{\alpha_3 x'_3})\]  
(B.36)

\[g_{31}(k_\parallel, \omega \mid x_3, x'_3) = R_t (\Gamma_t (\Lambda_2 e^{-\alpha_3 x_3} + \Lambda_1 e^{\alpha_3 x'_3}) - \Gamma_t e^{-\alpha_3 x'_3})\]

\[+ S_t (\Gamma_t e^{\alpha_3 x_3} - \Gamma_t (\Lambda_1 e^{-\alpha_3 x'_3} + \Lambda_2 e^{\alpha_3 x'_3}))\]  
(B.37)

\[g_{33}(k_\parallel, \omega \mid x_3, x'_3) = X_t (\Gamma_t (\Lambda_2 e^{-\alpha_3 x_3} + \Lambda_1 e^{\alpha_3 x'_3}) - \Gamma_t e^{-\alpha_3 x'_3})\]

\[+ Y_t (\Gamma_t e^{\alpha_3 x_3} - \Gamma_t (\Lambda_1 e^{-\alpha_3 x'_3} + \Lambda_2 e^{\alpha_3 x'_3}))\]  
(B.38)

(3) \(z_0 < x_3, \quad 0 < x'_3 < z_0\)

\[g_{11}(k_\parallel, \omega \mid x_3, x'_3) = R'_t e^{-\alpha'_3 x_3} + R'_t e^{-\alpha'_3 x'_3}\]  
(B.39)

\[g_{13}(k_\parallel, \omega \mid x_3, x'_3) = X'_t e^{-\alpha'_3 x_3} + X'_t e^{-\alpha'_3 x'_3}\]  
(B.40)
B. Elastic Green’s Function

\[ g_{22}(k_{\parallel}, \omega \mid x_3, x'_3) = V'_i e^{-\alpha_i|x_3|} \quad (B.41) \]

\[ g_{31}(k_{\parallel}, \omega \mid x_3, x'_3) = -(\Gamma'_i R'_i e^{-\alpha_i x_3} + \Gamma'_i R'_i e^{-\alpha_i x'_3}) \quad (B.42) \]

\[ g_{33}(k_{\parallel}, \omega \mid x_3, x'_3) = -(\Gamma'_i X'_i e^{-\alpha_i x_3} + \Gamma'_i X'_i e^{-\alpha_i x'_3}) \quad (B.43) \]

(4) \( z_0 < x_3, \quad z_0 < x'_3 \)

\[ g_{11}(k_{\parallel}, \omega \mid x_3, x'_3) = g^{(B)}_{11}(k_{\parallel}, \omega \mid x_3, x'_3) + \Lambda'_i e^{-\alpha_i x_3} + \Lambda'_i e^{-\alpha_i x'_3} \quad (B.44) \]

\[ g_{13}(k_{\parallel}, \omega \mid x_3, x'_3) = g^{(B)}_{13}(k_{\parallel}, \omega \mid x_3, x'_3) + G'_i e^{-\alpha_i x_3} + G'_i e^{-\alpha_i x'_3} \quad (B.45) \]

\[ g_{22}(k_{\parallel}, \omega \mid x_3, x'_3) = g^{(B)}_{22}(k_{\parallel}, \omega \mid x_3, x'_3) + E'_i e^{-\alpha_i x_3} \quad (B.46) \]

\[ g_{31}(k_{\parallel}, \omega \mid x_3, x'_3) = g^{(B)}_{31}(k_{\parallel}, \omega \mid x_3, x'_3) - (\Gamma'_i A'_i e^{-\alpha_i x_3} + \Gamma'_i A'_i e^{-\alpha_i x'_3}) \quad (B.47) \]

\[ g_{33}(k_{\parallel}, \omega \mid x_3, x'_3) = g^{(B)}_{33}(k_{\parallel}, \omega \mid x_3, x'_3) - (\Gamma'_i G'_i e^{-\alpha_i x_3} + \Gamma'_i G'_i e^{-\alpha_i x'_3}) \quad (B.48) \]

