PHONONIC BRAGG REFLECTORS FOR THERMAL ISOLATION OF SEMICONDUCTOR QUBITS

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ABSTRACT

This is still the wrong abstract

In recent years, the experimental capability in realizing and exercising full control over multiple coupled quantum dots in semiconductor heterostructures has advanced to the point where tuning the dots to the few-electron regime required for quantum computation applications will become impractical to perform manually, establishing the demand for automated procedures in this area. Moreover, charge stability diagrams, which represent a crucial tool in the tuning of quantum dot systems, become increasingly complex to understand and analyze due to the growing number of parameters influencing their structure. The goal of this thesis is to take a first step towards a fully computer-automated implementation of the tuning process by focusing on the coarse tuning of the system to the zero-electron regime.

I simulate charge diagrams of multiple coupled quantum dots in a linear array using a classical capacitive model, reproducing the honeycomb structure of double quantum dot charge diagrams. In order to automatically recognize the zero-electron regime in double-dot charge diagrams by identifying the charge transitions, I introduce a line detection algorithm using the Radon transform of the charge diagram able to detect lines even in noisy images by exploiting the fact that, in a suitable charge diagram detail, several transitions of the same kind and hence the same slope will show. The strong noise performance of the algorithm promises fast scan times during the tuning process. Finally, I present and test an algorithm that attempts to automatically tune a simulated double-dot system to the zero-electron regime using the line detection algorithm developed.

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INTRODUCTION

Introduction to notation

- notation of vectors and tensors

2

THEORY

In order to understand the complexity of the problem and the utilised solving method, it is reasonable to revisit some fundamental concepts in the following chapter. At the same time, a consistent notation is introduced. At first, the tensor formalism for elastic properties of rigid bodies is introduced. It should be noted in advance, that vectors are denoted by a single underline and tensors or tensor fields of higher order by a number of underlines corresponding to their order.
After that, elastic waves are derived and analysed further. This will be mostly based on [1], if not otherwise stated.

justification for modelling with elastic waves

check if description still applies, citation?

2.1 ELASTIC PROPERTIES OF MATERIALS

In the following, the formalism for bulk elastic properties of materials is introduced. As only small deformations are relevant for the considerations in this thesis, they are assumed to be in the regime of linear elastic behaviour, neglecting plastic or nonlinear behaviour.

In one dimension this can be described simply by Hooke's law, which states that a small displacement Δl caused by a force F is proportional to the displacement. Considering an object of length l and cross-sectional area A, **stress** and **strain** can be defined as

$$\text{Stress} \qquad \sigma := \frac{F}{A} \qquad\qquad \text{Strain} \qquad \epsilon := \frac{\Delta l}{l} \tag{2.1}$$

Hooke's law can now be reformulated as

$$\sigma = C\,\epsilon \tag{2.2}$$

with **Young's Modulus C** as proportional constant.

2.1.1 *Stress Tensor*

For finite size objects stress can be defined locally on infinitesimal, cubic volume elements. These volume elements get deformed by forces that are applied to

the object. If we consider a general force $\Delta\underline{F}$ acting on a surface element ΔA we can always divide this force into a normal component $\Delta\underline{F}_n$ and two mutually perpendicular tangential components $\Delta\underline{F}_{t1}$ and $\Delta\underline{F}_{t2}$. This implies the general definition of the stress tensor as

$$\sigma_{ij} = \frac{\text{force in direction i}}{\text{surface with normal in direction j}} \tag{2.3}$$

picture of stress definition?

whereas indices i and j denote denote one of the spatial directions x,y or z. If we claim the volume element to be static, it follows, that the normal forces on opposite sites and tangential forces on neighbouring sides equal each other. The latter can be expressed over $\sigma_{ij} = \sigma_{ji}$. This leaves 6 independent components, the three normal stresses σ_{ii} and the three shear stresses σ_{ij}.

2.1.2 *Strain Tensor*

Deformation of a three dimensional object can be described using the displacement field $\underline{u}(\underline{r},t) := \underline{r}' - \underline{r}$, which defines a displacement vector for each point $\underline{r}$ in space in comparison to the deformed position $\underline{r}'$. Local stress only relates to change in displacement relative to neighbouring positions which allows to consider the Taylor expansion in first order

$$\underline{u}(\underline{r} + \Delta\underline{r}, t) = \underline{u}(\underline{r},t) + \underline{\underline{\nabla}} u(\underline{r},t)\ \Delta\underline{r} \tag{2.4}$$

with the Jacobian matrix $(\underline{\underline{\nabla}} u)_{ij} = \frac{\partial u_i}{\partial r_j}$. This in turn can be decomposed into a symmetric part and an antisymmetric part. The symmetric part is defined as strain tensor:

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right) \tag{2.5}$$

It is a dimensionless measure for local deformation in contrast to the antisymmetric part, which represents local rotation.

reference to lecture 2?

