PERIODIC ORBIT THEORY APPLIED TO ACOUSTICS

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Introduction

About 25 years ago an interesting connection was found by Gutzwiller between the classical orbits of a system and the semi-classical spectrum of the corresponding Schrödinger operator. Gutzwiller managed to express the spectral density as a sum over periodic orbits. Gutzwiller's ideas have been refined and developed into a branch of physics called quantum chaos (for an introduction see ref. [27] and his book ref. [15]). For instance it is now possible to make a relatively good estimate of the energy levels of the helium atom by using just the classical periodic orbits. A few years ago it was shown by Gabor Vattay ref. [33] how to derive results similar to Gutzwiller without employing the so-called path-integrals (used by the latter). Basically it consisted in 3 steps: First go to the classical limit, ie. perform the WKB-expansion (cf. chapter 2) of the Schrödinger equation, second construct a suitable evolution operator, and finally take its trace. Step 1 was derived a long time ago whereas step 2 and 3 are the main achievement. The trace so derived does contain the Gutzwiller spectrum, but, unfortunately, it turns out that the corresponding spectrum is not the best possible, since it in e.g. for the 3-disc system (sect. 1.3) also includes non-quantum mechanical eigenvalues.

The purpose of this thesis is to show the same for acoustics as in ref. [33] in quantum mechanics. Thus we will somehow try to find a "classical" limit, construct an appropriate evolution operator, whose trace relates the sound spectrum to classical periodic orbits. In this thesis we shall investigate the so-called crystal acoustics, where one considers the interior vibrations of materials like quartz, sapphire, and aluminium. Crystals are known as very good resonators used in clocks and even gravity wave detectors! But this also means that they are excellent for testing the above ideas of the relationship between the frequencies and periodic orbits of a system. However, the wave equation for crystal acoustics is different from the scalar Schrödinger equation since it is vectorial and does not contain a small parameter like Planck's constant $\hbar$. It turns out that the above acoustic "classical" limit gives the desired results when one uses the high-frequency limit. The first step, the WKB-expansion, ends up being very similar to the quantum case and the derivations of the second step (the evolution operator) and the third step (taking the trace) are very general so we find for crystal acoustics almost the same formulas as in the semi-classical quantum mechanics of Vattay.

The main new result of this thesis not available in the literature (to the best knowledge of the author) is an isotropic acoustic determinant formula ((5.56)):

$$\det(1-\mathcal{L}) = \exp\left(-\sum_{p,r}\frac{s_p^r\sqrt{f_p^r}}{r|\Lambda_p^r|}\frac{e^{(i\omega T_p - i m_p\pi/2)r}}{(1-1/\Lambda_p^r)^2}\Delta_{p,r}\right)$$

where

$$\Delta_{p,r} = \frac{|\Lambda_p^r|^{1/2}+|\Lambda_p^r|^{-5/2}}{1-1/\Lambda_p^{2r}}.$$

Here $|\Lambda_p|$ is the product of all the expanding eigenvalues of the orbit, T_p is the flightime, m_p its Maslov phase and f_p (resp. s_p) is square root of the product of

all energy flux (resp. of the sign of all the amplitude ratios) ratios for every hit at the boundary. We remark that this determinant of Vattay contains extraneous zeroes, which one still not has procedure of excluding. But it leads to a Gutzwiller spectrum described by a zeta function

$$\frac{1}{\zeta} = \prod_p (1 - t_p)$$

with orbit weight

$$t_p = s_p \sqrt{f_p} \frac{e^{i\omega T_p - i m_p \pi/2}}{\sqrt{|\Lambda_p|}}.$$

in accordance with the results already derived by ref. [26] using different methods.

The thesis is organised as follows: First a review of periodic orbit theory with the main results together with the main results of ref. [33]. Second, an introduction to acoustics and the corresponding WKB-expansion. Third, some numerical predictions of the above theory applied to the 3-disc system in an isotropic acoustic medium. The escape rate (classical) and the leading scattering resonances (quantum mechanics, acoustics) are calculated by means of periodic orbits.

Chapter 1

Periodic orbit theory

Here follows a quick tour of the periodic orbit theory as described in refs. [3, 4, 7, 8, 9, 10, 32]. This theory was initiated by Ruelle [28]. We shall construct suitable evolution operators for a dynamical system and relate their traces to the periodic orbits in the corresponding flow. This statement that the periodic orbits should influence on these evolution operators might sound innocent but it is not. In chaotic systems there are infinitely many orbits and figuring out how the various orbits contribute is not a trvial task.

1.1 Flows and "wave" splitting

This section describes what happens when we evolve densities in a dynamical system. We also wish to include wave splitting.

The mental picture one should consider is the following. We think of a swarm of particles each of the same "type". With "type" we mean particles with a give polarisation, spin etc. in physical applications. The free flight evolution of such a swarm is classically described by an evolution operator acting on densities when one goes to the continuum limit. We start describing the free flight. Each particle is following the trajectory of a dynamical system:

$$\dot{\vec{x}} = \vec{F}(x). \tag{1.1}$$

Here the vector field $\vec{F}(x)$ gives rise to a one parameter group f^t acting on points:

$$\vec{x}(t) = f^t(\vec{x}) \tag{1.2}$$

fulfilling the semi group property

$$f^{s+t} = f^t \circ f^s. \tag{1.3}$$

Since the particle number is conserved we find in the continuum limit an equation of continuity:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho\, \vec{v}) = 0, \tag{1.4}$$

here the density distribution of the particles is called ρ and $\vec{v} = \dot{\vec{x}} = \vec{F}(x)$.

1.1.1 The Liouville formula

The Liouville formula (ref. [24]) is very important when one wants to solve so-called transport equations, like the continuity equation. Suppose we have a dynamical system

$$\frac{d\vec{x}}{dt} = \vec{F}(\vec{x}). \tag{1.5}$$

For a given $\vec{x}_0$ we can find a solution $\vec{x}(t)$ such that $\vec{x}(0) = \vec{x}_0$.

Now how does the volume around $\vec{x}$ change as we move with the flow? For this we introduce the Jacobian

$$j^t(\vec{x}_0) = \mathrm{Det}\left(\frac{\partial \vec{x}(t)}{\partial \vec{x}_0}\right) = \frac{dx_1(t) \wedge ... \wedge dx_n(t)}{dx_1 \wedge ... \wedge dx_n} \tag{1.6}$$

ie. the ratio of the final volume element to the initial volume element. Calculating in the exterior calculus cf. ref. [5]

$$\frac{d}{dt}\left(dx_1(t) \wedge ... \wedge dx_n(t)\right) = dF_1(x(t)) \wedge dx_2(t) \wedge ... \wedge dx_n(t) + ... + dx_1(t) \wedge ... \wedge dF_n(x(t))$$

$$= (\vec{\nabla} \cdot \vec{F}(x(t)))dx_1(t) \wedge ... \wedge dx_n(t)$$

and using that

$$dx_1(t) \wedge ... \wedge dx_n(t) = j^t(x)\, dx_1 \wedge ... \wedge dx_n$$

with the initial point $\vec{x}$ independent of t we find Liouville's result

$$\frac{d(\ln(j))}{dt} = \vec{\nabla} \cdot \vec{F}(\vec{x}). \tag{1.7}$$

1.1.2 Evolution operator for densities

Given an initial distribution $\rho_0(x)$ one can find the distribution of particles $\rho_t(x)$ at a later time t by means of the integral kernel

$$\mathcal{L}^t(y, x) = \delta(y - f^t(x)). \tag{1.8}$$

Indeed

$$\rho_t(x) = \int dy\ \mathcal{L}^t(x, y)\rho_0(y) \tag{1.9}$$

and this operator also fulfils the semi group property:

$$\mathcal{L}^{s+t} = \mathcal{L}^s \circ \mathcal{L}^t. \tag{1.10}$$

Now from a statistical point of view one should focus at the density evolution rather than at the individual particles. Therefore the eigenvalues of $\mathcal{L}^t$ are of interest. Because of the semi group property these eigenvalues necessarily have the form $e^{-\lambda t}$. One finds that the leading eigenvalue contains information about the escape rate and the next leading the decay of correlations.

We now assume that the swarm of particles is moving in some billiard and eventually at a certain time collides with the boundary. We impose a probabilistic rule that tells us with what probability a particle of a given type will bounce in a new direction and change its type. Instead of a precise formal definition let us just consider an example from acoustics in 2 dimensions: There are two kinds of particles: P (pressure) and S (shear) each moving with its own velocity. A particle can either reflect (P$\rightarrow$ P or S $\rightarrow$ S) or refract (P $\rightarrow$ S or S $\rightarrow$ P) following the law of reflection respectively Snell's law of refraction ((4.41)). The probabilities are chosen to correspond to the conservation of energy flux in the direction normal to the boundary. Thus for example the probability of going from an S particle to a P particle is given as the ratio of the outgoing P energy flux to the incoming S energy flux. In the continuum limit we will see that our swarm of particles will split into 2 smaller swarms when it hits the boundary. For a sufficiently localised incoming wave packet, a $\delta-$function, the height diminishes with the probabilities, ie. the above mentioned energy flux ratio factors. It is now possible to write an integral kernel describing this evolution. Let us denote the type of density with a_i and the reflection and the flight is denoted with an $R_{a_{i+1}a_i}$ respectively F_{a_i}. We find in the case of n bounces

$$\mathcal{L}^t_{a_n a_1} = \sum_{a_{n-1},\ldots,a_2} F^{t_n}_{a_n} \circ R_{a_n a_{n-1}} \circ \ldots \circ R_{a_2 a_1} \circ F^{t_1}_{a_1}, \tag{1.11}$$

where we sum over intermediate types and the intermediate flight times sum up to the total $t = t_1 + \ldots + t_n$. The reflection operators are just the probabilities of conversion from one type to another [1] and the flight operators are the above free flight integral kernel. By construction also the operator (1.11) is multiplicative (a semi group) so again the eigenvalues are of the form $e^{-\lambda t}$. We shall see what to do with these multiplicative operators.

1.2 Evolution operators, traces and determinants

In this section we take our point of departure in integral kernels basically of the form

$$\mathcal{L}^t_{\beta\alpha}(y,x) = \delta(y - f^t(x)) g^t_{\beta\alpha}(x). \tag{1.12}$$

Here the delta-function kernel is multiplicative since it is assumed that the flow function f^t is a one parameter group. The $g^t_{\beta\alpha}(x)$ is any multiplicative weight along the trajectory, and the indices refer to possible extra matrix structure:

$$\mathbf{g} = (g_{\beta\alpha}). \tag{1.13}$$

[1] For dimensions higher than 2 the reflection operators do not have to have the same reflection planes. If one uses a clever set of coordinates like parametrising with respect to the principal axes one will in general gain a reduction in coordinates describing the system. For instance in 3-d it suffices to use a total of 4 coordinates to parametrise phase space. However when we change from one reflection plane to the proceeding we have to use a rotation in order to relate the in general different tangent spaces. Since we only consider 2 dimensions in this thesis we will not consider this further (see Andreas Wirzba's "Non-paper about 3-d billiard Jacobians" in ref. [8]), who pointed this out to me.

What we want to find is the spectrum of such operators.

Basically all calculations start by evaluating the trace:

$$\mathrm{tr}\,(\mathcal{L}^t) = \sum_\alpha \int dx \mathcal{L}^t_{\alpha\alpha}(x,x). \tag{1.14}$$

For non-zero times this trace exactly gets a contribution from every periodic orbit. This sum over periodic orbits can be written as a sum over all primitive periodic orbits (prime orbits) and their repetitions. The trace is evaluated by integrating along the points on a periodic orbit. One therefore splits the integration into two: one along, $x_{||}$, and one orthogonal, $x_\perp$, to the orbit. The result is

$$\mathrm{tr}\,(\mathcal{L}^t) = \sum_p T_p \sum_{r=1}^{\infty} \delta(t - rT_p) \frac{\mathrm{tr}\,\mathbf{g}_p^r}{|\det(\mathbf{1} - \mathbf{J}_p^r)|}. \tag{1.15}$$

The $\mathbf{J}_p$ is the differential of the transverse flow. This differential is called the stability- or the monodromy matrix.

By a Laplace transform of the trace we go to the frequency domain:

$$\mathrm{tr}\,\mathcal{L}(s) = \int_{0+}^{\infty} dt\; e^{st} \mathrm{tr}\,(\mathcal{L}^t) = \sum_p T_p \sum_{r=1}^{\infty} \frac{e^{sT_p r}\mathrm{tr}\,\mathbf{g}_p^r}{|\det(\mathbf{1} - \mathbf{J}_p^r)|}. \tag{1.16}$$

The operators considered are evolution operators and therefore have eigenvalues of the form $e^{-\lambda t}$. The reason for the minus sign is explained by the exponential decay of e.g. the particle number in open systems, cf. ref. [8] for the 3-disc system. The above Laplace transform therefore has poles at the eigenvalues. So the spectrum corresponds to the poles of the trace.

From linear algebra, however, one has a function, the characteristic polynomial, whose zeros correspond to the spectrum of a linear operator. It turns out that it is much more convenient from a numerical point of view to study such a function. First it is more easy to search for a zero and second the function we find has good convergence properties. It also is much prettier because of its resemblance to the Riemann zeta-function. We therefore study the following function:

$$F = \det(1 - \mathcal{L}) \tag{1.17}$$

which has meaning if the operator $\mathcal{L}$ is trace class (see e.g. ref. [8]). The most important "trick" appears to be $exp(trace(\cdot)) = det(exp(\cdot))$ which we will apply now to this characteristic polynomial look-alike:

$$F(s) = e^{\mathrm{tr}\,(\log(1-\mathcal{L}))} = e^{-\sum_{n=1}^{\infty} \frac{1}{n} \mathrm{tr}\,(\mathcal{L}^n)}. \tag{1.18}$$

Actually this is the definition of determinant for trace class operators - the theorem becomes the definition. In the frequency domain this gives the so called Fredholm determinant

$$F(s) = \exp\left(- \sum_p \sum_{r=1}^{\infty} \frac{1}{r} \frac{e^{sT_p r}\mathrm{tr}\,\mathbf{g}_p^r}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} \right). \tag{1.19}$$

Here we used the above trace calculation on the operators $\mathcal{L}^n$.

We remark that the trace is minus the logarithmic derivative of the Fredholm determinant:

$$\mathrm{tr}\,\mathcal{L}(s) = -\frac{d}{ds}\log F(s). \tag{1.20}$$

The Fredholm determinant can be shown to be entire for (the unfortunately small class of) Axiom A systems to which the open disc billiards belong.

Now we specialise to the case of hyperbolic flows with none of the eigenvalues marginal (ie. all the eigenvalues are different from 1). Let the contracting eigenvalues be $\lambda_1, ..., \lambda_e$ and the expanding $\lambda_{e+1}, ..., \lambda_d$. The determinant becomes:

$$\frac{1}{|\det(\mathbf{1} - \mathbf{J}^{\mathbf{r}}_{\mathbf{p}})|} = \frac{1}{|\Lambda_p|^r}\prod_{a=1}^{e}\frac{1}{1-1/\lambda_{p,a}^r}\prod_{a=e+1}^{d}\frac{1}{1-\lambda_{p,a}^r}, \tag{1.21}$$

where Λ_p is the product of the expanding eigenvalues of the orbit. Expanding the fractions $\frac{1}{1-1/\lambda_{p,a}^r}$ and $\frac{1}{1-\lambda_{p,a}^r}$ in geometric series we find that the Fredholm determinant can be written as an infinite product of zeta functions:

$$det(1-\mathcal{L}) = \prod_{k_1,...,k_e}\prod_{l_{e+1},...,l_d}\frac{1}{\zeta_{k_1,...,l_d}}$$

$$1/\zeta_{k_1,...,l_d}(z) = \prod_p \mathrm{Det}\left(1 - \frac{e^{sT_p}\mathbf{g}_p}{|\Lambda_p|}\frac{\lambda_{p,e+1}^{l_{e+1}}...\lambda_{p,d}^{l_d}}{\lambda_{p,1}^{k_1}...\lambda_{p,e}^{k_e}}\right). \tag{1.22}$$

The leading part corresponds to the zeta function $\zeta_{0...0}$:

$$1/\zeta(s) = \prod_p \mathrm{Det}(1-t_p)$$

$$t_p = \frac{1}{|\Lambda_p|}\mathbf{g}_p e^{sT_p}. \tag{1.23}$$

This is also called the dynamical zeta function and it gives the leading eigenvalue. Hereby we see that unstable orbits with large $|\Lambda_p|$ are suppressed. If the evolution operator does not have a matrix part the determinant, "Det", shall be omitted in the above (1.23).