where

\[ g^{(A)}_{11}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{k_{\parallel}^2}{2 \alpha_i \omega^2} \right) [e^{-\alpha_i|x_3 - x'_3|} - \xi e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(A)}_{13}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{i k_{\parallel}}{2 \omega^2} \right) sgn(x_3 - x'_3) [e^{-\alpha_i|x_3 - x'_3|} - e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(A)}_{22}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{1}{2 \alpha_i v_i^2} \right) e^{-\alpha_i|x_3 - x'_3|} \]

\[ g^{(A)}_{31}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{i k_{\parallel}}{2 \omega^2} \right) sgn(x_3 - x'_3) [e^{-\alpha_i|x_3 - x'_3|} - e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(A)}_{33}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{k_{\parallel}^2}{2 \alpha_i \omega^2} \right) [e^{-\alpha_i|x_3 - x'_3|} - \xi e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(B)}_{11}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{k_{\parallel}^2}{2 \alpha_i \omega^2} \right) [e^{-\alpha_i|x_3 - x'_3|} - \xi e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(B)}_{13}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{i k_{\parallel}}{2 \omega^2} \right) sgn(x_3 - x'_3) [e^{-\alpha_i|x_3 - x'_3|} - e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(B)}_{22}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{1}{2 \alpha_i v_i^2} \right) e^{-\alpha_i|x_3 - x'_3|} \]

\[ g^{(B)}_{31}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{i k_{\parallel}}{2 \omega^2} \right) sgn(x_3 - x'_3) [e^{-\alpha_i|x_3 - x'_3|} - e^{-\alpha_i|x_3 - x'_3|}] \]

\[ g^{(B)}_{33}(k_{\parallel}, \omega \mid x_3, x'_3) = -\left( \frac{k_{\parallel}^2}{2 \alpha_i \omega^2} \right) [e^{-\alpha_i|x_3 - x'_3|} - \xi e^{-\alpha_i|x_3 - x'_3|}] \]

\[ \alpha_i(k_{\parallel} \omega) = \begin{cases} 
\frac{(k_{\parallel}^2 - \omega^2/v_i^2)^{1/2}}{2} & \text{if } k_{\parallel}^2 > \omega^2/v_i^2 \\
-i(\omega^2/v_i^2 - k_{\parallel}^2)^{1/2} & \text{if } k_{\parallel}^2 < \omega^2/v_i^2 
\end{cases} \]
\[
B. \text{ Elastic Green's Function}\]

\[
\alpha_i'(k\|\omega) = \begin{cases} \frac{(k^2 - \omega^2/v^2)^{1/2}}{k^2} & \text{if } k^2 > \omega^2/v^2 \\ -i\left(\omega^2/v^2 - k^2\right)^{1/2} & \text{if } k^2 < \omega^2/v^2 \end{cases}
\]

\[
\alpha_i(k\|\omega) = \begin{cases} (k^2 - \omega^2/v^2)^{1/2} & \text{if } k^2 > \omega^2/v^2 \\ -i\left(\omega^2/v^2 - k^2\right)^{1/2} & \text{if } k^2 < \omega^2/v^2 \end{cases}
\]

\[
\alpha'_i(k\|\omega) = \begin{cases} (k^2 - \omega^2/v^2)^{1/2} & \text{if } k^2 > \omega^2/v^2 \\ -i\left(\omega^2/v^2 - k^2\right)^{1/2} & \text{if } k^2 < \omega^2/v^2 \end{cases}
\]

\[
\xi = \frac{\alpha_i(k\|\omega)\alpha_i'(k\|\omega)}{k^2}, \quad \xi' = \frac{\alpha'_i(k\|\omega)\alpha'_i(k\|\omega)}{k^2}
\]

\[
\Gamma_1 = i \left(\frac{\omega^2 p^A + c_{44}^A c_i^2 - c_{11}^A k^2}{\alpha_i(c_{12} + c_{44}^A) k^2}\right), \quad \Gamma_1' = i \left(\frac{\omega^2 p^B + c_{44}^B c_i^2 - c_{11}^B k^2}{\alpha_i(c_{12} + c_{44}^B) k^2}\right)
\]