2.1.3 *Stress-Strain Relations*

With stress and strain tensor introduced, equation 2.2 can be generalised to three dimensions taking anisotropies of the material into account:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl} \qquad \text{or} \qquad \underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{C}}}} \cdot \underline{\underline{\epsilon}} \tag{2.6}$$

This defines the **Elasticity tensor** as order 4 tensor with unit force / area. In general this tensor contains 81 components. However, stress and strain tensor are

symmetric, so that $C_{ijkl} = C_{jikl} = C_{ijlk}$. This reduces the number of independent components to 36 and makes it possible to describe the Elasticity tensor as 6×6 matrix. For this representation, the so called Voigt notation maps pairs of coefficients of elasticity, strain and stress tensor to a single index as in table 2.1 This simplifies the notation of elasticity significantly, but it should be treated

$$xx \to 1 \quad yy \to 2 \quad zz \to 3 \quad yz = zy \to 4 \quad xz = zx \to 5 \quad xy = yx \to 6$$

Table 2.1: Voigt notation

carefully. Tensors written in Voigt notation do not transform like vectors in each index.

One can also proof, that $C_{ijkl} = C_{klij}$ considering elastic energy (see section 4.3.1 of [1]) which leads to 21 independent components. Further simplifications derive from crystal symmetry or limitations in anisotropy. In the following treatment, the material is assumed to be isotropic, which reduces the number of independent components to 2. These are typically introduced as Lamé constants λ and μ defined by the relation

$$\sigma_{ij} = \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij} \tag{2.7}$$

which derives from equation 2.6 by regarding isotropy of the material [2]. From this equation the elasticity tensor can be expressed by a simplified 6×6 matrix as in:

mention of einstein convention?

$$\underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{C}}}} \cdot \underline{\underline{\epsilon}} = \begin{pmatrix} \lambda+2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda+2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda+2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\mu \end{pmatrix} \cdot \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{pmatrix} \tag{2.8}$$

2.2 ELASTIC WAVES

This formalism can now be used to introduce elastic waves. Their existence and behaviour depends on the equations of motion of the regarded medium. To obtain these, we consider at first a small volume $\Delta V = \Delta x \Delta y \Delta z$, that is subject to a stress $\sigma_{xx}(x)$ on the one side and to $\sigma_{xx}(x + \Delta x)$ on the other side. The resulting net force becomes thus

$$\Delta F_x = [\sigma_{xx}(x + \Delta x) - \sigma_{xx}(x)] \Delta x \Delta y = \frac{\partial \sigma_{xx}}{\partial x} \Delta x \Delta y \Delta z \tag{2.9}$$

by approximating $\sigma_{xx}(x+\Delta x)$ in first order and setting the frame of reference to the center of mass of the volume. The force leads to a displacement u_x of the volume in x direction and equals the product of the mass $\rho\Delta x\Delta y\Delta z$ and acceleration in x direction $\frac{\partial^2 u_x}{\partial t^2}$. This yields the one dimensional partial differential equation

$$\rho\frac{\partial^2 u_x}{\partial t^2} = \frac{\partial \sigma_{xx}}{\partial x} \tag{2.10}$$

Assuming an isotropic material and using relation 2.6 we get

$$\rho\frac{\partial^2 u_x}{\partial t^2} = C_{11}\frac{\partial \epsilon_{xx}}{\partial x} = C_{11}\frac{\partial^2 u_x}{\partial x^2} \tag{2.11}$$

In an anisotropic medium the other stress components need to be taken into account leading to the general wave equation

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} = C_{ijkl}\frac{\partial^2 u_l}{\partial x_j \partial x_k} \tag{2.12}$$

2.2.1 *Solution for Isotropic Materials*

In the following analysis, only isotropic media will be considered. In this case the isotropic stress strain relation, equation 2.8, can be inserted to the wave equation which yields

$$\rho\frac{\partial^2 \underline{u}}{\partial t^2} = (\lambda+\mu)\,\underline{\nabla}(\underline{\nabla}\cdot\underline{u}) + \mu\,\underline{\nabla}^2\underline{u} \tag{2.13}$$

By using the relation $\nabla^2\underline{u} = \underline{\nabla}(\underline{\nabla}\cdot\underline{u}) - \underline{\nabla}\times(\underline{\nabla}\times\underline{u})$ for the vector laplace operator one can express it as

$$\rho\frac{\partial^2 \underline{u}}{\partial t^2} = (\lambda+2\mu)\,\underline{\nabla}(\underline{\nabla}\cdot\underline{u}) - \mu\,\underline{\nabla}\times(\underline{\nabla}\times\underline{u}) \tag{2.14}$$

If we now consider the Helmholtz decomposition of the displacement fields

$$\underline{u} = \underline{\nabla}\Phi + \underline{\nabla}\times\underline{\Psi} \tag{2.15}$$

with elastic potentials Φ and Ψ and insert it into 2.14, it decouples to the two equations (see [3])

$$\frac{\partial^2 \Phi}{\partial t^2} = c_L^2\,\underline{\nabla}^2\Phi \tag{2.16}$$

$$\frac{\partial^2 \underline{\Psi}}{\partial t^2} = c_T^2\,\underline{\nabla}^2\underline{\Psi} \tag{2.17}$$

$$\text{with } c_L = \left(\frac{\lambda+2\mu}{\rho}\right)^{1/2} \quad \text{and} \quad c_T = \left(\frac{\mu}{\rho}\right)^{1/2} \tag{2.18}$$

Those equations represent four wave equations for the elastic potentials with phase velocities c_L and c_T.