1.3 Cycle expansions

It turns out that the above trace formulas are associated with divergences. This is not a surprise since we sum over (in general) infinitely many primitive orbits and their repeats. In the Gutzwiller derivation it is seen that the imaginary part of the trace corresponds to the level density which is a sum of delta functions. So from a mathematical point of view (ie. distributions) we have no reason to expect that the trace is well-behaved. The good thing about the Fredholm determinants and zeta functions is now that it replaces the search for divergences with the search for zeroes. However, one still has to organise the sum over periodic orbits.

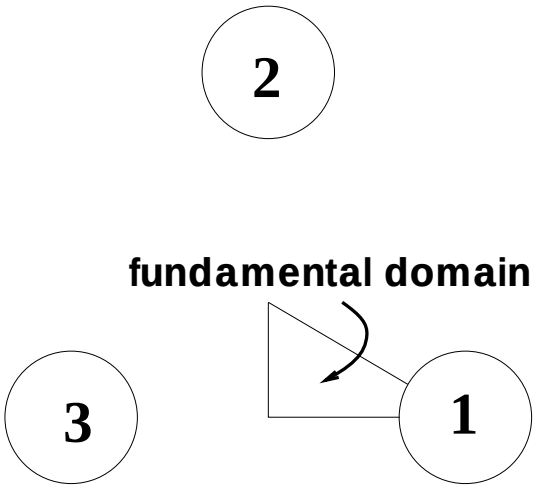


Figure 1.1: The 3-disc system.

For the 3-disc systems it turns out that one can use the symbolic description of the orbits as a guiding principle in how to sum the orbits.

Let us first describe the symbolic dynamics of the 3-disc system used in ref. [8]. We can label which discs we visit giving us an alphabet with 3 letters, say 1,2,3. But is also possible to label the orbits in a much more clever way. We simply write a "0" if the emitted particle hits one disc and return to the original disc. If the particle continues to the next (ie. third and last) disc we write a "1". Thus we have an alphabet with 2 letters. For the open 3-disc system with sufficiently distance between the discs (e.g. $R/a = 6$) in fact every symbol string or word is realized as a physical orbit. We write (1) for the orbit which visits the discs (123) (and also (132) and with cyclic permutations). Thus there are no forbidden rules (no pruning), the grammar is complete. Above we introduced weights of the primitive periodic orbits t_p. Because the weights are sufficiently smooth it turns out that:

$$t_{ab} \approx t_a t_b, \tag{1.24}$$

where a and b are 2 different symbol strings e.g. "0" and "01". This is so because the orbit ab consists of parts in phase space which are "close" to the occupied parts of the smaller orbits a and b. Thus we say that the large orbit ab is shadowed by the smaller orbits a and b.

How is this shadowing exploited? Formally we simply introduce a book-keeping variable z and replaces the above weights by putting $t_p := z^{n_p} t_p$ where the word length n_p is introduced. We then expand the zeta-function in powers of z and finally puts $z = 1$ in the end. Hereby we find

$$1/\zeta = 1 - t_0 - t_1 - (t_{01} - t_0 t_1) - (t_{001} - t_0 t_{01} - t_{01} t_1) - ... \tag{1.25}$$

where we have collected terms in increasing powers of z. The same can be done for the trace and the Fredholm calculations. The introduction of the variable z

in the trace becomes

$$\sum_p n_p \sum_{r=1}^{\infty} z^{n_p r} \frac{e^{sT_p r} \mathrm{tr}\, \mathbf{g}_p^r}{|\det(\mathbf{1} - \mathbf{J}_p^r)|}. \tag{1.26}$$

This means that if we have found words up to length 10 and wants to calculate the curvature expansion we only let the smaller orbits e.g. "0" and "001" contribute 10 and 3 times in their repeats. This way of summing the orbits is called the curvature expansion and it makes the above sums highly convergent (das Buch).

That the trace is minus the logarithmic derivative of the Fredholm (with respect to the variable s) now also holds in a modified form when we use our book keeping variable z :

$$\mathrm{tr}\, \mathcal{L}(z) = -z \frac{d}{dz} \log F(z). \tag{1.27}$$

Writing the trace and the Fredholm as

$$\mathrm{tr}\, \mathcal{L}(z) = \sum_{n=1}^{\infty} C_n z^n$$

and

$$F(z) = 1 - \sum_{n=1}^{\infty} c_n z^n \tag{1.28}$$

(z not yet put equal to 1)
we find the coefficients of the Fredholm as

$$c_1 = C_1$$

and

$$c_n = \frac{1}{n}(C_n - C_{n-1}c_1 - ... - C_1 c_{n-1}). \tag{1.29}$$

This is the way we calculate Fredholms.

1.4 Symmetry factorisations

The purpose of this chapter is to recapitulate the results of ref. [10] on the factorisation of how in case of zeta functions and Fredholm determinants factorise in presence of discrete symmmetries. This decomposition improves considerably the convergence of the above functions and is a necessary practical step.

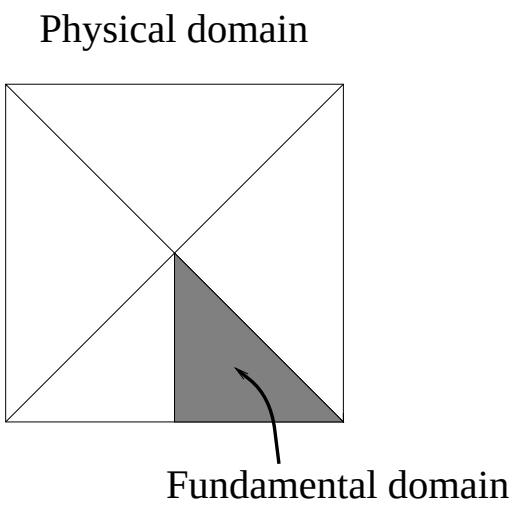


Figure 1.2: The physical domain and the fundamental domain.

1.4.1 Tiling generated by a fundamental tile

We assume that our domain M can be tiled by smaller identical tiles by an application of the group elements on the smallest piece which we call the fundamental domain, $\tilde{M}$. For example, in the case of a square the fundamental piece could be the triangle cut out along the diagonal and a symmetry axis, of one eighth of the whole square, see fig. 1.2. If we apply reflections along the diagonals resp. axes and rotations by $\pi/2$ on this piece we can tile the whole square. We write this as

$$M = \sum_{g \in G} g \cdot \tilde{M}, \tag{1.30}$$

where it is understood that $\cdot$ is the action of the group G on points in the fundamental domain, $\tilde{x} \in \tilde{M}$.

The flow should be invariant under the symmetries, ie. we have for $y = f^t(x)$ that $g \cdot y = f^t(g \cdot x)$.

Because of the symmetries the evolution operator is invariant with respect to the group G, ie.

$$\mathcal{L}(y, x) = \mathcal{L}(gy, gx). \tag{1.31}$$

Thus the "weight" associated with going from x to y is just the same as the one after a transformation.

1.4.2 Decomposition of the evolution operator

Given a finite group acting via the representation $g \mapsto U(g)$ there exist projection operators (ref. [16]) P_α defined by

$$P_\alpha = \frac{d_\alpha}{|G|} \sum_{g \in G} \chi_\alpha(g) g^{-1} \cdot . \tag{1.32}$$

Here α labels the sum which is over all irreducible representations α and χ_α is the corresponding character and d_α its dimension. These operators are projection operators in the sense that $P_a P_b = \delta_{ab} P_a$ and $\sum_\alpha P_\alpha = \mathbf{1}$. Here $\mathbf{1}$ is the identity transformation (on the space where G acts). In that way we decompose the space where the group acts into subspaces, one for each irreducible representation.

We have that $\phi(y) = \int \mathcal{L}(y,x)\phi(x)dx$. Inserting the identity we get

$$\phi(y) = \sum_\alpha P_\alpha \phi(y) = \sum_\alpha \frac{d_\alpha}{|G|} \sum_{g\in G} \chi_\alpha(g) g^{-1} \cdot \phi(y) \equiv \sum_\alpha \frac{d_\alpha}{|G|} \sum_{g\in G} \chi_\alpha(g)\phi(g^{-1}y)$$

$$\equiv \sum_\alpha \frac{d_\alpha}{|G|} \sum_{g\in G} \chi_\alpha(g) \int \mathcal{L}(g^{-1}y,x)\phi(x)dx. \tag{1.33}$$

Hence we conclude that $\mathcal{L}(y,x) = \sum_\alpha \mathcal{L}_\alpha(y,x)$, where

$$\mathcal{L}_\alpha(y,x) = \frac{d_\alpha}{|G|} \sum_{g\in G} \chi_\alpha(g)\mathcal{L}(g^{-1}y,x). \tag{1.34}$$

1.4.3 The trace

The trace of the full space evolution operator is a sum of traces:

$$\mathrm{tr}\,(\mathcal{L}) = \sum_\alpha \mathrm{tr}\,(\mathcal{L}_\alpha) = \sum_\alpha \frac{d_\alpha}{|G|} \sum_{g\in G} \chi_\alpha(g) \int_M \mathcal{L}(g^{-1}x,x)dx. \tag{1.35}$$

Let us use the tiling to restrict to the integration to the fundamental domain:

$$\mathrm{tr}\,(\mathcal{L}) = \sum_\alpha \mathrm{tr}\,\mathcal{L}_\alpha = \sum_\alpha d_\alpha \sum_{g\in G} \chi_\alpha(g) \int_{\tilde{M}} \mathcal{L}(g^{-1}x,x)dx. \tag{1.36}$$

We now recognise the trace of the regular representation $D(g)$:

$$\mathrm{tr}\, D(g) = \sum_\alpha d_\alpha \chi_\alpha(g). \tag{1.37}$$

See the appendix A.1 for further information about the regular representation.

All this means that instead of the original evolution operator we could use a matrix evolution operator $\mathbf{D}(h)\mathcal{L}$ in the fundamental domain as described in ref. [8]. Taking this point of view one finds

$$\mathrm{tr}\,(\mathcal{L}) = \sum_{g\in G} \int_{\tilde{M}} dx\; tr(D(g))\mathcal{L}(g^{-1}x,x), \tag{1.38}$$

which indeed is correct since the trace $tr(D(h)) = |G|\delta_{h,e}$ makes sure that only orbits that close in the physical domain are picked out. Note that the $1/|G|$-factor is cancelled. Given an orbit with degeneracy m_p we simply get as cycle weight

$$(1-t_p)^{m_p} = \mathrm{Det}(1 - D(h_{\tilde{p}})). \tag{1.39}$$

Let us now consider a fixed representation.

1.4.4 Sum over group elements

The formula (1.35) sums over all group element that closes the orbit in the fundamental domain.

Let us start with the case when this sum reduces to one group element, h_p. By splitting the integration in parts along the orbit, resp. transverse the orbit, we find as usual:

$$\mathrm{tr}\,\mathcal{L}^t = \sum_\alpha \sum_{\tilde{p}} T_{\tilde{p}} \sum_{r=1}^{\infty} \delta(t - rT_{\tilde{p}})\chi_\alpha(h_{\tilde{p}}^r) \frac{\mathrm{tr}\,\mathbf{g}_{\tilde{p}}^r}{|\mathrm{Det}(\mathbf{1} - (h_{\tilde{p}}\mathbf{J}_p)^r)|}. \tag{1.40}$$

Performing a Laplace transform $\mathrm{tr}\,\mathcal{L}(s) = \int_{0+}^{\infty} dt e^{st} \mathrm{tr}\,\mathcal{L}^t$ we get

$$\mathrm{tr}\,\mathcal{L}(s) = \sum_\alpha \sum_{\tilde{p}} T_{\tilde{p}} \sum_{r=1}^{\infty} \chi_\alpha(h_{\tilde{p}}^r) e^{srT_{\tilde{p}}} \frac{\mathrm{tr}\,\mathbf{g}_{\tilde{\mathbf{p}}}^{\mathbf{r}}}{|\mathrm{Det}(\mathbf{1} - (h_{\tilde{p}}\mathbf{J}_p)^r)|}. \tag{1.41}$$

The corresponding Fredholm is related to the trace by minus the logarithmic derivative:

$$\mathrm{tr}\,\mathcal{L}(s) = -\frac{d}{ds}\log F(s). \tag{1.42}$$

This gives

$$F(s) = \prod_\alpha F_\alpha^{d_\alpha}(s), \tag{1.43}$$

where

$$F_\alpha(s) = \exp\left(- \sum_{\tilde{p}} \sum_{r=1}^{\infty} \frac{1}{r} \chi_\alpha(h_{\tilde{p}}^r) e^{srT_{\tilde{p}}} \frac{\mathrm{tr}\,\mathbf{g}_{\tilde{p}}^r}{|\mathrm{Det}(\mathbf{1} - (h_{\tilde{p}}\mathbf{J}_p)^r|)} \right). \tag{1.44}$$

This is the symmetry factorisation of the Fredholm determinant. When we look for the spectra of the evolution operator we now check the Fredholm F_α for each subspace of the representation α. Using our favourite trick exp(tr())=det(exp()) on the the product trace $\chi_\alpha \cdot \mathrm{tr}$ we get when we expand the determinant, the cycle weight

$$t_{tildep} = \mathrm{Det}\left(1 - D_\alpha(h_p) \otimes \mathbf{g}_{\tilde{p}} \frac{e^{sT_{\tilde{p}}}}{|\Lambda_{\tilde{p}}|}\right) \tag{1.45}$$

in agreement with (1.23). Here D_α is the irreducible matrix representation (unique up to equivalence) of the group labeled by α. If our evolution operator has no a matrix part, ie. is a scalar, the product $\otimes$ becomes the usual product. Anyway since the determinant always can be expanded in terms of traces and the trace of the (tensor) product is just the product of the traces, we never need any explicit matrix representation of our symmetry group in our actual calculations. All we need are the irreducible characters of the symmetry group.

In this section we have assumed that we only had one closing element. Sometimes we actually have several closing elements in the case of boundary orbits, ie. orbits running on the boundary of the fundamental domain. This is described further in the appendix A.2.

Chapter 2

WKB method for scalar fields

In the preceeding chapter we got a taste of the periodic orbit theory. In the following we shall consider various WKB-like ansatz'es making a particle description (in some approximation) of wave phenomena possible. This will lead to two kinds of partial differential equations of first order of an unknown function. These equations can be solved, at least locally, by means of characteristics, resp. bicharacteristics. Therefore here is a short reminder - in a physicist style - of how to use these methods. In some sense they are just what one needs in periodic orbit theory, because you do not look for the whole solution, but only the solution along an orbit. For a short overview see ref. [11].

2.1 Some basic tools in partial differential equations

2.1.1 Method of characteristics

Suppose we want to solve:

$$a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = 0,\ a = a(x,y),\quad b = b(x,y) \tag{2.1}$$

in some region Ω of the plane. Now consider the curve obtained by integrating

$$\frac{dx}{d\tau} = a \quad \frac{dy}{d\tau} = b, \tag{2.2}$$

$$\vec{r}(0) = (x,y)(0) = \vec{r}_0. \tag{2.3}$$

Suppose further that we know the value of u at the initial point $\vec{r}(0)$.

It is now possible to find u along the curve $r(t)$ consistent with the global solution on Ω, without solving for the whole of Ω

First we calculate the change of u along the curve:

$$\frac{du}{d\tau} = \frac{\partial u}{\partial x}\frac{dx}{d\tau} + \frac{\partial u}{\partial y}\frac{dy}{d\tau} = \frac{\partial u}{\partial x}a + \frac{\partial u}{\partial y}b. \tag{2.4}$$

Thus we can make the function u a solution of the partial differential equation on the curve if we demand that $\frac{du}{d\tau} = 0$. This equation has a solution - even a unique one - since we know u at the initial point.