\[
\Lambda_1 = \frac{1}{k^2} \left[\begin{array}{c} \gamma_t \\ \gamma_t \end{array}\right], \quad \Lambda_1' = \frac{1}{k^2} \left[\begin{array}{c} \gamma_t' \\ \gamma_t' \end{array}\right]
\]

\[
\Lambda_2 = \frac{1}{k^2} \left[\begin{array}{c} \gamma_t \\ \gamma_t \end{array}\right], \quad \Lambda_2' = \frac{1}{k^2} \left[\begin{array}{c} \gamma_t' \\ \gamma_t' \end{array}\right]
\]

\[
\Upsilon_t = -(\alpha_t - ik\|\Gamma_t), \quad \Upsilon_t' = -(\alpha_t' - ik\|\Gamma_t')
\]

\[
\Pi_t = c_{12}^A k - ic_{44}^A \alpha_t \Gamma_t, \quad \Pi_t' = c_{12}^B k - ic_{44}^B \alpha_t' \Gamma_t'
\]

The coefficients in equations (B.29) to (B.48) will be determined from the following block matrix equation which was obtained from the boundary conditions for the Green's functions:

\[
\begin{pmatrix}
A & 0 & 0 & 0 & 0 & 0 \\
0 & A & 0 & 0 & 0 & 0 \\
0 & 0 & H & 0 & 0 & 0 \\
0 & 0 & 0 & Q & 0 & 0 \\
0 & 0 & 0 & 0 & Q & 0 \\
0 & 0 & 0 & 0 & 0 & K
\end{pmatrix}
\begin{pmatrix}
X_1 \\
X_2 \\
X_3 \\
X_4 \\
X_5 \\
X_6
\end{pmatrix}
=
\begin{pmatrix}
Y_1 \\
Y_2 \\
Y_3 \\
Y_4 \\
Y_5 \\
Y_6
\end{pmatrix}
\]

(B.49)

where \(A\) is a 4 \times 4 matrix, \(H\) is a 2 \times 2 matrix, \(Q\) is a 6 \times 6 matrix, \(K\) is a 3 \times 3 matrix, \(X_1, X_2, Y_1,\) and \(Y_2\) are single-column matrices which have four elements, \(X_3\) and \(Y_3\) are single-column matrices which have two elements, \(X_4, X_5, Y_4,\) and \(Y_5\) are single-column matrices which have six elements, and \(X_6\) and \(Y_6\) are single-column matrices which have two elements.
matrices which have three elements. Their elements are given by

\[ A(1, 1) = c_{44}^A \left[ \gamma_t e^{-\alpha_t z_0} - \gamma_t (\Lambda_2 e^{-\alpha_t z_0} + \Lambda_1 e^{\alpha_t z_0}) \right] \]

\[ A(1, 2) = -c_{44}^A \left[ \gamma_t e^{\alpha_t z_0} - \gamma_t (\Lambda_1 e^{-\alpha_t z_0} + \Lambda_2 e^{\alpha_t z_0}) \right] \]

\[ A(1, 3) = -c_{44}^B \gamma_t e^{-\alpha_t z_0} \]

\[ A(1, 4) = -c_{44}^B \gamma_t e^{-\alpha_t z_0} \]

\[ A(2, 1) = \Pi_t e^{-\alpha_t z_0} - \Pi_t (\Lambda_2 e^{-\alpha_t z_0} - \Lambda_1 e^{\alpha_t z_0}) \]

\[ A(2, 2) = \Pi_t e^{\alpha_t z_0} + \Pi_t (\Lambda_1 e^{-\alpha_t z_0} - \Lambda_2 e^{\alpha_t z_0}) \]

\[ A(2, 3) = -\Pi_t e^{-\alpha_t z_0} \]

\[ A(2, 4) = -\Pi_t e^{-\alpha_t z_0} \]

\[ A(3, 1) = e^{-\alpha_t z_0} - \Lambda_2 e^{-\alpha_t z_0} + \Lambda_1 e^{\alpha_t z_0} \]

\[ A(3, 2) = e^{\alpha_t z_0} + \Lambda_1 e^{-\alpha_t z_0} - \Lambda_2 e^{\alpha_t z_0} \]