In analogy to electromagnetic waves we can now make the harmonic plane wave ansatz $\Phi(\underline{x},t) = u_L\, e^{i(\underline{k}_L\underline{x}-\omega t)}$ and $\underline{\Psi}(\underline{x},t) = \underline{u}_T\, e^{i(\underline{k}_T\underline{x}-\omega t)}$ with arbitrary amplitudes $u_L \in \mathbb{C}$ and $\underline{u}_T \in \mathbb{C}^3$. At this, the vector $\underline{k} = \frac{2\pi}{\lambda}$ denotes the wave vector defined over the wavelength λ and ω is the circular frequency defined over the oscillation frequency f with $\omega = 2\pi f$. The differentiation between $\underline{k}_L$ and $\underline{k}_T$ is necessary because of the different phase velocities for the elastic potentials resulting in different wave numbers according to $c = \frac{\omega}{|\underline{k}|}$.

Substituting the wave ansätze into equation 2.15, we get

$$\underline{u} = u_L\underline{k}\, e^{i(\underline{k}_L\underline{x}-\omega t)} + \underline{k} \times \underline{u}_T\, e^{i(\underline{k}_T\underline{x}-\omega t)} \tag{2.19}$$

Here we can see now, that the elastic potential Φ is responsible for waves with longitudinal polarisation and $\underline{\Psi}$ for waves with transversal propagation. Furthermore we can identify an orthonormal polarisation basis depending on the propagation direction $\hat{\underline{k}} = \frac{\underline{k}}{|\underline{k}|}$ so that $\underline{u}$ decomposes to

$$\underline{u} = a_L\, \underline{p}_L\, e^{i(\underline{k}_L\underline{x}-\omega t)} + (a_{TH}\, \underline{p}_{TH} + a_{TV}\, \underline{p}_{TV})\, e^{i(\underline{k}_T\underline{x}-\omega t)} \tag{2.20}$$

In general, the polarisation vector for longitudinal polarisation $\underline{p}_L$ is fixed to be $\vec{\underline{k}}$. If scattering at an interface is considered, a plane of incidence can be defined that is spanned by $\hat{\underline{k}}$ and the normal vector of the interface. The transversal polarisation vectors are then defined as transversal horizontal polarisation $\underline{p}_{TH}$ pointing out of the plane of incidence and transversal vertical polarisation lying in plane of incidence orthonormal to $\hat{\underline{k}}$.

The coefficients a_i may be complex to express an additional phase between the components. However, it should be noted, that this is merely convenient for calculation and that the physical wave behaves like the real part of the shown equations.

2.2.2 *Elastic Wave Scattering at an Interface*

Boundary Conditions

On the way to describe wave propagation through complex layer structures it is useful to consider a single interface first. In the upper half space S_1 and lower half space S_2 we assume homogeneous materials with different elastic constants and thus different sound velocities. At the interface, which is chosen to be the xy-plane the elastic properties are discontinuous. However, we can assume that

those layers connected strongly so that the displacement field and normal stresses are continuous at the boundary [4, pp. 182, 185]. This leads to the boundary conditions:

$$\underline{u}^{(1)}(\underline{r},t)|_{\underline{r}\in\partial S_1} = \underline{u}^{(2)}(\underline{r},t)|_{\underline{r}\in\partial S_2} \tag{2.21}$$

$$\sigma^{(1)}_{13}(\underline{r},t)|_{\underline{r}\in\partial S_1} = \sigma^{(2)}_{13}(\underline{r},t)|_{\underline{r}\in\partial S_2} \tag{2.22}$$

$$\sigma^{(1)}_{23}(\underline{r},t)|_{\underline{r}\in\partial S_1} = \sigma^{(2)}_{23}(\underline{r},t)|_{\underline{r}\in\partial S_2} \tag{2.23}$$

$$\sigma^{(1)}_{33}(\underline{r},t)|_{\underline{r}\in\partial S_1} = \sigma^{(2)}_{33}(\underline{r},t)|_{\underline{r}\in\partial S_2} \tag{2.24}$$

In these six equations displacement and stress from upper and lower medium are differentiated by the given superscript index.