Hence $u(\tau) = u_0$ along the curve.

The inhomogeneous case is solved in the same way

$$a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = c,\ a = a(x,y)\ b = b(x,y),\ c = c(x,y) \tag{2.5}$$

leads to $\frac{du}{d\tau} = c$ so

$$u = \int_0^t c d\tau + u_0. \tag{2.6}$$

Let us now go to the next step: Assuming not only that the partial differential equation holds at the initial point but on a whole initial hyper surface with u continuous on that surface we can in principle solve for u on any curve starting at this surface. In that way we at least locally find a solution to the partial differential equation in the domain. Of course this initial hyper surface has to in some sense be transversal to the flow generated by the partial differential equation along which we integrate. If not we cannot "cover" a region of the same dimensionality as the domain. One now invokes the uniqueness of such a global u to get the validity of the found u.

2.1.2 Method of bicharacteristics:

The examples above was characterised by the linearity of the equations. We now turn to the general case:

$$H(\vec{x}, \frac{\partial S}{\partial \vec{x}}) = 0, \tag{2.7}$$

where $x \in \Omega$ and H is some not necessarily linear function. What we want to find is the function $S = S(\vec{x})$. Let us put

$$\vec{p} = \frac{\partial S}{\partial \vec{x}} \tag{2.8}$$

and consider $\vec{p}$ as an independent variable. In this way we enlarge our space to x and p coordinates. This space is called the phase space. The idea is now to construct a curve in this extended space, the so-called bicharacteristic curve:

$$\frac{d\vec{x}}{d\sigma} = \frac{\partial H}{\partial \vec{p}} \tag{2.9}$$

and

$$\frac{d\vec{p}}{d\sigma} = -\frac{\partial H}{\partial \vec{x}}. \tag{2.10}$$

(Besides the configuration space curve we also get one in p-space, probably this is why one calls this "bi"-characteristic).

As above, we assume boundary conditions $(x,p)(0) = (x_0, p_0)$ and at this initial point $S = S_0$. Furthermore we actually assume that the partial differential equation holds in this point, ie. $H(x_0, p_0) = 0$.

Now using the same arguments as in analytical mechanics:

$$\frac{dH}{d\sigma} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{d\vec{x}}{d\sigma} + \frac{\partial H}{\partial \vec{p}} \cdot \frac{d\vec{p}}{d\sigma} = \frac{\partial H}{\partial \vec{x}} \cdot \frac{\partial H}{\partial \vec{p}} + \frac{\partial H}{\partial \vec{p}} \cdot (-\frac{\partial H}{\partial \vec{x}}) = 0. \tag{2.11}$$

We conclude that H is conserved along our bicharacteristic. Thus our partial differential equation holds along the bicharacteristic. Furthermore S evolves as

$$S = \int_{start}^{end} dS + S_0 = \int_{start}^{end} \frac{\partial S}{\partial \vec{x}} \cdot d\vec{x} + S_0 = \int_{start}^{end} \vec{p} \cdot d\vec{x} + S_0. \tag{2.12}$$

This means just as for the method of characteristics that we are able to solve for S along some curve. Actually it is not just some curve but the one corresponding to the classical path.

2.2 Applications to scalar fields

In this section we shall familiarise ourselves with the WKB method. First we consider the Helmholtz equation and then an equation for thin plates.

2.2.1 Helmholtz equation

We wish here to study the high frequency solution of the Helmholtz equation following ref. [24]. The reason for this is that this equation is very similar to the anisotropic acoustic wave equation. It will turn out that once we have a WKB-like solution of the former we are not very far from a solution of the latter. The wave equation

$$(\triangle - n^2 \partial_t^2) u(x,t) = 0; \tag{2.13}$$

with a constant frequency

$$u(\vec{x},t) = f(\vec{x}) e^{-i\omega t} \tag{2.14}$$

becomes the Helmholtz equation

$$(\triangle + n^2 \omega^2) f(\vec{x}) = 0. \tag{2.15}$$

Here $n = n(x)$ is the index of refraction. Let us find the high frequency solution of the above, using the oscillatory ansatz:

$$f = a e^{i\omega T}. \tag{2.16}$$

Here $T = T(x)$ is a function only depending of spatial variable and of dimension time - hence the symbol capital T.

T plays the same formal role as the action in the quantum mechanical analogue the WKB approximation. There we recall that the "momentum" was given as the gradient of the phase function S:

$$\vec{p} = \frac{\partial S}{\partial \vec{x}}. \tag{2.17}$$

Now in the high frequency case we conclude that the corresponding momentum is of dimension inverse velocity:

$$\vec{s} = \frac{\partial T}{\partial \vec{x}}. \tag{2.18}$$

Here we will call $\vec{s}$ slowness[1].

The product of the slowness with the angular velocity corresponds to the more familiar wave vector, as seen from the case of a plane wave

$$e^{i(\vec{k}\cdot\vec{x}-\omega t)} = e^{i\omega(\frac{\vec{k}}{\omega}\cdot\vec{x}-t)} = e^{i\omega(\vec{s}\cdot\vec{x}-t)}. \tag{2.19}$$

The prefactor $a = a(x)$ will be called the amplitude as in QM. The Laplacian operator acts on the oscillatory ansatz (2.16) as

$$\triangle f = (\triangle a + i\omega(2(\vec{s}\cdot\vec{\nabla})a + a\vec{\nabla}\cdot\vec{s}) - a\omega^2 s^2)e^{i\omega T}. \tag{2.20}$$

Now let us concentrate on the most important terms, ie. we will omit the quantum potential-like term $\triangle a$. Let us also factor out $e^{i\omega T}$. The equation corresponding to ω^2 is the very simple:

$$s^2 = n^2. \tag{2.21}$$

This is actually an equation in the first order partial derivatives of T. Hence we can introduce a Hamiltonian system give by the Hamiltonian

$$H = \frac{1}{2}(s^2 - n^2). \tag{2.22}$$

We investigate the phase space by means of the classical trajectories, the bicharacteristics:

$$\vec{v} = \frac{d\vec{x}}{d\tau} = \frac{\partial H}{\partial \vec{s}} = \vec{s} \tag{2.23}$$

$$\frac{d\vec{s}}{d\tau} = -\frac{\partial H}{\partial \vec{x}} = \vec{\nabla}_x(n^2/2). \tag{2.24}$$

Here τ is some affine parameter of this curve in phase space. We can find the "acceleration" $\frac{d^2}{d\tau^2}\vec{x} = \vec{\nabla}(n(x)^2/2)$ and conclude that the square of the index of refraction is like a negative potential. These considerations explain the existence of mirages, since now a varying index will lead to curved light rays. However if there is no spatial variation of the index of a refraction, the potential is flat and we will get straight trajectories.

The phase will change as

$$\Delta T = \int \frac{\partial T}{\partial \vec{x}} \cdot d\vec{x} = \int \vec{s}\cdot d\vec{x}. \tag{2.25}$$

[1]This object appears not to be defined in the literature, therefore I have chosen to refer to it as "slowness" by analogy to the acoustic case, see sect. 4.2

Finally, frp, the terms proportional to ω in (2.20) we find the transport equation

$$(\vec{v}\cdot\vec{\nabla})a+\frac{1}{2}a\vec{\nabla}\cdot\vec{v}=0, \tag{2.26}$$

where the velocity is defined in (2.23). The method of characteristics gives us $\frac{d\vec{x}}{d\tau}=\vec{v}$ and $\frac{da}{d\tau}=-\frac{1}{2}a\vec{\nabla}\cdot\vec{v}$. Here we recognise the derivative of the velocity field and use the Liouville formula (1.7) to find the solution

$$a(x(\tau))=e^{-\frac{1}{2}\int\vec{\nabla}\cdot\vec{v}d\tau'}a(x)=\frac{1}{\sqrt{j^\tau(x)}}a(x). \tag{2.27}$$

Thus the whole oscillatory ansatz therefore evolves in the high frequency limit approximately as

$$u(x(\tau))=\frac{1}{\sqrt{j^\tau(x)}}e^{i\omega\int\vec{s}\cdot\vec{dx}}u(x) \tag{2.28}$$

(we recall that we have omitted the term Δa, which was of lower order).

When we introduce the wave vector $\vec{k}=\omega\cdot\vec{s}$, we may write this as

$$u(x(\tau))=\frac{1}{\sqrt{j^\tau(x)}}e^{i\int k(\vec{x})\cdot\vec{dx}}u(x). \tag{2.29}$$

It is possible to extend the solution beyond turning points by inclusion of a Maslov phase, see below sect. 2.4.1.

2.2.2 Bending waves of plates

As our second example we apply the WKB method on the partial differential equation for thin plates.

For a plate of small thickness h one may study the small vibrations perpendicular to the plate. We assume that the medium of the plate is isotropic. It turns out that the corresponding wave equation is not like the ordinary wave equation. It has the following form ([18]):

$$\rho\frac{\partial^2\zeta}{\partial t^2}+\frac{Eh^2}{12(1-\sigma^2)}\Delta^2\zeta=0. \tag{2.30}$$

The constants E and σ are referred to as the Young modulus and the Poisson ratio respectively. The small parameter in this problem is the thickness h. The field ζ is the deformation of the plate normal to its relaxed state. Because of the square of the Laplacian in the wave-equation for ζ we have a fourth-order spatial derivative instead of the just a second order as in the ordinary scalar wave-equation $(\frac{\partial^2}{\partial t^2}-\frac{1}{v^2}\triangle)u=0$. Again it is possible to do a WKB expansion. The expansion parameter will be the thickness h and not $\hbar$ but otherwise everything is pretty much like the quantum mechanical case. The oscillatory ansatz will be

$$\zeta=ae^{iS/h}, \tag{2.31}$$

where a and S are called the amplitude, resp. phase function. Just as ζ, a and S are assumed to depend on space (x and y coordinates) and time t. As in QM we will set

$$\vec{p} = \frac{\partial S}{\partial \vec{x}} \tag{2.32}$$

and

$$\epsilon = -\frac{\partial S}{\partial t}. \tag{2.33}$$

The equation for the phase, ie. the highest ranking equation, corresponds to the Hamilton-Jacobi equation. We find

$$-\epsilon^2 + Ap^4 = 0, \tag{2.34}$$

where the constant A is

$$\frac{E}{12\rho(1-\sigma^2)}. \tag{2.35}$$

So a Hamiltonian for this problem could be $H = -\epsilon^2 + Ap^4$. The bicharacteristics are found from the corresponding Hamilton's equations. The full derivative is with respect to a curve parameter called τ. We find

$$\dot{\vec{x}} = \frac{\partial H}{\partial \vec{p}} = 4Ap^3\vec{p}/p = 4Ap^2\vec{p}. \tag{2.36}$$

$$\dot{t} = \frac{\partial H}{\partial (S_t)} = -\frac{\partial H}{\partial \epsilon} = 2\epsilon. \tag{2.37}$$

For the conjugate momenta we find nothing but conserved quantities, since we assume that A is a spatial and temporal constant:

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{x}} = \vec{0} \tag{2.38}$$

and

$$\dot{\epsilon} = -\dot{S}_t = -(-\frac{\partial H}{\partial t}) = 0. \tag{2.39}$$

We notice that since ϵ is a constant along the curve t is proportional to the curve parameter τ. The physical velocity in the x-y space is

$$\frac{d\vec{x}}{dt} = \dot{\vec{x}}/\dot{t} = \frac{2Ap^2\vec{p}}{\epsilon} = \sqrt{4A}\vec{p}. \tag{2.40}$$

Here we used the "velocities" in the x,y,t-space and that H=0. Let us introduce a wave-vector $\vec{k} = \vec{p}/h$ and a angular velocity $\omega = \epsilon/h$ so that the velocity becomes

$$\frac{d\vec{x}}{dt} = \sqrt{4Ah^2}\vec{k}, \tag{2.41}$$

(just as in ref. [18]).

The transport equation is found by straightforward albeit long derivations: Basically one just has to derive four times with respect to the spatial coordinates and then contract the 2 pairs of indices to get the the square of the Laplacian. One should keep only the 2 most important terms in the development in powers of the thickness h. The second order time derivative which is present also has to be considered.

Let us denote the coordinates (x,y,t) collectively by $\vec{u}$. Vectorially in x,y,t-space we find

$$\dot{\vec{u}} \cdot \vec{\nabla}_u a + \frac{1}{2}(\nabla_u \cdot \dot{\vec{u}})a = 0, \tag{2.42}$$

which looks just like an ordinary continuity equation. Now however the dynamical system also has an evolution of the time and what parametrises the state of the system is no longer the time, t, but our parameter τ. But Liouville's formula (1.7) is still applicable. The divergence of the velocity is still the logarithmic derivative of the ratio between the infinitesimal evolved volume element and the original volume element:

$$\nabla_u \cdot \dot{\vec{u}} = \frac{d \ln j^\tau(u)}{d\tau}. \tag{2.43}$$

The transport equation therefore integrates to

$$a(\tau) = \frac{1}{\sqrt{j^\tau(x_0, y_0, t_0)}} a(x_0, y_0, t_0). \tag{2.44}$$

In order to project down to the plate, x, y-space, we now consider the evolution an infinitesimal element of volume $dx \wedge dy \wedge dt$. Let us specify the initial conditions in the following way: ϵ is constant (constant frequency) on the initial hyper surface corresponding to the time "ticks" with the same speed everywhere.

Then if $t_\pm$ are two initial times, they will in curve-time τ evolve to $t_\pm(\tau) = 2\epsilon\tau + t_\pm$ and therefore $\Delta t = t_+ - t_- = t_+(\tau) - t_\tau = \Delta t(\tau)$. We therefore conclude that the differential dt is conserved. So the Jacobian in x,y,t-space

$$j^\tau(x, y, t) = \mathrm{Det}\left(\frac{\partial(x, y, t)(\tau)}{\partial(x, y, t)}\right) = \frac{dx(\tau) \wedge dy(\tau) \wedge dt(\tau)}{dx \wedge dy \wedge dt}$$

$$= \frac{dx(\tau) \wedge dy(\tau)}{dx \wedge dy} = j^t(x, y), \tag{2.45}$$

is nothing but the Jacobian in x,y-space.

The change of phase when we go from one point to another on the plate is by the chain rule

$$\Delta S = \vec{p} \cdot \Delta\vec{x} - \epsilon \Delta t. \tag{2.46}$$

Collecting the above expressions we find using (1.7):

$$\zeta(\vec{x}(t), t) = \frac{1}{\sqrt{j^t(\vec{x}_0)}} e^{i(\vec{k} \cdot \vec{\Delta} x - \omega t)} \zeta(\vec{x}, 0), \tag{2.47}$$

with the same form as in (2.29), in leading order in the small constant h.

Also here it is possible to extend the solution beyond turning points by inclusion of Maslov's phase.

The free boundary conditions are very complex (even Landau and Lifshitz think so: ref. [18] formulae 12.6 and 12.7) whereas the conditions for clamped plates are much simpler:

$$\zeta = 0, \quad \frac{\partial \zeta}{\partial n} = 0. \tag{2.48}$$

2.3 WKB in QM

In this section we want to focus on a local WKB-solution of the Schrödinger equation in the semiclassical limit. We mean by "semiclassical" nothing more than $\hbar \to 0$. We will not go into detail in the extension of solutions through caustics. For this we refer to refs. [24, 19, 17, 21, 23].