\[ A(3, 3) = -e^{-\alpha_t z_0} \]

\[ A(3, 4) = -e^{-\alpha_t z_0} \]

\[ A(4, 1) = \gamma_t (\Lambda_2 e^{-\alpha_t z_0} + \Lambda_1 e^{\alpha_t z_0}) - \gamma_t e^{-\alpha_t z_0} \]

\[ A(4, 2) = \gamma_t e^{\alpha_t z_0} - \gamma_t (\Lambda_1 e^{-\alpha_t z_0} + \Lambda_2 e^{\alpha_t z_0}) \]

\[ A(4, 3) = -\gamma_t e^{-\alpha_t z_0} \]

\[ H(1, 1) = c_{44}^A \gamma_t (e^{\alpha_t z_0} - e^{-\alpha_t z_0}) \]

\[ H(1, 2) = c_{44}^A \gamma_t e^{\alpha_t z_0} \]

\[ Q(1, 1) = \gamma_t \]

\[ Q(1, 2) = -\gamma_t \]

\[ Q(1, 3) = \gamma_t \]

\[ Q(1, 4) = -\gamma_t \]

\[ Q(2, 1) = Q(2, 2) = \Pi_t \]

\[ Q(2, 3) = Q(2, 4) = \Pi_t \]

\[ Q(2, 5) = Q(2, 6) = 0 \]

\[ Q(3, 1) = c_{44}^A \gamma_t e^{-\alpha_t z_0} \]

\[ Q(3, 2) = -c_{44}^A \gamma_t e^{\alpha_t z_0} \]

\[ Q(3, 3) = c_{44}^A \gamma_t e^{-\alpha_t z_0} \]

\[ Q(3, 4) = -c_{44}^A \gamma_t e^{\alpha_t z_0} \]

\[ Q(3, 5) = -c_{44}^B \gamma_t e^{-\alpha_t z_0} \]

\[ Q(3, 6) = -c_{44}^B \gamma_t e^{-\alpha_t z_0} \]

\[ Q(4, 1) = \Pi_t e^{-\alpha_t z_0} \]

\[ Q(4, 2) = \Pi_t e^{\alpha_t z_0} \]

\[ Q(4, 3) = \Pi_t e^{-\alpha_t z_0} \]

\[ Q(4, 4) = \Pi_t e^{\alpha_t z_0} \]

\[ Q(4, 5) = -\Pi_t e^{-\alpha_t z_0} \]

\[ Q(4, 6) = -\Pi_t e^{-\alpha_t z_0} \]

\[ Q(5, 1) = e^{-\alpha_t z_0} \]

\[ Q(5, 2) = e^{\alpha_t z_0} \]

\[ Q(5, 3) = e^{-\alpha_t z_0} \]

\[ Q(5, 4) = e^{\alpha_t z_0} \]

\[ Q(5, 5) = -e^{-\alpha_t z_0} \]

\[ Q(5, 6) = -e^{-\alpha_t z_0} \]

\[ Q(6, 1) = \gamma_t e^{-\alpha_t z_0} \]

\[ Q(6, 2) = -\gamma_t e^{\alpha_t z_0} \]

\[ Q(6, 3) = \gamma_t e^{-\alpha_t z_0} \]

\[ Q(6, 4) = -\gamma_t e^{\alpha_t z_0} \]

\[ Q(6, 5) = -\gamma_t e^{-\alpha_t z_0} \]

\[ Q(6, 6) = -\gamma_t e^{-\alpha_t z_0} \]

\[ K(1, 1) = 1 \]

\[ K(1, 2) = -1 \]

\[ K(1, 3) = 0 \]

\[ K(2, 1) = c_{44}^A \gamma_t e^{-\alpha_t z_0} \]

\[ K(2, 2) = -c_{44}^A \gamma_t e^{\alpha_t z_0} \]

\[ K(2, 3) = -c_{44}^B \gamma_t e^{-\alpha_t z_0} \]

\[ K(3, 1) = e^{-\alpha_t z_0} \]