Law of Refraction

If we now consider a plane wave that is incident on that interface, we can define a plane of incidence as in section 2.2.1 and rotate the coordinate system so that it equals the yz-plane. This is only valid if we assume an isotropic material as stated before. In that setting, the wave vector $\underline{k}_i$ for a particular mode $i \in \{L, TV, TH\}$ can be parametrised by the angle of incidence θ as

consistent mode description

$$\underline{k}_i = \frac{\omega}{c_i}(0,\ \sin(\theta_i),\ -\cos(\theta_i)\ )^T \tag{2.25}$$

The polarisation basis can then be defined as

$$\underline{p}_L = \hat{\underline{k}} = (0,\ \sin(\theta_i),\ -\cos(\theta_i)\ )^T \tag{2.26}$$

$$\underline{p}_{TH} = (\ 1,\ 0,\ 0)^T \tag{2.27}$$

$$\underline{p}_{TV} = \underline{p}_L \times \underline{p}_{TH} = (0,\ -\cos(\theta), -\sin(\theta))^T \tag{2.28}$$

It is now possible to extract a law of refraction from the boundary conditions in equation 2.21 (see [4, 168ff]). A simple approach is to consider scattering of the transversal horizontal mode (TH) so that the displacement is only in x-direction. An incoming plane wave with wave vector $\underline{k}_{in}$ is partially reflected to a wave along $\underline{k}_r$ and partially transmitted through the interface to a wave with $\underline{k}_t$. Also, different frequencies ω_i are assumed for the scattered waves so that the wave in the upper medium is

$$u^{(1)}_1 = a_{in}\ e^{i(k_{in}\sin\theta_{in}y - \omega_{in}t)} + a_r\ e^{i(k_r(\sin\theta_r y - \omega_r t)} \tag{2.29}$$

and in the lower medium

$$u^{(2)}_1 = a_t\ e^{i((k_t\sin\theta_t y - \omega_t t)} \tag{2.30}$$

Here it was used, that the interface is at $z = 0$ which simplifies the following derivation. According to the boundary conditions, these displacements must equal each other at any time and for all points on the interface. This leads to the immediate conclusion, that

$$\omega = \omega_{in} = \omega_r = \omega_t \tag{2.31}$$

After removing the common factor $e^{-i\omega t}$ from the equation and expressing the wave numbers by frequency and sound velocity over $k = \frac{\omega}{c}$, we get

$$a_{in}\ e^{i\frac{\omega}{c_{T,1}}\sin\theta_{in}y} + a_r\ e^{i\frac{\omega}{c_{T,1}}\sin\theta_r y} = a_t\ e^{i\frac{\omega}{c_{T,2}}\sin\theta_t y} \tag{2.32}$$

This however can be only fulfilled for all $y \in \mathbb{R}$, if the relations

$$a_{in} + a_r = a_t \tag{2.33}$$

$$\frac{\sin\theta_{in}}{c_{T,1}} = \frac{\sin\theta_r}{c_{T,1}} = \frac{\sin\theta_t}{c_{T,2}} \tag{2.34}$$

are met. Equation 2.34 can be also interpreted as the equality of the wave vector component parallel to the interface $k_y = \sin\theta_i \frac{\omega}{c_i}$.

The same procedure can be applied to the y and z component of the displacement field, where transversal vertical (TV) and longitudinal (L) modes need to be considered [4, p. 185]. However, one significant difference is that even for a single incident mode, both L and TV mode are possible after being reflected or transmitted. This will only add a term of the form $a_i\ e^{i\frac{\omega}{c}\sin\theta_i y}$ to each side of equation 2.32, but will result in analogous relations to 2.31 and 2.34, namely the invariance of frequency ω and k_2 of each mode under scattering at the interface.

To conclude, the angle θ_{out} of any outgoing polarisation mode can be determined from the incoming wave's angle θ_{in} and the sound velocities for incoming and outgoing wave c_{in}, c_{out} by

$$\frac{\sin\theta_{in}}{c_{in}} = \frac{\sin\theta_{out}}{c_{out}} \tag{2.35}$$

This can be transferred to the optical law of snellius by introducing an effective refraction index $n_i = \frac{1}{c_i}$. Consequently, TH-polarised waves scatter like electromagnetic waves and for example the reflected angle is always the incident angle. The main difference to optics becomes clear for L and TV polarised waves. Scattering within the same polarisation mode is the same as for the TH mode, but now those modes can scatter into each other. Equation 2.35 still applies, but energy is also emitted to additional modes as shown in figure 2.1.

It is also possible to get the analytical solutions for refraction of a single mode at an interface by evaluating the remaining boundary conditions and the results

from continuity of displacement. The results are usually expressed by defining a reflection coefficient r_i and a transmission coefficient t_i for participating mode $i \in \{L, TH, TV\}$ as

$$r_i := \frac{a_{r,i}}{a_{in,i}} \tag{2.36}$$

$$t_i := \frac{a_{t,i}}{a_{in,i}} \tag{2.37}$$

Usually those coefficients have a functional dependency on the incident angle.