2.3.1 Hamilton-Jacobi and the transport equation

In order to solve the Schrödinger equation

$$(-\frac{\hbar^2}{2m}\triangle + V)\psi = i\hbar\frac{\partial \psi}{\partial t} \tag{2.49}$$

Wentzel, Kramers and Brillouin used an ansatz of the form

$$\psi = ae^{iS/\hbar}. \tag{2.50}$$

where a is the amplitude and S is the action. The motivation for these names we shall soon see. This ansatz is then put into the Schrödinger equation and after some calculation one realizes that there are terms proportional to different powers of the Planck constant $\hbar$. The terms proportional to $\hbar^0$ yield the Hamilton-Jacobi equation:

$$\frac{\partial S}{\partial t} + H(\vec{x}, \vec{\nabla}_x S) = 0 \tag{2.51}$$

and the terms proportional to $\hbar$ yield the transport equation

$$\frac{\partial a}{\partial t} + \frac{1}{m}\vec{\nabla}_x S \cdot \vec{\nabla}_x a = -a\frac{1}{2m}\frac{\partial^2 S}{\partial \vec{q} \cdot \partial \vec{q}}. \tag{2.52}$$

Here we have dropped in the Hamilton-Jacobi equation the addition of the so-called Quantum Potential $-\frac{\hbar^2}{2m}\frac{1}{a}\triangle a$, which is of order $\hbar^2$. This approximation is called the WKB-approximation. So all we have to do is to solve the Hamilton-Jacobi and the transport equation. The strategy is to solve the former first and then use the solution for S in the latter. What we have gained is that the solution is reduced to ordinary differential equations, whereas we have lost some information by dropping the quantum potential. The WKB-method has been refined to use an asymptotic series in $\hbar$ instead of just the simple ansatz. Here we neglect terms of order $O(\hbar^2)$, but it is possible to go beyond. That means that, it is possible to solve (at least formally) the hierarchy of equations arising from each term in the asymptotic series ([24, 14]).

2.3.2 Hamilton's equations

Let us solve the Hamilton Jacobi equation by means of bicharacteristics. In order to do that we have to identify the conjugate momenta. First there is the spatial momentum

$$\vec{p} \equiv \frac{\partial S}{\partial \vec{q}} \tag{2.53}$$

We remark that we also have a time derivative present

$$\frac{\partial S}{\partial t} = -H(\vec{q}, \vec{p}) \equiv -E. \tag{2.54}$$

Therefore we define a Hamiltonian:

$$H'(q, t, p, E) = -E + H(\vec{q}, \vec{p}) \tag{2.55}$$

corresponding to the Hamilton-Jacobi equation:

$$H'(q, t, p, E) = 0. \tag{2.56}$$

This gives rise to bicharacteristics in the (x, t, p, E)-space:

$$\frac{d\vec{q}}{d\tau} = \frac{\partial H'}{\partial \vec{p}} = \frac{\partial H}{\partial \vec{p}} \tag{2.57}$$

and

$$\frac{d\vec{p}}{d\tau} = -\frac{\partial H}{\partial \vec{p}} \tag{2.58}$$

and for the time and energy we get

$$\frac{dt}{d\tau} = \frac{\partial H'}{\partial (S_{,t})} = -\frac{\partial H'}{\partial E} = 1 \tag{2.59}$$

respectively

$$\frac{dE}{d\tau} = -\frac{\partial H'}{\partial t} = 0. \tag{2.60}$$

We observe that the evolution of our time t is trivial $dt = d\tau$, and we may therefore just consider the bicharacteristics in q,p-space:

$$\frac{d\vec{q}}{d\tau} = \frac{\partial H}{\partial \vec{p}} \tag{2.61}$$

and

$$\frac{d\vec{p}}{d\tau} = -\frac{\partial H}{\partial \vec{q}}. \tag{2.62}$$

Thus we get the Hamilton's equations from the Hamilton-Jacobi equation as is well known, and in order to obtain the WKB-solution we have to go along the classical paths.

The change of the phase is given by

$$dS = \frac{\partial S}{\partial \vec{q}} \cdot d\vec{q} + \frac{\partial S}{\partial t} dt = \vec{p} \cdot d\vec{q} - Edt = Ldt, \tag{2.63}$$

where $L = \frac{1}{2}mv^2 + V(q)$ is the Lagrange function. Thus knowing an initial value of the phase S we can always recover it at a point later on a classical trajectory by integration of the Lagrangian along the trajectory. Quantum mechanics is not forgotten however since the phase is measured in units of $\hbar$.

2.3.3 Transport equation

The transport equation for the amplitude is equivalent to the continuity equation:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0, \tag{2.64}$$

when we put $\rho = a^2$ and the velocity $\vec{v} = \vec{p}/m$. The transport equation can be recast as

$$\frac{da}{dt} = -\frac{1}{2}(\vec{\nabla} \cdot \vec{v})a, \tag{2.65}$$

so formally the solution is

$$a(x(t)) = e^{-\frac{1}{2}\int_{t_0}^{t} \vec{\nabla} \cdot \vec{v} dt'} a(x). \tag{2.66}$$

Using (1.7) we therefore find (at least locally)

$$a(x(t)) = \frac{1}{\sqrt{j^t(x)}} a(x). \tag{2.67}$$

Thus we conclude that the semi classical wave function at a point later on a classical trajectory is related to an initial value by:

$$\psi(x(t)) = \frac{1}{\sqrt{j^t(x)}} e^{i\Delta S/\hbar} \psi(x). \tag{2.68}$$

This result is equivalent to the previously obtained in (2.29) and (2.47).

2.4 Vattay's evolution operator

When our WKB-solution evolves, the phase $S = S(\vec{q}, t)$ and the amplitude $a = a(\vec{q}, t)$ change. These changes can be described by the action of a so-called evolution operator which relates the initial solution at time $t = 0$ to the solution at a time t later. It is not enough to know the initial point in configuration space, one also has to know the initial momenta- which is related to the gradient of the phase - in order to find the final point. Similarly the amplitude has to change and that is in principle found by sending out small volume elements in configuration space following the trajectories of the projected phase space curves. The initial volume element is described by vectors $\delta\mathbf{q}_1, ..., \delta\mathbf{q}_d$. In order to evolve these vectors we also have to know the initial momentum vectors, and these vary

over the volume element with $\delta\mathbf{p}_1, ..., \delta\mathbf{p}_d$. The variation of the initial momenta can be found just by keeping track of the curvature matrix

$$\mathbf{M} = \frac{\partial^2 S}{\partial\vec{x}\partial\vec{x}}, \tag{2.69}$$

since

$$\delta\mathbf{p} = \mathbf{M}\cdot\delta\mathbf{q}. \tag{2.70}$$

The curvature matrix plays the following role in the transport equation (2.65):

$$\dot{\kappa} = -\frac{1}{m}\mathrm{Tr}\,\mathbf{M}, \tag{2.71}$$

where $\kappa = \log(a^2)$, since

$$\vec{\nabla}\cdot\vec{v} = \frac{1}{m}\vec{\nabla}\cdot\vec{p} = \frac{1}{m}\vec{\nabla}\cdot\vec{\nabla}S = \frac{1}{m}\ \mathrm{Tr}\ \left(\frac{\partial^2 S}{\partial\vec{q}\partial\vec{q}}\right) = \frac{1}{m}\mathrm{Tr}\,\mathbf{M}.$$

Taking this point of view (ref. [33]) we therefore start picking a solution of the Hamilton-Jacobi equation ((2.51)) $S(q,t)$. The wave function is evolved according to the initial momenta ∇S and the $\mathbf{D}^2 S(q,t) = \mathbf{M}$-matrix. But this evolution depends on the initial curvature matrix.

Hence we will extend the space to also include the curvature matrices and evolve densities of the form

$$\tilde{\psi}(\mathbf{q},\mathbf{p},\mathbf{M},t) = \psi(\mathbf{q},t)\delta(\vec{p}\,' - \vec{\nabla}S(\vec{q}\,',0))\delta(\mathbf{M}' - \mathbf{D}^2 S(\vec{q}\,',0)), \tag{2.72}$$

Here ψ is the usual wave function. The evolution is given by the integral operator

$$\tilde{\psi}(\mathbf{q}',\mathbf{p}',\mathbf{M}',t) = \int dqdpd\mathbf{M}\mathcal{L}(\mathbf{q}',\mathbf{p}',\mathbf{M}',t|\mathbf{q},\mathbf{p},\mathbf{M})\tilde{\psi}(\mathbf{q},\mathbf{p},\mathbf{M},0), \tag{2.73}$$

with the kernel

$$\mathcal{L}(\mathbf{q}',\mathbf{p}',\mathbf{M}',t|\mathbf{q},\mathbf{p},\mathbf{M}) = e^{i(\frac{1}{\hbar}\int L dt + \frac{1}{2m}\int_0^t)d\tau \mathrm{tr}\,\mathbf{M}^\tau}(q',p',\mathbf{M}')$$

$$\times\delta(\vec{q}' - \vec{q}'^t)\delta(\vec{p}' - \vec{p}'^t)\delta(\mathbf{M}' - \mathbf{M}^t(q,p,\mathbf{M})). \tag{2.74}$$

We compute in the above formula $\vec{\nabla}S(q,t)$ and $\mathbf{D}^2 S(q,t)$ from their initial values and replace these with $\vec{p}'^t$ and $\mathbf{M}^t$.

We remark that the original wave function can be recovered from the extended since:

$$\psi(q,t) = \int dpd\mathbf{M}\psi(q,p,\mathbf{M}). \tag{2.75}$$

The nice geometrical fact is that for problems with constant potential the curvature matrix $\mathbf{M}$ is the curvature matrix of the wave front (modulo some constant factor). The reason for this is that in such cases the length of the momentum is conserved. Thus $\mathbf{M} \propto \nabla\mathbf{n}$, where $\mathbf{n} = \vec{p}/p$ is the normal vector to the wavefront. But the 2-tensor $-\nabla\mathbf{n} \equiv \gamma$ is Gauss's curvature matrix (see any book in differential geometry). The eigenvalues of this symmetric matrix are the

principal curvatures of the surface. Thus the evolution operator above includes the geometric information of curvatures of the wavefront.

Let us commence the evaluation of the trace of the quasi-classical evolution operator:

By the usual manipulations we find the trace over the phase space variables q, p:

$$tr\mathcal{L}^t = \sum_p T_p \sum_{r=1}^{\infty} \frac{\delta(t - rT_p)e^{irS_p/\hbar}}{|\mathrm{Det}(1 - \mathbf{J}_p^r)|}\Delta_{p,r}. \tag{2.76}$$

The remaining $\mathbf{M}-$ trace restricted to prime cycles and their repeats is

$$\Delta_{p,r} = \int d\mathbf{M}\delta(\mathbf{M}' - \mathbf{M}(q,p,M))\sqrt{j}^{rT_p}(q,p,M), \tag{2.77}$$

when we include the $\sqrt{j}$ from the evolution operator. It is now possible to actually do this trace. The good thing is that we do not need any new information which is not already contained in the phase space Jacobian $\mathbf{J}$.

We shall concentrate on the case of 2-d hyperbolic Hamiltonian flows. For general dimension see ref. [12]. In the 2-d case the derivation of the quasi classical trace formula is very simple. The $[2\times 2]$-dimensional phase space Jacobian matrix is

$$\begin{bmatrix} \delta q' \\ \delta p' \end{bmatrix} = \mathbf{J} \begin{bmatrix} \delta q \\ \delta p \end{bmatrix}.$$

In the 2-d phase space the curvature matrix $\mathbf{M}$ is $[1\times 1]$, ie. the scalar $\kappa := \partial p/\partial q$. Divide through with δq.

$$\frac{dq'}{dq}\begin{bmatrix} 1 \\ \kappa' \end{bmatrix} = \mathbf{J} \begin{bmatrix} 1 \\ \kappa \end{bmatrix}. \tag{2.78}$$

Writing $\mathbf{J} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ we have

$$j(\kappa) = \frac{dq'}{dq} = A + B\kappa\,, \qquad \kappa' = M(\kappa) = \frac{C + D\kappa}{A + B\kappa}\,.$$

For a periodic orbit there are two solutions

$$\mathbf{J}\begin{bmatrix} 1 \\ \kappa_\pm \end{bmatrix} = \Lambda_\pm \begin{bmatrix} 1 \\ \kappa_\pm \end{bmatrix}$$

so the configuration volume ratio $j(\kappa) = \frac{dq'}{dq}$ is for a periodic orbit simply the eigenvalue of the phase space Jacobian. Since the flow is Hamiltonian and hyperbolic $\det\mathbf{J} = 1$ and thus $j(\kappa) = \Lambda_\pm = \Lambda^{\pm 1}$. The κ part of the trace is

$$\int d\kappa\,\delta(\kappa - M(\kappa)) = \frac{1}{\left|1 - \frac{\partial M}{\partial \kappa}\right|}\,. \qquad \frac{\partial M}{\partial \kappa} = \frac{\det\mathbf{J}}{(A + B\kappa)^2} = \frac{1}{\Lambda_\pm^2}$$

so the curvature matrix contribution to the trace is

$$\int d\kappa\, \delta(\kappa - M(\kappa)) \left|\frac{dq'}{dq}\right|^{1/2} = \sum_{j(\kappa)} \frac{\sqrt{j(\kappa)}}{(1-1/j(\kappa)^2)} = \frac{|\Lambda_+|^{1/2}}{|1-1/\Lambda_+^2|} + \frac{|\Lambda_-|^{1/2}}{|1-1/\Lambda_-^2|}$$

Substituting into the trace (2.76) yields the Fredholm determinant

$$\begin{aligned} \det(\mathbf{1}-\mathcal{L}) &= \exp\left(-\sum_{p,r}\frac{1}{r\mid\Lambda_p^r\mid}\frac{e^{irS_p(E)+im_p\pi}}{(1-1/\Lambda_p^r)^2}\Delta_{p,r}\right) \\ \Delta_{p,r} &= \frac{\mid\Lambda_p^r\mid^{1/2}}{1-1/\Lambda_p^{2r}} + \frac{\mid\Lambda_p^r\mid^{-5/2}}{1-1/\Lambda_p^{2r}}\,, \end{aligned} \tag{2.79}$$

This result is of fundamental importance. One is now tempted to do exactly the same in other areas where a WKB expansion is possible. Thus the result derived by the authors in ref. [33] should be considered as the starting point of this thesis.

The determinant (2.79) can be manipulated further to find the dynamical zeta function. Expanding $1/(1-1/\Lambda_{p,i}^r)^2$ and $1/(1-1/\Lambda_{p,i}^{2r})$ in series we find to leading order a dynamical zeta function with the orbit weight

$$t_p = \frac{e^{iS_p/\hbar - i\pi\frac{m_p}{2}}}{\sqrt{|\Lambda_p|}}. \tag{2.80}$$

2.4.1 Maslov index

One of the problems of the WKB method is that we have turning points in the configuration space. These can also be described as folds in the phase space. Suppose that the dimension of space is 1 for simplicity. In these points $dv/dx = \frac{1}{m}dp/dx \to \infty$ because in the phase space the flow turns vertical, see fig. 2.1. The projection down to x-space there has a caustic, a place where light "burns". There are several methods to overcome the problem: analytical continuation ref. [19], boundary layer methods (ref. [17]) and Fourier transformation (ref. [24]). The end result is the same: the solution acquires a phase shift of $-\pi/2$ through each passage across a caustic. To keep track of these phase changes Maslov has developed a theory - Maslov indices (ref. [24]).

Another way to see that we will get phases is in the amplitude prefactor is the following: The prefactor which turns up in transport equations is

$$1/\sqrt{j^t} = \frac{1}{\sqrt{\frac{dx_1(t)\wedge\ldots\wedge dx_n(t)}{dx_1\wedge\ldots\wedge dx_n}}}.$$

When we send out our volume element on a little trip there might be orientation changes with respect to the original volume element defined with respect the projection on to the x-coordinates. An orientation change will give us a factor -1 in the ratio. So when we take the square root we get say a factor i. The phase shift therefore is effectively a multiplication by $e^{-im_p\pi/2}$.

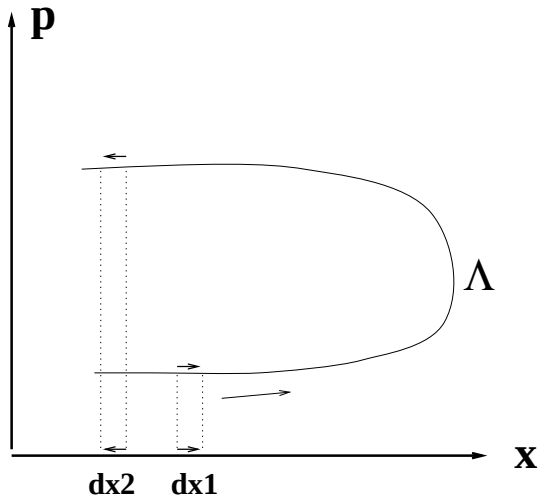


Figure 2.1: The projected volume element is sent out on a tour on the manifold Λ. After the passage of the fold the volume element, when projected down to the x-plane, is seen to have changed its orientation.