\[ K(3, 2) = e^{\alpha_t z_0} \]

\[ K(3, 3) = -e^{-\alpha_t z_0} \]
B. Elastic Green’s Function

\[ Y_1(1) = \frac{c_{44}^2}{2\omega^2} e^{-\alpha_i(x_3' - n_3)} - \frac{k_1^2}{\omega} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_1(2) = -\frac{k_1}{\omega} \left[ (c_{12}^1 - c_{12}^A) e^{-\alpha_i(x_3' - n_3)} - (c_{11}^1 - \frac{k_1^2}{\alpha_i^2} c_{12}^1) \alpha_i e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_1(3) = -\frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_1(4) = i \frac{k_1}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_2(1) = -\frac{k_1}{\omega} \left[ (c_{12}^1 - c_{12}^A) e^{-\alpha_i(x_3' - n_3)} - \left( \frac{k_1^2}{\alpha_i^2} \right) (1 + \frac{k_1^2}{\alpha_i^2}) e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_2(2) = -\frac{k_1^2}{\omega} \left[ (c_{11}^1 - c_{12}^1) e^{-\alpha_i(x_3' - n_3)} + (c_{11}^2 - \frac{k_1^2}{\alpha_i^2} c_{11}^1) e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_2(3) = -\frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_2(4) = \frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_3(1) = -\frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_3(2) = -\frac{1}{2\alpha_i^2 \omega} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_4(1) = \frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \frac{k_1^2}{\omega} e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_4(2) = \frac{k_1^2}{\omega} \left[ \alpha_i c_{12}^1 - c_{12}^A \right] e^{-\alpha_i(x_3' - n_3)} + \alpha_i (c_{11}^1 - c_{12}^A) e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_4(3) = \frac{k_1^2}{\omega} \left[ \alpha_i c_{12}^1 - c_{12}^A \right] e^{-\alpha_i(x_3' - n_3)} - \frac{k_1^2}{\omega} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_4(4) = \frac{k_1^2}{\omega} \left[ \alpha_i c_{12}^1 - c_{12}^A \right] e^{-\alpha_i(x_3' - n_3)} + \alpha_i (c_{11}^1 - c_{12}^A) e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_4(5) = \frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_4(6) = \frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_5(1) = \frac{k_1^2}{\omega} \left[ \alpha_i (1 + \frac{k_1^2}{\alpha_i^2}) e^{-\alpha_i(x_3' - n_3)} - 2\alpha_i e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_5(2) = -\frac{k_1^2}{\omega} \left[ (c_{11}^1 - c_{12}^A) e^{-\alpha_i(x_3' - n_3)} + (c_{12}^2 - \frac{k_1^2}{\alpha_i^2} c_{11}^1) e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_5(3) = i \frac{k_1^2}{\omega} \left[ \alpha_i (1 + \frac{k_1^2}{\alpha_i^2}) e^{-\alpha_i(x_3' - n_3)} - 2\alpha_i e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_5(4) = i \frac{k_1^2}{\omega} \left[ \alpha_i (1 + \frac{k_1^2}{\alpha_i^2}) e^{-\alpha_i(x_3' - n_3)} - 2\alpha_i e^{-\alpha_i(x_3' - n_3)} \right] \]
\[ Y_5(5) = i \frac{k_1^2}{\omega} \left( e^{-\alpha_i(x_3' - n_3)} - \xi e^{-\alpha_i(x_3' - n_3)} \right) \]
\[ Y_5(6) = -\frac{1}{2\alpha_i^2 \omega} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_6(1) = -\frac{1}{2\alpha_i^2 \omega} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_6(2) = \frac{c_{44}^2}{2\omega^2} e^{-\alpha_i(x_3' - n_3)} \]
\[ Y_6(3) = \frac{1}{2\alpha_i^2 \omega} e^{-\alpha_i(x_3' - n_3)} \]

\[ \tilde{X}_1 = (R_1, S_1, A_1', A_1') \]
\[ \tilde{X}_2 = (X_1, Y_1, G_1', G_1') \]
\[ \tilde{X}_3 = (V_1, E_1') \]
\[ \tilde{X}_4 = (A_t, B_t, A_l, B_l, R'_t, R'_l) \]
\[ \tilde{X}_5 = (G_t, H_t, G_l, H_l, X'_t, X'_l) \]
\[ \tilde{X}_6 = (E_t, F_t, V'_t) \]
APPENDIX C