Total Internal Reflection

Total internal reflection is known as the phenomenon, when a wave is totally reflected at a boundary for incident angles greater than a critical angle θ_{tot}. If c_1 and c_2 are the phase velocities first and second medium, the outgoing angle

$$\theta_2 = \arcsin\left(\frac{c_1}{c_2}\sin(\theta_1)\right) \quad c_2 < c_1 \tag{2.38}$$

has no real solution for $\theta_1 > \theta_{tot} = \arcsin\frac{c_2}{c_1}$. There is however a complex solution and this resulting complex angle can be interpreted in the given wave formalism [5, p. 5]. This interpretation also allows to extend the concept to two arbitrary polarisation modes that the wave can scatter inbetween, regardless of propagation direction.

Considering the case $\theta_1 > \theta_{tot}$, θ_2 takes the shape of $\theta_2 = \frac{\pi}{2} + i\alpha,\ \alpha \in \mathbb{R}$. Inserting this into the general wave solution equation 2.20, we need to calculate the wave vector $\underline{k}$ as in equation 2.25. This results in

$$k_y = k\sin\theta_2 = k\cosh\alpha \qquad k_z = k\cos\theta = ik\sinh\alpha \tag{2.39}$$

This complex wave vector inserted into the factor $e^{ik_z z}$ results in $e^{-k\sinh\alpha z}$ which represents an evanescent wave. This type of wave is attenuated exponentially so that the wave behaves as expected.

In case of Frustrated total internal reflection this exponential behaviour becomes relevant, when another interface is close to the first reflecting interface. Then it is possible for the usually totally reflected mode to transmit intensity into a mode of the third medium.

Conservation of Energy at a Single Interface

According to [4, p. 166] the transmitted time averaged power per unit area of a transversal elastic wave in a homogeneous medium is

$$I_L = \frac{1}{2}(\lambda + 2\mu)\frac{\omega^2}{c_L}|a_L|^2 \tag{2.40}$$

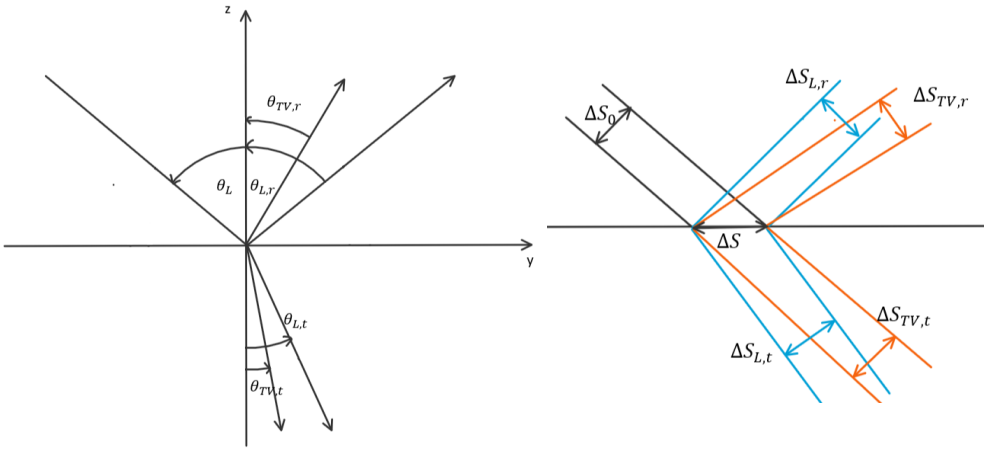
and similarly for a transversal elastic wave of a single polarisation mode

$$I_T = \frac{1}{2}\mu\frac{\omega^2}{c_T}|a_T|^2 \tag{2.41}$$

where a_T is either a_{TV} or a_{TH} depending on the regarded mode. This quantity is also known as time averaged intensity. By using the definition of c_L and c_T from equation 2.18 we get the more general relation

$$I_p = \frac{\rho\omega^2}{2}|a_p|^2 c_p \tag{2.42}$$

with $p \in \{L, TH, TV\}$ denoting the polarisation mode. It should be noted that the referred unit area is perpendicular to the direction of propagation.



(a) Refraction of a Longitudinal Elastic Wave

(b) Conservation of Energy at Surface Element ΔS for an TV polarized beam

Figure 2.1

In the setting of an arbitrary polarised wave scattered at an interface, there are six possible outgoing modes as discussed previously. To get an energy relation

between the intensities of each participating mode we consider the energy balance of a surface element ΔS of the interface, on which an arbitrary polarised beam with cross-sectional area ΔS_0 and intensity I_{in} is incident. The cross-sectional areas of the outgoing beams are named according to figure 2.1b which can be also transferred to the case of an incident TH polarised wave.

The power each beam transmits or emits is given by the product $P_p = I_p\ \Delta S_p$. ΔS_p is related to ΔS by $\Delta S_p = \cos\theta_p\ \Delta S$, p denoting any of the depicted beams and $theta_p$ being the according angle.