Chapter 3

Mini-course in acoustics

This chapter is a short introduction to some acoustic terms. It should not be considered as a full exposition of acoustics, but rather as a summary of important results and their derivations. The material is take from refs. [19, 25, 2].

First some definitions:

Consider the fig. 3.1 of a continuous medium undergoing an elastic deformation. We use $\vec{r}$ to denote the original position of an infinitesimal volume element and $\vec{r}\,'$ the position after a deformation of the body. Now what matters is the relative change in position, the displacement

$$\vec{u} = \vec{r}\,' - \vec{r}. \tag{3.1}$$

The body is referred to by Ω and the border by $\partial\Omega$. Finally at the border we let $d\vec{A} = \vec{n}dA$ denote the directed infinitesimal area, where $\vec{n}$ is the outward normal

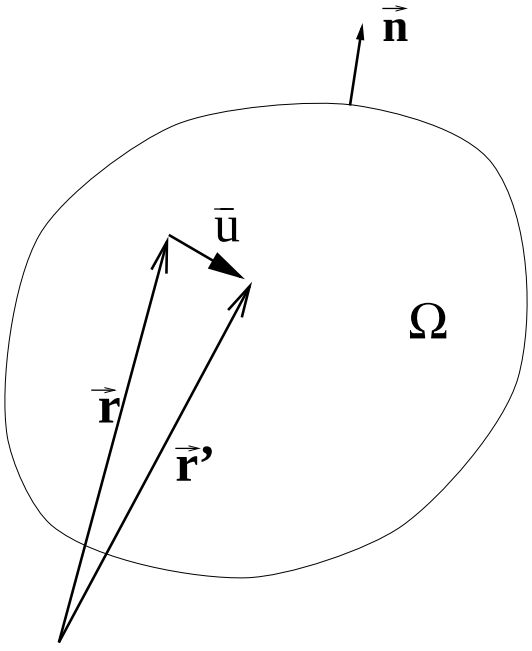


Figure 3.1: The continuous medium; notation.

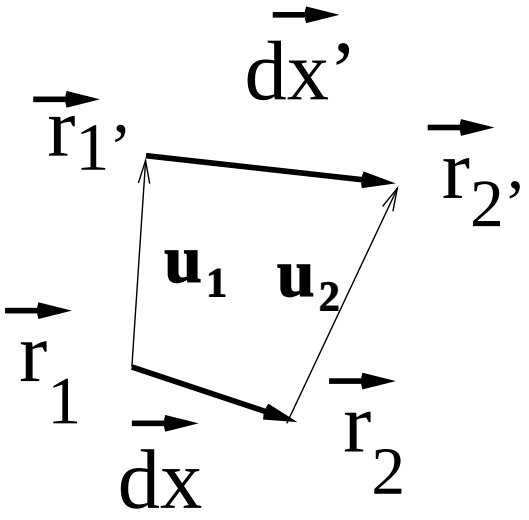


Figure 3.2: The deformation of the line element

of the boundary. We fix the dimension of space to 3.

3.1 Kinematical description: the strain-field

We wish to describe the deformations with a geometric field. This field should be non-zero when we deform the body. That field turns out not to be the displacement field as defined in (3.1). If we, say, translate the whole body, the displacement is a constant non-zero vector, but we have not actually deformed the body. In the same way our field must be zero when we perform a rotation of the body. What counts is how the infinitesimal neighbourhood around some interior point in the body is distorted. This can be investigated by means of the metric tensor (squared distance):

$$dl^2 = dx_1^2 + dx_2^2 + dx_3^2, \tag{3.2}$$

where $\vec{dx} = \vec{r_2} - \vec{r_1}$ with $\vec{r_2}, \vec{r_1}$ two infinitesimally close vectors before the deformation, see fig. 3.2. After the deformation (transition to primed vectors) the two initial vectors change to $\vec{r_2}', \vec{r_1}'$. We see that $d\vec{x}' = d\vec{x} + d\vec{u}$ and therefore also the squared distance is changed as:

$$dl'^2 = dx'^2 = dx^2 + 2\vec{dx} \cdot \vec{du} + du^2 = dl^2 + 2dx_i u_{i,k} dx_k + u_{i,k} u_{i,j} dx_k dx_j$$

$$= dl^2 + 2u_{ik} dx_i dx_k, \tag{3.3}$$

where

$$u_{ik} = \frac{1}{2}(u_{i,k} + u_{k,i} + u_{l,i} u_{l,k}). \tag{3.4}$$

Here the repeated indices are summed over (unless explicitly stated otherwise).

This rank 2-tensor u_{ik} is called the strain tensor. The strain tensor describes what is called the strain field. In the linear theory of elasticity, which we will consider here, the displacements are assumed small. In that approximation the strain field is just

$$u_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}). \tag{3.5}$$

This is the field that describes deformations. It is sensible that the field only contains derivatives of the displacements, since global translations and rotations should not give any field. One may ask, why not use the more general 2-tensor $\vec{\nabla}\vec{u}$? Let us decompose such a tensor in its symmetric and antisymmetric part:

$$\vec{\nabla}\vec{u} = (\vec{\nabla}\vec{u})_s + \vec{\nabla}\vec{u}_a. \tag{3.6}$$

Now a local rotation is felt by the antisymmetric part, since $(\nabla\vec{u}_a)_{ij} \propto \epsilon_{ijk}(\vec{\nabla}\times\vec{u})_k$ and the curl measures the infinitesimal rotation around a point. However, a local rotation will not produce any interior stress since the distance between two neighbouring points is conserved. Therefore we end up with only the symmetric part, which again is nothing but the strain field in the linear approximation. As a final remark on the strain field we should bear in mind that for general coordinates we should use covariant derivatives in order to have a covariant (2-tensor) field.

3.2 Dynamical description: the stress field

The last section dealt with the geometrical description of a deformed body. In this chapter we describe the internal stresses producing these deformations. In some texts on continuum mechanics one simply introduces the stress tensor by definition as follows: consider an infinitesimal element of area $d\vec{A}$ in a deformed medium. The corresponding force $d\vec{f}$ acting on this area element is assumed to be of the form

$$d\vec{f} = \vec{\vec{\sigma}} \cdot d\vec{A}, \tag{3.7}$$

where $\vec{\vec{\sigma}}$ is the stress tensor. This tensor is thus a 2-tensor (described by a 3x3-matrix in three dimensions). A motivation for such a definition is given in ref. [18]. We assume that the forces have very short range so that the total force exerted on the body comes from the surroundings of the body. Here we use Newton's third law. The force on the body is given as an integral of the force per volume element

$$\int_\Omega \vec{f} dV. \tag{3.8}$$

Now this integral can be transformed to a surface integral if $\vec{f}$ is a divergence of a 2-tensor σ : ie.

$$f_i = \sigma_{ik,k} \tag{3.9}$$

(the force comes from the surroundings). In such a case the total force's component is

$$\int_\Omega f_i dV = \int_{\partial\Omega} \sigma_{ik} dA_k \tag{3.10}$$

written in vector notation as

$$\int_\Omega \vec{f} dV = \int_{\partial\Omega} \vec{\vec{\sigma}} \cdot d\vec{A}. \tag{3.11}$$

So we conclude that the force on the area-element $d\vec{A}$ is $d\vec{f} = \vec{\vec{\sigma}} \cdot d\vec{A}$. The condition for a free boundary is therefore

$$\vec{t} \stackrel{\text{def}}{=} \vec{\vec{\sigma}} \cdot \vec{n} = \vec{0}. \tag{3.12}$$

Here $\vec{t}$ is called the traction. The traction is a vector describing the force per unit area on the surface, cf. the definition of the stress tensor (3.7).

We can argue that the stress tensor is symmetric by considering the moment

$$M_{ik} = \int_\Omega (f_i x_k - f_k x_i) dV = \int_\Omega (\sigma_{il,l} x_k - \sigma_{kl,l} x_i) dV$$

$$= \int_\Omega ((\sigma_{il} x_k - \sigma_{kl} x_i)_{,l} - (\sigma_{il} x_{k,l} - \sigma_{kl} x_{i,l})) dV$$

$$= \int_{\partial\Omega} (\sigma_{il} x_k - \sigma_{kl} x_i) dA_l + \int_\Omega (\sigma_{ki} - \sigma_{ik}) dV. \tag{3.13}$$

Again if the moment should only be a boundary integral the last term has to vanish, ie. $\sigma_{ik} = \sigma_{ki}$.

3.3 Free energy

We start by determining the work done on the elastic medium by the surroundings when the body suffers a deformation $\delta\vec{u}$. This will be accompanied by a change in energy $dE = dQ + dW$ per unit volume. The force is given by (3.9) and therefore

$$-\Delta W = \int \vec{f} \cdot \delta\vec{u} dV = \int \vec{\nabla} \cdot \vec{\vec{\sigma}} \cdot \delta\vec{u} dV = \int d\vec{A} \cdot \vec{\vec{\sigma}} \cdot \delta\vec{u} - \int \sigma_{ik} \frac{\partial \delta u_i}{\partial x_k} dV. \tag{3.14}$$

We assume that the deformation $\delta\vec{u} \to 0$ at infinity. Hence the first term vanishes, whereas by symmetry of the stress tensor the last term gives

$$-\Delta W = -\int \sigma_{ik} \delta u_{ik} dV, \tag{3.15}$$

where $u_{ik} = \frac{1}{2}(u_{i,j} + u_{j,i})$ is the strain field. We conclude that

$$dE = dQ + \sigma_{ik} du_{ik} \tag{3.16}$$

per unit volume. The case where $\sigma_{ik} = -p\delta_{ik}$ (hydrostatic compression) gives us the familiar thermodynamics relation $dW = -pdV$. The argument for this goes as

follows: First we diagonalize the strain (since it is symmetric there is no problem) then we consider the deformed squared infinitesimal line element:

$$dl'^2 = dl^2 + 2u_{ik}dx_i dx_k = (1+2u_1)dx_1^2 + (1+2u_2)dx_2^2 + (1+2u_3)dx_3^2.$$

Therefore the volume element changes to:

$$dV' = \sqrt{g}\, dx_1 dx_2 dx_3 = \sqrt{1+2u_1}\sqrt{1+2u_2}\sqrt{1+2u_3}\, dx_1 dx_2 dx_3$$

$$\approx (1 + (u_1 + u_2 + u_3))dx_1 dx_2 dx_3 = (1 + \mathrm{tr}\,(u))dx_1 dx_2 dx_3. \tag{3.17}$$

So the trace of the strain is the relative change of volume, but in the above case we were calculating per unit volume.

By a Legendre transformation $F = E - TS$ we find the free energy as usual. A change in the free energy is given by:

$$dF = -SdT + \sigma_{ik}du_{ik}. \tag{3.18}$$

3.4 Elasticity tensor

The generalised Hooke's law says how the free energy depends on the strain (the energy of a spring depends on the displacement). Its name suggests it should be very much as for the case of a spring, ie. $U = \frac{1}{2}Kx^2$. By (3.18) $\sigma_{ik} = \frac{\partial F}{\partial u_{ik}}$. In the following we will assume constant temperature. Furthermore we will only assume a stress when there is a strain. The Taylor expansion of the free energy, F, in terms of the strain-tensor therefore does not have a linear term. So in general $F = \frac{1}{2}c_{iklm}u_{ik}u_{lm}$, omitting the constant term and terms of order higher than quadratic. This is like a spring - therefore the name generalised Hooke's law.

This form of the free energy is correct since F has to be a scalar and since the strain field is described by a 2-tensor. The 4-tensor c_{iklm} is called the elasticity tensor and because of the symmetries of the strain field we see that it has the following symmetries:

$$c_{iklm} = c_{kilm} = c_{ikml} = c_{lmik}. \tag{3.19}$$

Here the symmetries are with respect to exchange of the indices in either the pairs (12) resp. (34), and finally exchange of the pair (12) with the pair (34). By a counting argument it is not difficult to see that this gives in general 21 independent components of the elasticity tensor. First because of the exchange symmetry in each pair one labels (Voigt notation ref. [2]) each type of pair with a number from 1 to 6: $xx = 1$, $yy = 2$, $zz = 3$, $yz = 4$, $xz = 5$, $xy = 6$. There are indeed $3(3+1)/2 = 6$ (the number of independent elements in a symmetric matrix) labellings. Second because of the symmetry of the exchange of pair (12) with (34) we will have using Voigt notation say $c_{25} = c_{52}$. So using exactly the same argument as the first we find $6(6+1)/2 = 21$ different components. If other symmetries are present the number of components becomes further reduced. Let us consider 3 important cases: the isotropic, the cubic (aluminium) and the rhombohedral (quartz) case.

The isotropic case: Suppose we transform to coordinates:

$$x_i' = O_i^j x_j, \tag{3.20}$$

where O_i^j are the components of an orthogonal matrix. This corresponds to a rotation plus perhaps a reflection (depending on the sign of $\mathrm{Det}(O) = \pm 1$). The elastic tensor c_{ijkl} transforms as follows:

$$c'_{ijkl} = c_{abcd} O_i^a O_j^b O_k^c O_l^d. \tag{3.21}$$

In an isotropic body we demand that any tensor should be invariant under orthogonal transformations, hence actually

$$c_{ijkl} = c_{abcd} O_i^a O_j^b O_k^c O_l^d. \tag{3.22}$$

As an example of such a tensor we mention the identity transformation as an invariant 2-tensor:

$$\delta'_{rs} = \delta_{ab} O_r^a O_s^b = O_r^a O_s^a = \delta_{rs}, \tag{3.23}$$

since the rows are orthonormal in an orthogonal matrix. Using this tensor as a building block we arrive at the following isotropic candidate :

$$c_{rsmn} = \lambda \delta_{rs}\delta_{mn} + \mu \delta_{rm}\delta_{ns} + \nu \delta_{rn}\delta_{sm}. \tag{3.24}$$

Actually all isotropic 4-tensors have this form (see for example PC group theory). Then we invoke the symmetries of the elasticity tensor to reduce the above expression: by the symmetry of the last two indices, $c_{rsmn} = c_{rsnm}$:

$$\lambda \delta_{rs}\delta_{mn} + \mu \delta_{rm}\delta_{ns} + \nu \delta_{rn}\delta_{sm} = \lambda \delta_{rs}\delta_{nm} + \mu \delta_{rn}\delta_{ms} + \nu \delta_{rm}\delta_{sn} \tag{3.25}$$

we conclude that $\mu = \nu$. With this adjustment all the remaining symmetries are also accounted for. The elasticity tensor in the isotropic case therefore only depends on 2 parameters:

$$c_{ijkl} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{3.26}$$

The constants λ and μ are called the Lamé constants.

The rhombohedral case: An example is the material quartz cf. ref. [22]. Quartz is a very good resonator because of its high Q-value. Now by definition of this crystal class the symmetry group is D_3 , the symmetries of an equilateral triangle.

Let us assume that the triangle is lying in the $x - y$ -plane with its center of mass at the origin and with one of its vertices on the x-axis (see fig. 3.3). The symmetry axis is then aligned along the z-axis. The symmetry group is now generated by a rotation $2\pi/3$ around the origin and a rotationπ around the x-axis. We can use complex coordinates $\xi = x + iy$ resp. $\eta = x - iy$. Therefore the first rotation acts as $\xi \mapsto e^{i2\pi/3}\xi$ and $\eta \mapsto e^{-i2\pi/3}\eta$ whereas the last rotation is just conjugation $\xi \mapsto \eta$ and vice versa. The first operation leaves z unchanged $z \mapsto z$ whereas the rotation around the x-axis changes the sign of $z : z \mapsto -z$. Let

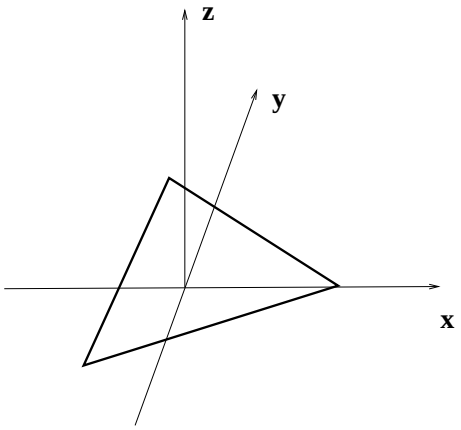


Figure 3.3: An equilateral triangle.

us start by considering only rotations around the z-axis. We remark that by our change of variables the rotation no longer mixes the symmetry plane coordinates. Therefore the elastic tensor's components which are conserved are only those with 3 $\xi's$ or 3 $\eta's$:

$$c_{\xi\xi\xi z}, c_{\eta\eta\eta z},$$

or with the same number of $\xi's$ and $\eta's$:

$$c_{\xi z\eta z}, c_{\xi\eta zz}, c_{\eta\xi\eta\xi}, c_{\eta\eta\xi\xi}$$

and finally with no $\xi's$ or $\eta's$:

$$c_{zzzz}.$$

The rotation around the x-axis now interchanges ξ with η and changes the sign of z, so we actually have in the above list of 7 components that

$$c_{\xi\xi\xi z} = -c_{\eta\eta\eta z}, \tag{3.27}$$

leaving us with a total of 6 independent components.