Effective Source Force Density

The source force due to electron-phonon interaction depends on the direction of propagation of the phonons. Therefore the effective force for a specific mode can be obtained using coordinate transformations. It is easier to use the effective force in \((x', y', z')\) coordinates (as shown in Figure 5.1) where the elastic Green's function can be decoupled into LA and TA phonon parts. First of all, we need to decouple the force into LA and TA parts using the phonon coordinates \((x, y, z)\) where the phonons are propagating along the \(z\)-direction [see Figure 5.1]. In the phonon coordinates, the \(x\)-, \(y\)-, and \(z\)-components of the force density \(F''\) are the effective force densities for LA, TA\(_1\), and TA\(_2\) phonons, respectively. Using the transformation matrix \(U\), the source force densities in the crystallographic coordinates \((X, Y, Z)\) and in the coordinates \((x', y', z')\) are related by

\[
F'(q_\parallel, x_3, \omega) = UF(q_\parallel, x_3, \omega)
\]
(C.1)

and using the transformation matrix \(R\), the relation between the source force densities in the phonon coordinates \((x, y, z)\) and in the coordinates \((x', y', z')\) is

\[
F'(q_\parallel, x_3, \omega) = R^{-1}F''(q, x_3, \omega)
\]
(C.2)

where \(F\), \(F'\), and \(F''\) are the source force densities in the \((X, Y, Z)\), \((x', y', z')\), and \((x, y, z)\) coordinates, respectively. Here \(F''\) is

\[
F'' = \begin{pmatrix} F^{(TA_1)} \\ F^{(TA_2)} \\ F^{(LA)} \end{pmatrix}
\]
(C.3)

where \(F^{(LA)}\) is the effective force density for LA phonons, and \(F^{(TA_1)}\) and \(F^{(TA_2)}\) are the effective force densities for P- and H- TA phonons. The source force density
C. Effective Source Force Density

$F$ itself can be easily obtained in the crystallographic coordinates. Then the source force density $F''$ in the phonon coordinates is

$$
F'' = \mathbf{aF} = \mathbf{RUF} = 
\begin{pmatrix}
\cos \theta \cos \phi F_1 + \cos \theta \sin \phi F_2 - \sin \theta F_3 \\
- \sin \phi F_1 + \cos \phi F_2 \\
\sin \theta \cos \phi F_1 + \sin \theta \sin \phi F_2 + \cos \theta F_3
\end{pmatrix}.
$$

(C.4)

Once the effective source force densities for each phonon mode in the phonon coordinates are obtained, the source force densities for each phonon mode in $(x', y', z')$ coordinates can be evaluated using equation (C.2)

$$
F' = \mathbf{R}^{-1}F'' = 
\begin{pmatrix}
\cos \theta F^{(TA_1)} + \sin \theta F^{(LA)} \\
F^{(TA_2)} \\
- \sin \theta F^{(TA_1)} + \cos \theta F^{(LA)}
\end{pmatrix}.
$$

(C.5)

In other words, the effective force densities for each phonon mode in $(x', y', z')$ coordinates are

$$
F^{(LA)} = 
\begin{pmatrix}
\sin \theta F^{(LA)} \\
0 \\
\cos \theta F^{(LA)}
\end{pmatrix},
$$

(C.6)

$$
F^{(TA_1)} = 
\begin{pmatrix}
\cos \theta F^{(TA_1)} \\
0 \\
- \sin \theta F^{(TA_1)}
\end{pmatrix},
$$

(C.7)

$$
F^{(TA_2)} = 
\begin{pmatrix}
0 \\
F^{(TA_2)} \\
0
\end{pmatrix}.
$$

(C.8)

Therefore we can calculate displacement vectors for each phonon mode using equation (5.56) and the above relations.


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