In conclusion, the energy balance results in

$$I_{in}\cos\theta_{in} = \sum_{i=L,TH,TV} I_{i,r}\ \cos\theta_{i,r} + I_{i,t}\ \cos\theta_{i,t} \tag{2.43}$$

From that we can define reflectivity $\mathscr{R}$ and transmittivity $\mathscr{T}$ of the interface as fraction of reflected and transmitted power by

$$\mathscr{R} := \frac{I_{L,r}\ \cos\theta_{L,r} + I_{TH,r}\cos\theta_{T,r} + I_{TV,r}\cos\theta_{T,r}}{I_{in}\cos\theta_{in}} \tag{2.44}$$

$$\mathscr{T} := \frac{I_{L,t}\ \cos\theta_{L,t} + I_{TH,t}\cos\theta_{T,t} + I_{TV,t}\cos\theta_{T,t}}{I_{in}\cos\theta_{in}} \tag{2.45}$$

$$\tag{2.46}$$

so that $\mathscr{R} + \mathscr{T} = 1$ is fulfilled. This can be later used to verify the obtained results.

2.2.3 *Scattering at a System of Layers*

The considerations of one interface can now be extended to a system of N interfaces as shown in figure 2.2. Each layer gets an index n starting from the uppermost layer of index $n = 0$. The first interface from the top is still located at $z_1 = 0$ and has index $n = 1$. The subsequent interfaces follow below at depths z_n. Their depth depends on the intermediate layer thicknesses $d_n = z_n - z_{n+1}$ with layer index n. Similar as before, we assume now the displacement field in each layer n as

$$\underline{u}^{(n)}(\underline{x},t) = \sum_{i\in\{L,TH,TV\}} t_{n,i}\underline{p}^{t}_{n,i}\ e^{i(\underline{k}^{t}_{n,i}\underline{x}-\omega t)} + r_{n,i}\underline{p}^{r}_{n,i}\ e^{i(\underline{k}^{r}_{n,i}\underline{x}-\omega t)} \tag{2.47}$$

This formula is a superposition of a down going wave with quantities denoted by t and a upgoing wave caused by reflections with quantities denoted by r. The upgoing $\underline{k}^r$ is flipped in z-direction compared to $\underline{k}^t$. Further, the complex amplitudes of down and upgoing modes are directly denoted by $t_{n,i}$ and $r_{n,i}$. As the angle $\theta_{n,i}$ between $\underline{k}$ and z-axis is changes by scattering, also $\underline{k}_{n,i}$ and polarisation vector $\underline{p}_{n,i}$ is different for each material.

To evaluate the transmission through the stack of layers, it is now the task to calculate the coefficients $t_{N,i}$ and $r_{1,i}$ under given coefficients $t_{1,i}$ and with the assumption $r_{N,i} = 0$ for all $i \in \{L, TH, TV\}$. We further choose exactly one $t_{1,i} = 1$ to mark the incident mode. This simplifies solving the problem and lets the coefficients $t_{N,i}$ and $r_{1,i}$ become the transmission and reflection coefficients of the layer system.

For this, all $6N$ boundary conditions need to be solved. These are constructed by inserting the general displacement field of each participating layer as in equation 2.47 in the boundary conditions for a single interface (equation 2.21). As a result each displacement field of an enclosed layer is evaluated twice, once at the upper boundary and once at the lower boundary. This results in a phase shift of $e^{-ik_z d_n}$ between upper and lower displacement.

As many systems of equations this problem can be formulated with matrices. In the following, two similar solution methods are introduced.

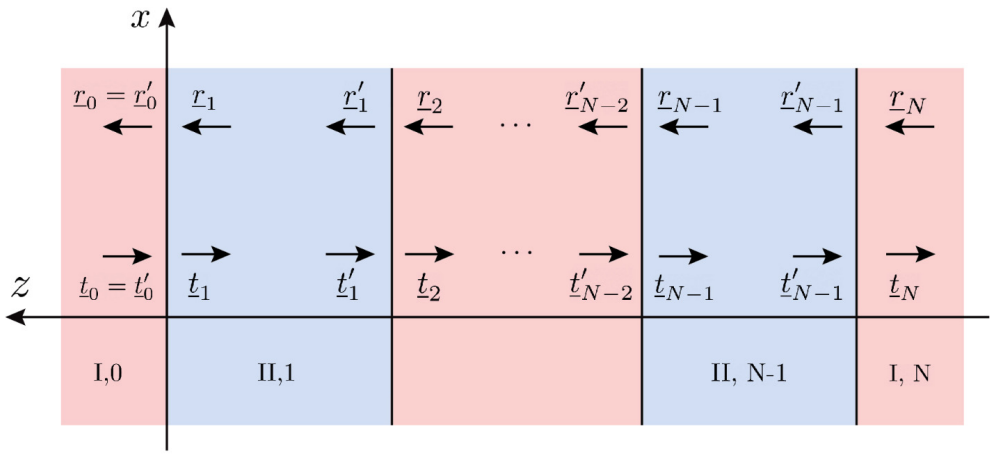


Figure 2.2: Geometry and amplitude nomenclature of a N layer strong bragg reflector