Finally **the cubic case**: This symmetry means that we have invariance with respect to 90° rotations around the z-axis:

$$x \mapsto y,\ y \mapsto -x,\ z \mapsto z.$$

Hence as independent components we may choose $c_{xxxx}, c_{zzzz}, c_{xxyy}, c_{xzzz}, c_{xyxy}$ and c_{xzxz}. If we then consider rotations around the x- and y - axis we mix z-coordinates with resp. $x-$ and y- coordinates:

$$x \mapsto x,\ y \mapsto -z,\ z \mapsto y.$$

respectively

$$x \mapsto -z,\ y \mapsto y,\ z \mapsto x.$$

Thus by a y-rotation the first 2 components are equal and similarly by x-rotations the remaining components are equal in pairs. Hence there are 3 independent components of the elasticity tensor in the cubic case, say: c_{xxxx}, c_{xxyy} and c_{xyxy}.

Chapter 4

Anisotropic acoustic wave equation

By Newton's second law the force per unit volume is given by

$$\vec{f} = \rho \frac{\partial^2 \vec{u}}{\partial t^2}, \tag{4.1}$$

where $\vec{u} = u(\vec{x}, t)$ is the displacement field and ρ is the mass-density which we shall assume constant. On the other hand, the force was the divergence of the stress-tensor (3.9) and the stress tensor was the derivative of the free energy density F with respect to the potential:

$$\sigma_{ik} = \frac{\partial F}{\partial u_{ik}} = \frac{\partial}{\partial u_{ik}} \frac{1}{2} c_{abcd} u_{ab} u_{cd} = c_{iklm} u_{lm}. \tag{4.2}$$

In components the force becomes

$$f_i = \sigma_{ik,k} = c_{iklm} u_{lm,k} = c_{iklm} u_{ml,k} = c_{iklm} u_{m,kl} \tag{4.3}$$

since the strain is symmetric and partial derivatives commute.

Thus in the interior of our body (Ω^o) we have the following vectorial second order linear partial differential equation:

$$\rho \frac{\partial^2 u_a}{\partial t^2} = c_{abcd} u_{d,bc}. \tag{4.4}$$

At the boundary ($\partial\Omega$) we assume that there is no force acting, ie. the free-boundary condition:

$$\vec{t} \stackrel{\text{def}}{=} \vec{\vec{\sigma}} \cdot \vec{n} = \vec{0}. \tag{4.5}$$

Here $\vec{n}$ is a vector normal to the boundary.

4.1 Dispersion relation

To analyse this linear partial differential equation it is convenient to use a plane wave ansatz

$$u_a = A_a e^{i(\vec{k} \cdot \vec{x} - \omega t)}. \tag{4.6}$$

The amplitude vector $\vec{A}$ is constant. This gives

$$c_{abcd}A_d k_b k_c = \rho\omega^2 A_a. \tag{4.7}$$

So a condition on k_a and ω for for non-trivial displacements A_a is that the matrix

$$M_{ad} = c_{abcd}k_b k_c - \rho\omega^2\delta_{ad} \tag{4.8}$$

is not invertible, ie.

$$\det(c_{abcd}k_b k_c - \rho\omega^2\delta_{ad}) = 0. \tag{4.9}$$

This gives us the dispersion relation. For a given frequency ω we can in general find 3 corresponding wave-vectors and associated polarisations, when the direction of the wave vector $\vec{n} = \vec{k}/k$ is specified. The 3 polarisations form an orthogonal set since the matrix $\mathbf{M}$ is symmetric in a and d:

$$c_{abcd}x_b x_c = c_{badc}x_b x_c = c_{dcba}x_c x_b = c_{dbca}x_b x_c, \tag{4.10}$$

for any vector x_a. Since both the wave vector and the frequency enter quadratically in the dispersion relation we actually have that k is proportional to ω. The mapping from ω and the k-direction to wave-vector-length is called the wave vector surface. This surface is 3-sheeted, since there are in general 3 different lengths of $\vec{k}$.

4.2 Slowness surface

Because of the proportionality of k to ω, acousticians have found it convenient to introduce the concept of slowness ([2, 25]). The slowness vector is defined as follows:

$$\vec{s} = \vec{k}/\omega. \tag{4.11}$$

By dimensional analysis

$$[s] = (1/L)/(1/T) = 1/(L/T) = 1/\text{Velocity}. \tag{4.12}$$

Also the velocity of the wave-front (ie. points of equal-phase) is $(\omega/k)\vec{k}/k$, so the slowness-vector is the slowness of the front. The plane wave expressed in terms of slowness is given

$$u_a = A_a e^{i\omega(\vec{s}\cdot\vec{x}-t)}, \tag{4.13}$$

which we will need later.

Corresponding to (4.7) we find

$$c_{abcd}A_d s_b s_c = \rho A_a. \tag{4.14}$$

The dispersion relation now becomes a relation between the components of the slowness:

$$S = \text{Det}(\mathbf{S}) = \text{Det}(S_{ad}) = \text{Det}(c_{abcd}s_b s_c - \rho\delta_{ad}) = 0. \tag{4.15}$$

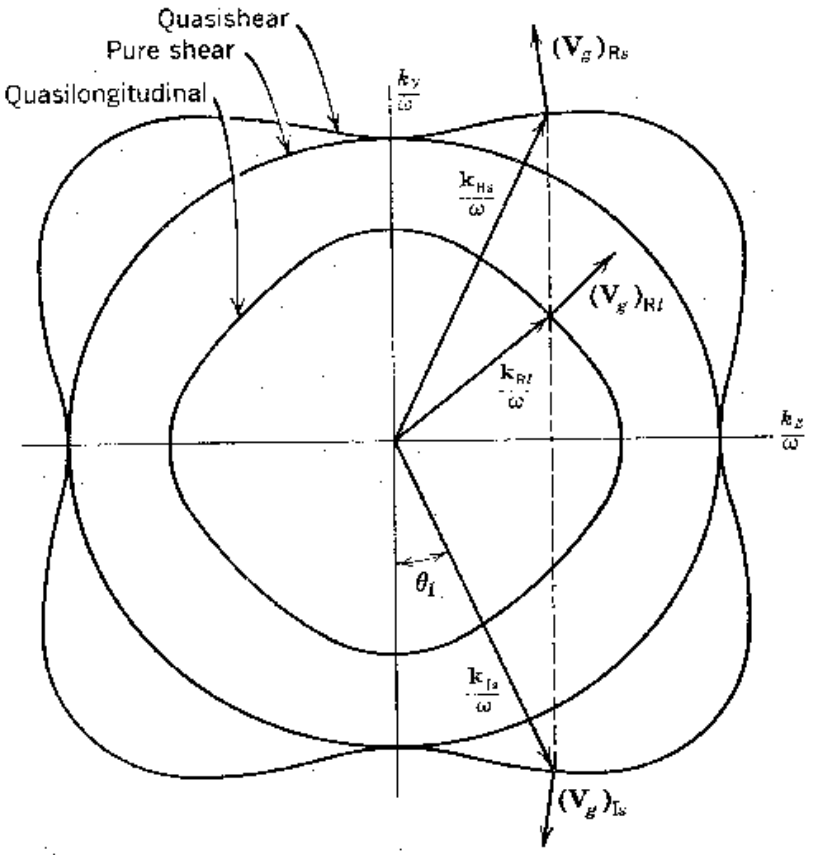


FIGURE 9.8. Quasishear scattering at an [010]-oriented free boundary of a cubic crystal. Incidence is in the (100) plane.

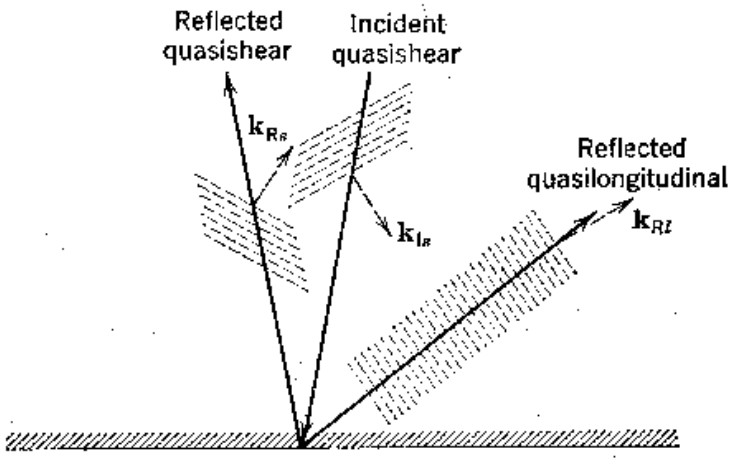


FIGURE 9.9. Ray vectors (solid arrows) and wave fronts (dashed lines) corresponding to Figure 9.8.

Figure 4.1: Figures from ref. [2] depicting a cut in the slowness surface of a cubic crystal. The 3 sheets now projects down to closed curves. The slowest wave number are the points on the so-called quasishear sheet. The names shear and longitudinal refers to the isotropic case cf. sect. 4.5 whereas "quasi" indicates that the wave vector is almost as in the isotropic case. Thus the quasilongitudinal mode has a displacement which is almost parallel to the wave vector (cf. the figure 9.9 using the ref. [2] -labelling). Remark that the group velocity V_g is orthogonal to the sheets.

The set of points (s_a) which fulfils this relation is called the slowness surface.

As a function of the direction of the front (ie. $\vec{n} = \vec{s}/s$) we have 3 different values of the slowness s. The slowness surface is therefore a surface consisting of 3 sheets. Sections of the surface is conveniently depicted in polar plots, see fig. 4.1. For each sheet we have an associated polarisation of the amplitude of the displacement and these polarisations constitute an orthogonal set (since **S** is symmetric).

Since the matrix **S** is a [3x3]-matrix and the slowness components s_a enter quadratically, the surface is an algebraic surface of order 6 (the set of zeroes of a 6 order polynomial). Furthermore, the roots to the equation $0 = S(\vec{s})$ come in complex pairs since the elasticity tensor and the density are assumed to be real quantities:

$$0 = \overline{S}(\vec{s}) = S(\overline{\vec{s}}). \tag{4.16}$$

4.3 Phase velocity

The speed of the phase is given as the inverse slowness $1/s$. The phase-velocity surface is therefore defined by:

$$\mathrm{Det}(c_{ijkl}n_j n_k - \rho v^2 \delta_{il}) = 0. \tag{4.17}$$

If the phase velocity has to be real, the matrix $\Gamma_{il} = c_{ijkl}n_j n_k$ should be positive definite. This we will show from the positivity of the potential energy $\propto c_{ijkl}u_{i,j}u_{k,l}$. The positivity of the strain energy implies that $c_{ijkl}t_{ij}t_{kl} \geq 0$ for every symmetric real matrix t_{ij}. Suppose that e_i is an eigenvector of Γ_{ik}. The corresponding eigenvalue will be

$$\lambda^{(e)} = \Gamma_{ij}e_i e_j = c_{iabj}e_i n_a n_b e_j = c_{iabj}t_{ia}t_{bj} \geq 0, \tag{4.18}$$

when we define $t_{ij} = \frac{1}{2}(e_i n_j + e_j n_i)$. Here we have used the symmetries of the elasticity tensor in the first and second pair. Since every eigenvalue is positive we therefore have positive definite matrix.

The order of the velocity surface is 12 however, (and not 6) since the direction vector contains a square root of the velocity: $n_i = v_i/\sqrt{v_j v_j}$.

4.4 Energy flux

The purpose of this section is to show that the energy flux is actually directed along the normal to the slowness surface. Later on in the WKB-section we will see that the group-velocity is also normal to the slowness surface, so we interpret this result by saying that the energy flux is just some multiple of the velocity. The flux, however, is not along the slowness-vector! This phenomenon is sometimes called extraordinary-refraction.

4.4.1 General displacement

The total energy within a wave front W is a sum of kinetic and potential energy

$$E = \frac{1}{2}\int_W dV(\rho \dot{u}_i \dot{u}_i + c_{ijkl} u_{i,j} u_{k,l}). \tag{4.19}$$

By the continuity equation for the energy, the energy flux through W becomes:

$$\int \vec{J}_e \cdot d\vec{A} = -\frac{dE}{dt}. \tag{4.20}$$

We find

$$\begin{aligned}\frac{dE}{dt} &= \int_W (\rho \dot{u}_i \ddot{u}_i + c_{ijkl} \dot{u}_{i,j} u_{k,l}) dV \\ &= \int_W (\rho \dot{u}_i c_{ijkl} u_{l,jk} + c_{ijkl} \dot{u}_{i,j} u_{l,k}) dV = \int_W (c_{ijkl} u_{l,k} \dot{u}_i)_{,j} dV \\ &= \int_W (c_{ijkl} u_{k,l} \dot{u}_i) dA_j, \end{aligned} \tag{4.21}$$

from which we deduce $(J_e)_j = -c_{ijkl} u_{k,l} \dot{u}_i = -\sigma_{ij} \dot{u}_i$. We conclude that energy flux is given by the time derivative of the displacement field and the stress tensor as

$$\vec{J}_e = -\vec{\vec{\sigma}} \cdot \dot{\vec{u}}. \tag{4.22}$$

4.4.2 Plane wave energy flux

We now consider only displacements of the form of a plane wave. The stress energy tensor depends on the displacement field as:

$$\sigma_{ij} = c_{ijkl} u_{kl} = c_{ijkl} u_{k,l}. \tag{4.23}$$

Since we do not have any imaginary displacements we have to take the real part of both the stress tensor and the displacement field in order to find the real energy flux: $\vec{J}_e = -Re(\vec{\vec{\sigma}}) \cdot Re(\dot{\vec{u}})$. Let us write the displacement field as

$$\vec{u} = A\vec{p} e^{i(\vec{k}\cdot\vec{x} - \omega t)} \tag{4.24}$$

in order to make the polarisation $\vec{p}, p^2 = 1$. explicit. The amplitude A is assumed real. This gives the flux:

$$(J_e)_i = -\frac{1}{4} c_{ijkl}[(u_{k,l} \cdot u_j^*) + (u_{k,l}^* \cdot u_j) + (u_{k,l} \cdot u_j + u_{k,l}^* \cdot u_j{}^*)]. \tag{4.25}$$

The last two terms will oscillate in time with exponential variation and will therefore not be seen in the average. The average flux therefore becomes:

$$\overline{(J_e)}_i = -\frac{1}{4} c_{ijkl}((u_{k,l} \cdot u_j^*) + (u_{k,l}^* \cdot u_j)). \tag{4.26}$$

Introducing $\omega' s$ to get the slowness we find

$$\overline{(J_e)}_i = \frac{1}{4}\omega^2 A^2 c_{ijkl}(p_k p_j^* s_l + p_k^* p_j s_l^*). \tag{4.27}$$

Let us now for simplicity assume real slowness and real polarisation. That gives us the final result:

$$\overline{(J_e)}_i = \frac{1}{2}\omega^2 A^2 c_{ijkl} p_j p_k s_l. \tag{4.28}$$

We shall later see in the WKB section chapter 5.1 that this expression is exactly proportional to the velocity. Let us at first content ourselves by showing that the energy flux is normal to the slowness surface in the case of non-cutting sheets in the surface:

By the defining relation of the slowness surface (4.15) the normal is along: $\frac{\partial S}{\partial s_a} = C_{bc}\frac{\partial S_{bc}}{\partial s_a} = 2C_{bc}c_{abcd}s_d$, where C_{bc} is the cofactor matrix of $[S_{bc}] \equiv \mathbf{S}$. Now this matrix can be decomposed in projectors, $\mathbf{S} = \sum_{\mathbf{i=1}}^{\mathbf{3}} \lambda_{\mathbf{i}} \vec{\mathbf{p}^{(\mathbf{i})}}\vec{\mathbf{p}^{(\mathbf{i})}}$ (dyadic notation). Its determinant is zero, so some of the eigenvalues are 0. If we choose a definite length of the slowness in order to get a definite polarisation, the eigenvalue associated with that given polarisation vanishes. What is left of $\mathbf{S}$ are 2 projectors orthogonal to that direction. The transpose of the cofactor of a matrix multiplied by the matrix is always equal to the determinant and since $\mathbf{S}$ is symmetric we have: $\mathbf{C}\cdot\mathbf{S} = \mathbf{S}\cdot\mathbf{C} = \det S = 0$. This implies that $\mathbf{C}$ has to live on the subspace orthogonal $\mathbf{S}$, ie. $\mathbf{S}$ is proportional to $\vec{p}\vec{p}$. We therefore conclude that the normal $\frac{\partial S}{\partial s_a}$ is proportional to

$$c_{abcd}p_b p_c s_d, \tag{4.29}$$

just as the energy flux.

