

PHONONIC BRAGG REFLECTORS FOR THERMAL ISOLATION OF SEMICONDUCTOR QUBITS

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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

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 [2], if not otherwise stated.

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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

$$\text{Stress} \quad \sigma := \frac{F}{A} \quad \text{Strain} \quad \epsilon := \frac{\Delta l}{l} \quad (2.1)$$

Hooke's law can now be reformulated as

$$\sigma = C \epsilon \quad (2.2)$$

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

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

whereas indices i and j 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

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

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

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

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

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:

$$\sigma_{ij} = C_{ijkl} \epsilon_{kl} \quad \text{or} \quad \underline{\underline{\sigma}} = \underline{\underline{C}} \cdot \underline{\underline{\epsilon}} \quad (2.6)$$

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

picture of stress definition?

reference to lecture 2?

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

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

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 [2]) 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

$$\sigma_{ij} = \lambda \delta_{ij} \epsilon_{kk} + 2\mu \epsilon_{ij} \quad (2.7)$$

which derives from equation 2.6 by regarding isotropy of the material [3]. From this equation the elasticity tensor can be expressed by a simplified 6×6 matrix as in:

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

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

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

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

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

Assuming an isotropic material and using relation 2.6 we get

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

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

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

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

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

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

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

If we now consider the Helmholtz decomposition of the displacement fields

$$\underline{u} = \underline{\nabla} \Phi + \underline{\nabla} \times \underline{\Psi} \quad (2.15)$$

with elastic potentials Φ and Ψ and insert it into 2.14, it decouples to the two equations (see [4])

$$\frac{\partial^2 \Phi}{\partial t^2} = \alpha^2 \underline{\nabla}^2 \Phi \quad (2.16)$$

$$\frac{\partial^2 \underline{\Psi}}{\partial t^2} = \beta^2 \underline{\nabla}^2 \underline{\Psi} \quad (2.17)$$

with $\alpha = \left(\frac{\lambda+2\mu}{\rho}\right)^{1/2}$ and $\beta = \left(\frac{\mu}{\rho}\right)^{1/2}$. Those equations represent four wave equations for the elastic potentials with phase velocities α and β .

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 $\Psi(\underline{x}, t) = \underline{u}_T e^{i(\underline{k}_T \underline{x} - \omega t)}$ 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

$$\underline{u} = u_L \underline{k} e^{i(\underline{k}_L \underline{x} - \omega t)} + \underline{k} \times \underline{u}_T e^{i(\underline{k}_T \underline{x} - \omega t)} \quad (2.18)$$

Here we can see now, that the elastic potential Φ is responsible for waves with longitudinal polarisation and Ψ 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

$$\underline{u} = a_L \underline{p}_L e^{i(\underline{k}_L \underline{x} - \omega t)} + (a_{TH} \underline{p}_{TH} + a_{TV} \underline{p}_{TV}) e^{i(\underline{k}_T \underline{x} - \omega t)} \quad (2.19)$$

In gernerel, the polarisation vector for longitudinal polarisation \underline{p}_L is fixed to be $\hat{\underline{k}}$. 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. This leads to the boundary conditions:

lookup citation from [1]

$$\underline{u}^{(1)}(\underline{r}, t)|_{\underline{r} \in \partial S_1} = \underline{u}^{(2)}(\underline{r}, t)|_{\underline{r} \in \partial S_2} \quad (2.20)$$

$$\sigma_{13}^{(1)}(\underline{r}, t)|_{\underline{r} \in \partial S_1} = \sigma_{13}^{(2)}(\underline{r}, t)|_{\underline{r} \in \partial S_2} \quad (2.21)$$

$$\sigma_{23}^{(1)}(\underline{r}, t)|_{\underline{r} \in \partial S_1} = \sigma_{23}^{(2)}(\underline{r}, t)|_{\underline{r} \in \partial S_2} \quad (2.22)$$

$$\sigma_{33}^{(1)}(\underline{r}, t)|_{\underline{r} \in \partial S_1} = \sigma_{33}^{(2)}(\underline{r}, t)|_{\underline{r} \in \partial S_2} \quad (2.23)$$

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 wavevector \underline{k}_i for a particular mode $i \in \{L, TV, TH\}$ can be parametrised by the angle of incidence θ as

$$\underline{k}_i = \frac{\omega}{c_i} (0, \sin(\theta_i), -\cos(\theta_i))^T \quad (2.24)$$

The polarisation basis can then be defined as

$$\underline{p}_L = \hat{\underline{k}} = (0, \sin(\theta_i), -\cos(\theta_i))^T \quad (2.25)$$

$$\underline{p}_{TH} = (1, 0, 0)^T \quad (2.26)$$

$$\underline{p}_{TV} = \underline{p}_L \times \underline{p}_{TH} = (0, -\cos(\theta), -\sin(\theta))^T \quad (2.27)$$

It is now possible to extract a law of refraction from the boundary conditions in equation 2.20 (see [5], pp.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

$$u_1^{(1)} = a_{in} e^{i(k_{in} \sin \theta_{in} y - \omega_{in} t)} + a_r e^{i(k_r (\sin \theta_r y - \omega_r t))} \quad (2.28)$$

and in the lower medium

$$u_1^{(2)} = a_t e^{i(k_t \sin \theta_t y - \omega_t t)} \quad (2.29)$$

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

$$\omega = \omega_{in} = \omega_r = \omega_t \quad (2.30)$$

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

$$a_{in} e^{i \frac{\omega}{c_{T,1}} \sin \theta_{in} y} + a_r e^{i \frac{\omega}{c_{T,1}} \sin \theta_r y} = a_t e^{i \frac{\omega}{c_{T,2}} \sin \theta_t y} \quad (2.31)$$

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

$$a_{in} + a_r = a_t \quad (2.32)$$

$$\frac{\sin \theta_{in}}{c_{T,1}} = \frac{\sin \theta_r}{c_{T,1}} = \frac{\sin \theta_t}{c_{T,2}} \quad (2.33)$$

are correct. Equation 2.33 can be also interpreted as the equality of the component parallel to the interface of wave vector $k_y = \sin \theta_i \frac{\omega}{c_i}$.

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. 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 an additional addend of the form $a_i e^{i \frac{\omega}{c} \sin \theta_i y}$ to each side of equation 2.31, but will result in analogous relations to 2.30 and ??, namely the invariance of frequency ω and k_2 of each mode under scattering at the interface.

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.

2.2.3 Solving Methods for Stratified Media

Transfer Matrix Method

Linear System of Equations

IMPLEMENTATION

ANALYSIS

CONCLUSION

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