Transfer Matrix Method

To introduce the matrix formalism it is useful to focus on a single interface with index n between layers $n-1$ and n located at depth z_n. We can define a generalised state vector $\underline{v}_i$ in each layer i as [6]

$$\underline{v}_i = (u_1^{(i)}, u_2^{(i)}, u_3^{(i)}, \sigma_{13}^{(i)}, \sigma_{23}^{(i)}, \sigma_{33}^{(i)})^T \tag{2.48}$$

Each of the components depends on location $\underline{x}$ and time t in the layer. We also introduce the superscript "+" for evaluating an arbitrary multidimensional function

of space and layer index n at interface $\mathscr{F}_n$ and superscript "-" for evaluating at $\mathscr{F}_{n-1}$ so that the boundary conditions at the n-th interface $\mathscr{F}_n$ are

$$\underline{v}_n^+ = \underline{v}_{n+1}^- \tag{2.49}$$

In addition to equation 2.47 the stress components in $\underline{v}$ can be evaluated as well. From stress strain relation 2.6 we get for an isotropic material

$$C_{1313}^{(n)} \epsilon_{13}^{(n),+} = C_{1313}^{(n+1)} \epsilon_{13}^{(n+1),-} \tag{2.50}$$

$$C_{2323}^{(n)} \epsilon_{23}^{(n),+} = C_{2323}^{(n+1)} \epsilon_{23}^{(n+1),-} \tag{2.51}$$

$$\sum_{i=1}^{3} C_{33ii}^{(n)} \epsilon_{ii}^{(n),+} = \sum_{i=1}^{3} C_{33ii}^{(n+1)} \epsilon_{ii}^{(n+1),+} \tag{2.52}$$

mention, that propagation of angles is needed first

Furthermore, the strain can be evaluated by inserting the general displacement field 2.47 into its definition $\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right)$.

At this point it is neccessary to know all angles at which the different modes propagate through each layer in order to construct the equations as linear relations. These can be obtained by following the considerations of section **??** Because of our limitation to one incident mode on the top layer, also only one propagation angle per distinct phase velocity in the medium is possible. From the structure of $\underline{u}^{(n)}$ it is possible to construct a 6×6 matrix M_n so that

$$\underline{v}_n(z) = \underline{\underline{M}}_n \, \underline{\underline{P}}_n(z - z_n) \underline{a}_n \tag{2.53}$$

The coefficient vector $\underline{a}_n$ of layer n is defined as

$$\underline{a}_n = (\underline{t}_n, \underline{r}_n)^T = (t_{n,L}, t_{n,TH}, t_{n,TV}, r_{n,L}, r_{n,TH}, r_{n,TV})^T \tag{2.54}$$

containing the wave amplitudes at the upper edge of each layer $z = z_n$. As an exeption, $r_{0,i}$ and $t_{0,i}$ are defined directly at the first interface.

$\underline{\underline{P}}_n(z)$ represents the phase factors due to wave propagation as diagonal matrix

$$\underline{\underline{P}}_n(z) = diag\{e^{ik_{z,n}^{(L)} z}, e^{ik_{z,n}^{(TH)} z}, e^{ik_{z,n}^{(TV)} z}, e^{-ik_{z,n}^{(L)} z}, e^{-ik_{z,n}^{(TH)} z}, e^{-ik_{z,n}^{(TV)} z}\} \tag{2.55}$$

The addend $k_{y,n} y$ was removed from the expression as it does not change at the boundary. This automatically sets the phase of the displacement wave to zero at the upper boundary of the layer. The coefficients at the lower boundary are in the following denoted by $\underline{a}'_n = \underline{\underline{P}}_n(-d_n) \, \underline{a}_n$.

As a result the boundary conditions at an individual interface between layers $n-1$ and n can be written as

$$\underline{\underline{M}}_{n-1}\,\underline{a}'_{n-1} = \underline{\underline{M}}_{n}\,\underline{a}_{n} \tag{2.56}$$

If we assume that $\underline{\underline{M}}_n$ is invertable, we can define the Transfermatrix S_n by

$$\underline{a}_n = \underline{\underline{M}}_n^{-1}\,\underline{\underline{M}}_{n-1}\underline{a}'_{n-1} = \underline{\underline{S}}_n\underline{a}'_n \tag{2.57}$$

which enables us to obtain the wave coefficients after scattering by a simple matrix multiplication.

With this knowledge we can assemble a global transfermatrix for all interfaces by

$$\underline{\underline{S}} = \underline{\underline{S}}_N \cdot \underline{\underline{P}}_N(z_N - z_{N-1}) \cdot \underline{\underline{S}}_{N-1} \cdot \underline{\underline{P}}_{N-1}(z_{N-1} - z_{N-2}) \cdots \underline{\underline{S}}_2 \cdot \underline{\underline{P}}_2(z_2 - z_1) \cdot \underline{\underline{S}}_1 \tag{2.58}$$

so that the final wave coefficients $\underline{a}_N$ below the lowest interface are

$$\begin{pmatrix} \underline{t}_n \\ \underline{r}_n \end{pmatrix} = S \cdot \begin{pmatrix} \underline{t}_1 \\ \underline{r}_1 \end{pmatrix} = \begin{pmatrix} \underline{\underline{T}} & \underline{\underline{C}}_1 \\ \underline{\underline{C}}_2 & \underline{\underline{R}} \end{pmatrix} \cdot \begin{pmatrix} \underline{t}_1 \\ \underline{r}_1 \end{pmatrix} \tag{2.59}$$