Sometimes the eigenvalues of the S-matrix coincide, ie. 2 sheets cut. This is for instance the case for transverse waves in an isotropic medium. The above derivation breaks down at such points. It is however still possible to show that the energy flux associated with a given polarisation is proportional to $c_{abcd}p_b p_c s_d$. The eigenvalue associated to the polarisation $\vec{p}$ is nothing but $c_{abcd}p_a s_b s_c p_d - \rho = c_{abcd}s_a p_b p_c s_d - \rho$. This expression may be considered to be a function whose zeros define a surface, one of the sheets of the slowness surface for the given polarisation $\vec{p}$. Derivation with respect to the slowness coordinate s_a gives us a normal with terms like $c_{abcd}p_b p_c s_d$ and terms containing derivatives of the polarisation vector. Fortunately these terms vanish (since the polarisation is an eigenvector and of unit length, see chapter 5.2.1). We therefore have the nice geometrical result that the average energy flux is always proportional to the normal of the corresponding slowness sheet.

4.5 Isotropic case

In this section we consider the special case of an isotropic medium, with the elasticity tensor (3.26).

The corresponding wave equation follows from the general expression (4.4)

$$\rho\frac{\partial^2 \vec{u}}{\partial t^2} = \mu\Delta(\vec{u}) + (\lambda+\mu)\vec{\nabla}(\vec{\nabla}\cdot\vec{u}). \tag{4.30}$$

By inserting a plane wave ansatz

$$u_a = A_a e^{i(\vec{k}\cdot\vec{x}-\omega t)} \tag{4.31}$$

one finds

$$(\mu k^2 \mathbf{1} + (\lambda+\mu)\vec{k}\vec{k}) \cdot \vec{A} = \rho\omega^2 \vec{A}. \tag{4.32}$$

Let us now introduce the longitudinal and transversal projectors

$$\mathbf{P}_{||} = \frac{\vec{k}\vec{k}}{k^2} \tag{4.33}$$

and

$$\mathbf{P}_{\perp} = \mathbf{1} - \mathbf{P}_{||} \tag{4.34}$$

in the above equation:

$$\frac{\lambda+2\mu}{\rho}\mathbf{P}_{||} + \frac{\mu}{\rho}\mathbf{P}_{\perp} = \frac{\omega^2}{k^2}\mathbf{P}_{||} + \frac{\omega^2}{k^2}\mathbf{P}_{\perp}. \tag{4.35}$$

From this decomposition we conclude that waves with amplitude vector parallel to the wave vector, so called pressure-waves or P-waves, have phase velocities (ie. inverse slowness $(|\vec{k}|/\omega)^{-1}$)

$$v_P = \sqrt{\frac{\lambda+2\mu}{\rho}} \tag{4.36}$$

whereas shear-waves or S-waves have

$$v_S = \sqrt{\frac{\mu}{\rho}}. \tag{4.37}$$

From the above equation we also see that the frequency is proportional to the wave vector, eg. for an S-wave

$$\omega = v_S k \tag{4.38}$$

so the group velocity

$$\frac{\partial\omega}{\partial\vec{k}} = \frac{\omega}{k}\frac{\vec{k}}{k} \tag{4.39}$$

is the phase velocity, resp. v_P and v_S. The ratio between the velocities

$$\kappa \equiv \frac{v_P}{v_S} = \sqrt{\frac{\lambda+2\mu}{\mu}} \tag{4.40}$$

is of order 1, eg. 1.429 (used in ref. [26] corresponding to a critical angle at $\approx 45°$). This ratio will be important when we have refraction at a boundary as we shall now show.

4.6 Reflection at a boundary

The physical situation is assumed to be the following: Let a plane wave of definite polarisation from the interior of the body hit the boundary at an angle. We consider the boundary to be free, ie. there is no traction. The goal is now to construct outgoing plane waves such that this boundary condition is fulfilled. This will enable us to take any sufficiently nice ingoing wave and find the outgoing waves.

First some definitions: Assume that we are in 3 dimensions. Let the boundary correspond to the coordinate $x_3 = 0$ and the interior of the body to $x_3 > 0$. The incident wave has the form $u_k^{(I)} = A^{(I)} p_k^{(I)} e^{i\omega(s^{(\vec{I})} \cdot \vec{x} - t)}$ and the outgoing waves are of the form $u_k^{(M)} = A^{(M)} p_k^{(M)} e^{i\omega(s^{(\vec{M})} \cdot \vec{x} - t)}$, where $M = 1, 2, 3$. Thus we assume the same time dependence. The slowness of the incoming wave is assumed to be entirely in the plane $x_1 = 0$. At the boundary $x_3 = 0$ and we therefore require, that the incoming slowness projected on the boundary is conserved: $s_2^{(I)} = s_2^{(M)}$ and $s_1^{(M)} = 0$. This gives us the first 2 components of the outgoing slowness and the last is found by looking at the cuts with the slowness surface of points with these first 2 components $(0, s_2^{(I)}, s_3^{(M)})$.

This in general leads to 3 possible slowness-vectors pointing into the domain. We choose these as slowness for our plane waves. To each of these choices there also correspond definite polarisation. This is illustrated at fig. 4.1 and fig. 4.2. Since the outgoing wave no longer have the same phase velocity this will lead to refracted waves. Just as in optics one therefore finds Snell's law:

$$\sin(\theta^{(M)}) / \sin(\theta^{(I)}) = v_{(M)} / v_{(I)}, \tag{4.41}$$

where θ refers to the incidence angle and v to the phase-velocity.

4.6.1 Interlude: Critical angle

The interesting thing happens when we do not cut all sheets of our slowness surfaces with the line $(0, s_2^{(I)}, s_3^{(M)})$ but only say 2, see fig. 4.3.

This is related to the concept of critical angles. Physically, there is a certain angle when the incident plane wave is no longer converted to all 3 modes. However if $s_3^{(M)}$ is chosen complex we can cut the slowness surface. This kind of wave will therefore suffer exponential attenuation. We can show following ref. [30] that the energy flux will run along the boundary. For this we will use the averaged energy flux with complex slowness. Except for some constants it is basically the complex vector:

$$J_i = c_{ijkl}(\overline{p}_j s_k p_l + p_j \overline{s}_k \overline{p}_l). \tag{4.42}$$

Let us investigate the flux in the direction of the slowness: We find

$$J_i s_i = c_{ijkl}(s_i \overline{p}_j s_k p_l + s_i p_j \overline{s}_k \overline{p}_l). \tag{4.43}$$

Using that $\vec{p}$ is an eigenvector we have:

$$\rho p_i = c_{ijkl} s_j s_k p_l \tag{4.44}$$

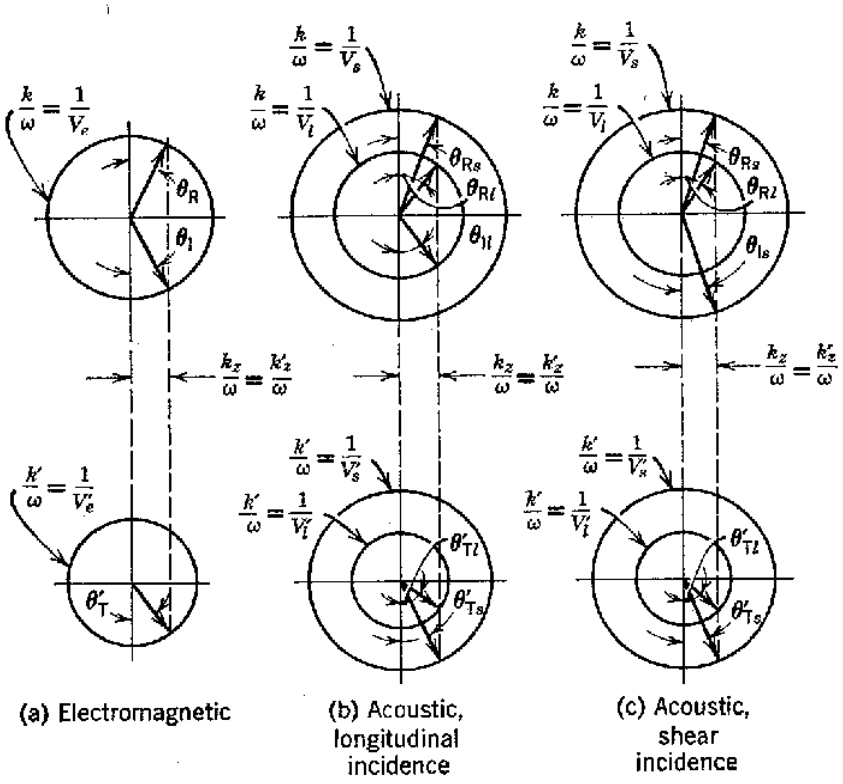


FIGURE 9.2. Derivation of Snell's Law relations from the slowness surface.

Figure 4.2: Figure from ref. [2] illustrating the law of refraction in the isotropic case. Because of isotropy the sheets of the slowness surface are spheres. Since shear waves are the slowest they have the largest radius. The reflection is here with respect to the horizontal axis. The vertical lines indicate that the projected slowness is conserved.

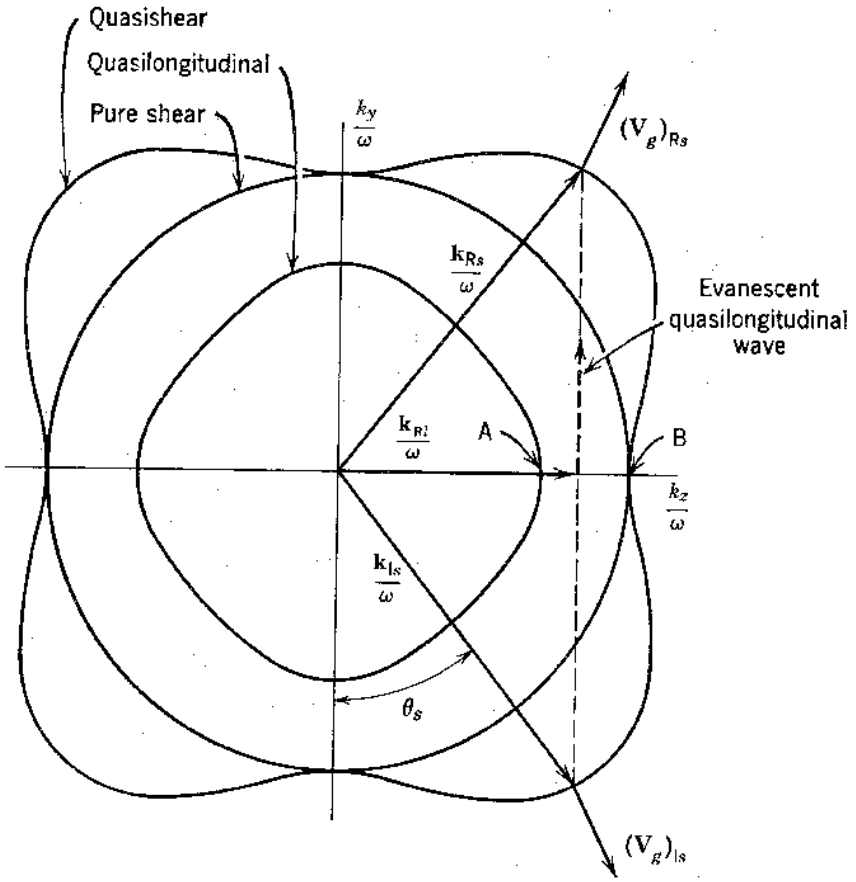


FIGURE 9.10(a). **Quasishear scattering at an [010]-oriented free boundary of a cubic crystal, with (100) plane propagation. Condition for the existence of an evanescent quasilongitudinal wave.**

Figure 4.3: Figure from ref. [2] depicting the case when we do not cut the slowness surface. Here the inner sheet of the quasilongitudinal mode is not hit by the incoming quasishear. However, if slowness is allowed complex we can cut the quasilongitudinal sheet.

and therefore

$$c_{ijkl}\overline{p}_i s_j s_k p_l = \rho |p|^2 \geq 0, \tag{4.45}$$

so the first term in $\vec{J} \cdot \vec{s}$ is real and positive. For the last term in $\vec{J} \cdot \vec{s}$ to be real and positive we use the positivity of the strain energy: For any real symmetric t_{ij} $c_{ijkl} t_{ij} t_{kl} \geq 0$. This implies for any complex symmetric t_{ij}, $c_{ijkl} t_{ij} \overline{t}_{kl} \geq 0$ (decompose in real and complex part). This we can use in the last term for the symmetric tensor $\vec{s} \odot \vec{p} = \vec{s}\vec{p} + \vec{p}\vec{s}$. By construction the flux is a real quantity, so we conclude

$$0 = J_i(s_i - \overline{s}_i) = 2 \cdot J_i Im(s_i). \tag{4.46}$$

By assumption only the slowness coordinate in the normal direction (3) was complex: $Im(s_3) \neq 0$. Hence the above sum reduces to the normal direction and we find

$$J_3 = 0. \tag{4.47}$$

The propagation of energy is therefore entirely along the boundary.

4.6.2 Amplitude ratios

Since now the dependencies on space and time and the polarisations of the plane wave have been found all we need is to find the new amplitudes.

Here we require that the force per unit area, the traction, should be zero. Since the normal vector is in the 3-direction we get:

$$\sigma_{3j}^{(I)} + \sum_{M=1,2,3} \sigma_{3j}^{(M)} = 0. \tag{4.48}$$

The stresses are calculated from the elasticity tensor as follows: $\sigma_{ij} = c_{ijkl} u_{kl} = c_{ijkl} u_{k,l}$. We find

$$\sigma_{3j}^{(I)} = i\omega c_{3jkl} A^{(I)} p_k^{(I)} s_l^{(I)} e^{i\omega(\vec{s}^{(I)} \cdot \vec{x} - t)}, \tag{4.49}$$

and

$$\sigma_{3j}^{(M)} = i\omega c_{3jkl} A^{(M)} p_k^{(M)} s_l^{(M)} e^{i\omega(\vec{s}^{(M)} \cdot \vec{x} - t)}, \tag{4.50}$$

ie. 3 linear equations in 3 unknowns

$$A^{(M)}/A^{(I)}, \tag{4.51}$$

the ratios of the outgoing and the incoming amplitudes. These equations are in the general anisotropic case solved numerically.

4.6.3 Ratios in the isotropic case

In the isotropic case it is possible find a closed expression for the amplitude ratios (ref. [18]).