Remembering that $\underline{r}_n = 0$, we can solve for $\underline{r}_1$ and $\underline{t}_n$

$$\underline{r}_1 = -\underline{\underline{R}}^{-1}\,\underline{\underline{C}}_2\,\underline{t}_1 \tag{2.60}$$

$$\underline{t}_n = \left(\underline{\underline{T}},\ \ \underline{\underline{C}}_1\right) \cdot \begin{pmatrix} \underline{t}_1 \\ -\underline{\underline{R}}^{-1}\underline{\underline{C}}_2\,\underline{t}_1 \end{pmatrix} \tag{2.61}$$

Linear System of Equations

As an alternative, a more direct solving approach is presented by solving the system of linear equations with the inversion of a single matrix. This method will be called from now on LSE-method (Linear System of Equations). Its advantages and disadvantages will be discussed later.

For this method the coefficients for upgoing waves are defined to have their phase origin at the lower interface instead of the upper interface as defined in 2.55, so that the P-matrix becomes

$$\underline{\underline{P}}_n(z) = diag\{e^{ik_{z,n}^{(L)}z}, e^{ik_{z,n}^{(TH)}z}, e^{ik_{z,n}^{(TV)}z}, e^{-ik_{z,n}^{(L)}(z+d_n)}, e^{-ik_{z,n}^{(TH)}(z+d_n)}, e^{-ik_{z,n}^{(TV)}(z+d_n)}\} \tag{2.62}$$

For better clarity in notation we can rewrite matrix $\underline{\underline{M}}_n$ as composition of two 6×3 matrices $\underline{\underline{M}}_n = (\underline{\underline{T}}_n, \underline{\underline{R}}_n)$ and $\underline{\underline{P}}_n$ as block diagonal of two 3×3 matrices $\underline{\underline{P}}_n =$

$diag\{\underline{\underline{D}}_n(z), \underline{\underline{D}}_n(-(z+d_n))\}$. The boundary conditions at interface n, below layer n are then

$$\left(\underline{\underline{T}}_n, \underline{\underline{R}}_n \cdot \underline{\underline{D}}_n(-d_n)\right)\begin{pmatrix}\underline{t}_n\\ \underline{r}_n\end{pmatrix} = \left(\underline{\underline{T}}_{n-1} \cdot \underline{\underline{D}}_{n-1}(-d_{n-1}), \underline{\underline{R}}_{n-1}\right)\begin{pmatrix}\underline{t}_{n-1}\\ \underline{r}_{n-1}\end{pmatrix} \tag{2.63}$$

With $\underline{\underline{T}}'_{n-1} = \underline{\underline{T}}_{n-1} \cdot \underline{\underline{D}}_{n-1}(-d_{n-1})$ and analogously for $\underline{\underline{R}}'_n$, this is equivalent to

$$\left(\underline{\underline{T}}'_{n-1}, \underline{\underline{R}}_{n-1} - \underline{\underline{T}}_n, -\underline{\underline{R}}'_n,\right)\begin{pmatrix}\underline{t}_{n-1}\\ \underline{r}_{n-1}\\ \underline{t}_n\\ \underline{r}_n\end{pmatrix} = 0 \tag{2.64}$$

This denotes now a 6×12 matrix for a single interface. In general the total system is constructed as $6N \times 6N$ matrix

$$\begin{pmatrix}
\underline{\underline{R}}_0 & -\underline{\underline{T}}_1 & -\underline{\underline{R}}'_1 & 0 & 0 & \cdots & 0\\
0 & \underline{\underline{T}}'_1 & \underline{\underline{R}}_1 & \underline{\underline{T}}_2 & \underline{\underline{R}}'_2 & \cdots & \vdots\\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots\\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots\\
0 & \cdots & \cdots & 0 & \underline{\underline{T}}'_{N-1} & \underline{\underline{R}}_{N-1} & \underline{\underline{T}}_N
\end{pmatrix}\begin{pmatrix}\underline{r}_0\\ \underline{t}_1\\ \underline{r}_1\\ \vdots\\ \underline{t}_N\end{pmatrix} = \begin{pmatrix}-\underline{\underline{T}}_0\ \underline{t}_0\\ 0\\ \vdots\\ \vdots\\ \underline{\underline{R}}_N\ \underline{r}_N\end{pmatrix} \tag{2.65}$$

to be able to invert it. By setting $\underline{r}_N = 0$ as before we obtain $\underline{r}_0$ and $\underline{t}_N$ after inverting the 16×16 matrix.

3

IMPLEMENTATION

4

ANALYSIS

5

CONCLUSION

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