It turns out that S-waves with amplitude orthogonal to the plane of incidence (ie. the plane between the boundary normal and the wave vector) do not couple to P-waves and vice versa. The remaining parts of the S-wave, however, do couple. Below we list the various possible amplitude ratios and here "S" refers to the S-waves that couple. With some calculational effort we find:

$$\alpha_{P\leftarrow P} = \frac{A_P^{out}}{A_P^{in}} = \frac{v_S^2 \sin(2\theta_S)\sin(2\theta_P) - v_P^2\cos^2(2\theta_S)}{v_S^2 \sin(2\theta_S)\sin(2\theta_P) + v_P^2\cos^2(2\theta_S)} \tag{4.52}$$

and

$$\alpha_{S\leftarrow P} = \frac{A_S^{out}}{A_P^{in}} = -\frac{2v_P v_S \sin(2\theta_P)\cos(2\theta_S)}{v_S^2 \sin(2\theta_S)\sin(2\theta_P) + v_P^2\cos^2(2\theta_S)} \tag{4.53}$$

respectively

$$\alpha_{S\leftarrow S} = \frac{A_S^{out}}{A_S^{in}} = \frac{v_S^2 \sin(2\theta_P)\sin(2\theta_S) - v_P^2\cos^2(2\theta_S)}{v_S^2 \sin(2\theta_P)\sin(2\theta_S) + v_P^2\cos^2(2\theta_S)} \tag{4.54}$$

and

$$\alpha_{P\leftarrow S} = \frac{A_P^{out}}{A_S^{in}} = \frac{2v_P v_S \sin(2\theta_S)\cos(2\theta_S)}{v_S^2 \sin(2\theta_P) sin(2\theta_S) + v_P^2\cos^2(2\theta_S)}. \tag{4.55}$$

We remark that the sum

$$\sum_M |A^{(M)}/A^{(I)}|^2 \neq 1! \tag{4.56}$$

However, by the principle of energy conservation the outgoing energy flux in the normal direction should be equal to the ingoing flux in the normal direction - what hits also gets back.

The energy flux is proportional to

$$F_i = c_{ijkl} p_j p_k s_l |A|^2. \tag{4.57}$$

In the isotropic case (3.26) P-waves with slowness parallel to the polarisation the flux becomes proportional to

$$\vec{F}_P = (\lambda + 2\mu)|A_P|^2 \vec{s_P} \tag{4.58}$$

whereas for S-waves with slowness orthogonal to the polarisation

$$\vec{F}_S = \mu |A_P|^2 \vec{s_S}. \tag{4.59}$$

For example the ratio between fluxes in the normal direction of an outgoing P-wave and an ingoing S-wave is given by

$$\epsilon_{P\leftarrow S} = \frac{\vec{F_P}\cdot\vec{n}}{|\vec{F_S}\cdot\vec{n}|} = \frac{(\lambda+2\mu)\ s_P\ \cos(\theta_P)}{\mu\ s_S\ \cos(\theta_S)} \frac{|A_P^{out}|^2}{|A_S^{in}|^2} = \frac{v_P\ \cos(\theta_P)}{v_S\ \cos(\theta_S)} \frac{|A_P^{out}|^2}{|A_S^{in}|^2}. \tag{4.60}$$

If, however, we consider no change of wave type , eg. P-wave to P-wave, the angles and the velocities are unchanged. Therefore in such cases the ratio of the fluxes reduces to the ratio of the squares of the amplitudes:

$$\epsilon_{P\leftarrow P} = \frac{|A_P^{out}|^2}{|A_P^{in}|^2}. \tag{4.61}$$

Chapter 5

Acoustic WKB

In this chapter we derive a high frequency approximation to the anisotropic acoustic wave equation (4.4). We get results similar to the Helmholtz equation derived in sect. 2.2.1.

5.1 Separation into eikonal and transport equations

The general acoustic wave equation is

$$\rho \frac{\partial^2 u_a}{\partial t^2} = c_{abcd} u_{d,bc}. \tag{5.1}$$

Here ρ is the mass-density, c_{abcd} the elasticity-tensor, and the partial derivative $\frac{\partial u}{\partial x^a}$ is denoted by "$u_{,a}$".

This equation compared to the Schrödinger case does not contain any small parameter like $\hbar$. Therefore one cannot just do a straightforward WKB approximation. We consider instead the limit of high frequencies (or short waves), and just as in QM we will observe a particle-like behaviour.

A solution of constant frequency

$$u_a(x,t) = u_a(x) e^{-i\omega t} \tag{5.2}$$

will lead us to an equation similar to the Helmholtz-equation. However this new equation will be vectorial:

$$c_{abcd} u_{d,bc} + \omega^2 \rho u_a = 0. \tag{5.3}$$

Let us introduce the oscillatory ansatz as in (2.16):

$$u_a = a_a e^{i\omega T}, \tag{5.4}$$

where T=T(x), a=a(x) which are of dimension time and displacement. After some calculation one gets

$$u_{d,bc} = (a_{d,bc} + i\omega(a_{d,c}T_{,b} + a_{d,b}T_{,c} + a_d T_{,bc}) - \omega^2 a_d T_{,b} T_{,c}) e^{i\omega T}. \tag{5.5}$$

In the high-frequency limit ω tends to infinity. Thus the most important terms are those proportional to ω^2, then ω and finally ω^0. This is just as in QM

with $1/\hbar$. In the following we shall omit the term of order ω^0 (no "quantum-potential").

With the slowness vector defined as in the scalar case (2.18)

$$s_a = T_{,a}\,, \tag{5.6}$$

we get an "eikonal" equation ($\propto \omega^2$):

$$c_{abcd}a_d s_b s_c - \rho a_a = 0 \tag{5.7}$$

and a transport equation ($\propto \omega^1$):

$$c_{abcd}(a_{d,c}\, s_b + a_{d,b}\, s_c + a_d s_{b,c}\,) = 0. \tag{5.8}$$

The ω^0 term omitted is of the form:

$$c_{abcd}a_{d,bc} = 0. \tag{5.9}$$

(Henceforth we shall omit the " " in "eikonal").

The reason for adopting the name "slowness" is the formal resemblance of (5.7) with the plane wave case cf. (4.14). Furthermore if the ansatz actually was a plane wave of constant amplitude the time function $T(x) = \vec{s}\cdot\vec{x}$, since

$$\vec{k}\cdot\vec{x} - \omega t = \omega(\vec{s}\cdot\vec{x} - t)$$

with $\vec{s} = \vec{k}/\omega$.

One could use a more refined technique and write the displacement field as an asymptotic series. One would start solving for the dominant terms and use the solution found on the next lower level. However here we will only be interested in the 2 leading terms of highest importance (just as in the quantum mechanical WKB-approximation).

5.2 Eikonal equation

In this section we will investigate the eikonal equation (5.7). The solution of the eikonal equation simply gives us the "classical paths" of the system. Its solution will then be used as "input" to the transport equation (5.8).

Before we start we remark that unlike the case of QM we actually have the amplitude present in the eikonal equation. In QM the corresponding equation, the Hamilton-Jacobi equation, is only an equation of the phase function S. How can we get rid of the amplitude vector a_i ?

First we treat the 2-tensor $c_{abcd}s_b s_c$. Because of the symmetries of the elasticity tensor, we immediately see that the 2-tensor is symmetric:

$$c_{abcd}s_b s_c = c_{bacd}s_b s_c = c_{cdba}s_b s_c = c_{dbca}s_b s_c. \tag{5.10}$$

Here the symmetries of the first 2 indices (12) and the pairs (12)(34) were exploited cf. sect. 3.4.

The unit-normal to the wave-surface T=Const. is an interesting quantity in its own right and therefore we introduce a new symmetric 2-tensor, $\mathbf{\Gamma}$, only depending on this normal:

$$\Gamma_{ad} = c_{abcd} n_b n_c. \tag{5.11}$$

With these notations we find in matrix-form:

$$\rho \vec{a} = s^2 \mathbf{\Gamma} \cdot \vec{a}. \tag{5.12}$$

Obviously the next step is to consider the i'th eigendirection of $\mathbf{\Gamma}$:

$$\mathbf{\Gamma} \cdot \vec{p}^{(i)} = \lambda_i \vec{p}^{(i)}. \tag{5.13}$$

This decomposition can also be used for the displacement field

$$\vec{a} = \sum_{i=1}^{d} a^i \vec{p}^{(i)}, \tag{5.14}$$

where d is the dimension of space. The vector $\vec{p}$ thus plays the role of polarisation, and we will also refer to it as the polarisation vector and to the different modes as polarisations. By projecting onto the i'th eigenmode we finally find:

$$\rho = s^2 \lambda^i, \tag{5.15}$$

independent of the amplitude. Actually the eigenvalue only depends on the direction of the slowness $\lambda = \lambda(\vec{n})$, and $\vec{n} = \vec{s}/s$. We emphasise that $\vec{s} = \frac{\partial T}{\partial \vec{x}}$, so what we actually have found is an equation in the first order derivatives of our time-function, $T = T(x)$. This equation is solved by introducing a Hamiltonian system cf. sect. 2.1.2, say

$$H^i(x,s) = H^i(x, \frac{\partial T}{\partial \vec{x}}) = \frac{1}{2}\left(\frac{\lambda(\vec{n})^i}{\rho} s^2 - 1\right) \tag{5.16}$$

with $H^i(x, \frac{\partial T}{\partial \vec{x}}) = 0$.

This Hamiltonian will provide us with bicharacteristics, corresponding to classical paths, no longer in (x,p)-space as in QM but rather in (x,s)-space. If the reader is uncomfortable with the slowness coordinate, he should only multiply with ω to get k-coordinates, where k is the wave-vector.

Since we have 3 modes for $d = 3$, we have in fact 3 Hamiltonian systems; one for each eigendirection. In the same way we will get 2 modes in $d = 2$. Let us consider one of these Hamiltonian systems.

5.2.1 Fixed mode

In what follows we shall consider a fixed eigendirection of our 2-tensor $\mathbf{\Gamma}$. For convenience we will put $p = p_i, \lambda = \lambda_i$. In this eigenspace the Hamiltonian we will use is

$$H = \frac{1}{2}\left(s^2 \frac{\lambda(\vec{n})}{\rho} - 1\right), \tag{5.17}$$

as above. The reason for this particular choice is that we want to define our slowness surface implicitly by the zeros of some function. In QM one has the similar idea of an energy surface which again is some surface defined implicitly by $H(x,p) = E$. For this we have added a 1 in the parenthesis defining H. We could also omit the -1, and just restrict the Hamiltonian to $1/2$. It is a matter of taste. Furthermore we multiplied with a non-zero factor one half. We could in fact have multiplied and added a lot of non-zero stuff without affecting the phase-space curves, but the above choice, however leads to slightly prettier formulas. Hamilton's equations

$$\frac{d\vec{x}}{d\tau} = \frac{\partial H}{\partial \vec{s}} \tag{5.18}$$

$$\frac{d\vec{s}}{d\tau} = -\frac{\partial H}{\partial \vec{x}} \tag{5.19}$$

will be investigated one by one. First the general anisotropic case is treated and second we check the results for the isotropic case.

We start with the "velocity equation", ie. the first equation: we notice that λ is in general only dependent on the direction $\vec{n}$. Here the direction is with respect to the direction of the slowness $\vec{s}$. The eigenvalue, however, does not depend on the actual size of the slowness, s.

The partial derivative of λ becomes

$$\frac{\partial \lambda}{\partial s_i} = \frac{\partial \lambda}{\partial n_j}\frac{\partial n_j}{\partial s_i} \tag{5.20}$$

and using $\vec{n} = \vec{s}/s$ we get

$$\vec{v} = \frac{s}{\rho}\left(\lambda\vec{n} + \frac{1}{2}(\mathbf{1} - \vec{n}\vec{n})\frac{\partial \lambda}{\partial \vec{n}}\right). \tag{5.21}$$

Now restricting to the slowness surface the relation of the eigenvalue $\rho = s^2\lambda^i$ corresponding to $H = 0$ holds. This gives in dyadic notation

$$\vec{v} = \frac{1}{s}\left(\vec{n} - (\mathbf{1} - \vec{n}\vec{n})\frac{1}{s}\frac{\partial s}{\partial \vec{n}}\right). \tag{5.22}$$

This shows explicitly that if we have anisotropy the velocity is no longer directed along the normal of constant phase $= T$, since $\mathbf{1} - \vec{n}\vec{n}$ is the transversal projector. This is different compared to the scalar phenomena such as the wave equation and the Schrödinger equation. At fig. 5.1 we see the corresponding extraordinary refraction in an experimental setting of quartz. And now a more mathematical remark to shed some light on the slowness surface. One may consider each of the Hamiltonians as functions whose zeros implicitly define each sheet of the slowness surface. We take the gradient of our Hamiltonians to find the velocity. The velocity is therefore directed along the normal of one of the chosen sheets of the slowness surface. So every time one knows the direction of the slowness' one finds the corresponding point on one sheet. At that point one

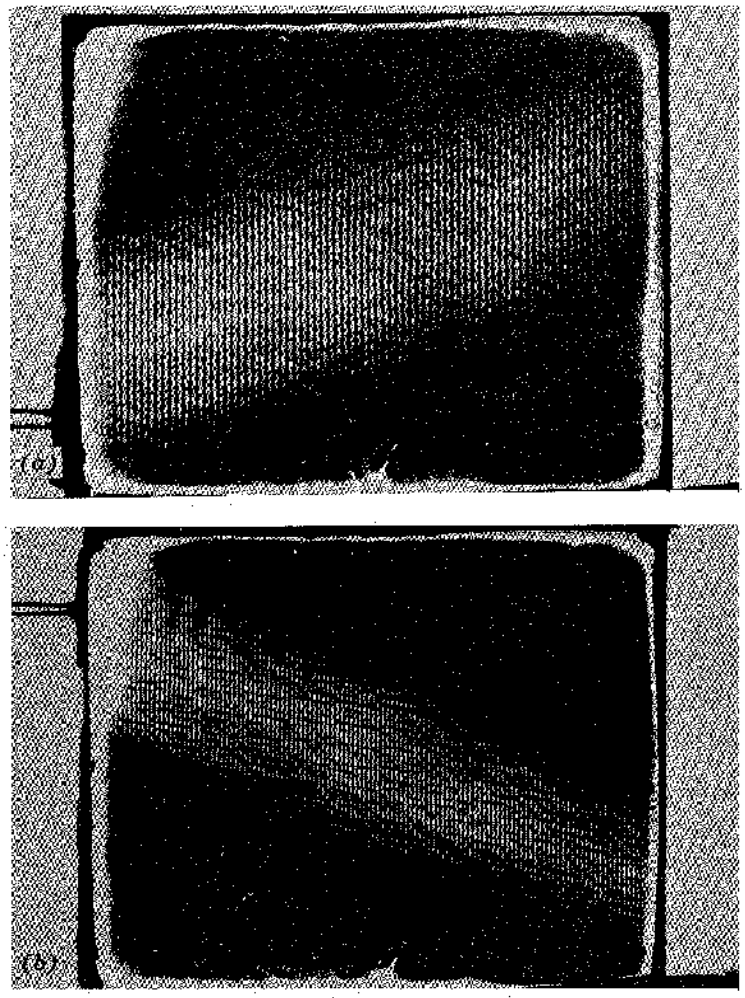


FIGURE 7.8. **Deflection of (a) quasilongitudinal and (b) quasishear acoustic beams with k parallel to the *Y* crystal axis in quartz. (After Staudt and Cook.)**

Figure 5.1: Figure from ref. [2] illustrating an elastic wave in quartz

raises the normal to find the direction of the velocity, see fig. 4.1. How about the size of the velocity? It is of course dependent of the factor chosen in front of the Hamiltonian; above we use 1/2. Choosing this factor we will get the physical velocities in the isotropic case.

We can find an explicit expression for the velocity in terms of the elasticity tensor, the slowness and the polarisation. First we re-express the product of the eigenvalue and the square of the slowness as:

$$\lambda \cdot s^2 = c_{ijkl} p_i p_l s_j s_k. \tag{5.23}$$

Then we derive with respect to the slowness, using the symmetries of the elasticity-tensor

$$\frac{\partial(\lambda \cdot s^2)}{\partial s_a} = 2 \cdot c_{ajkl} p_j p_k s_l, \tag{5.24}$$

since the terms with derivatives of the polarisation $\vec{p}$ cancel, eg. :

$$c_{ijkl} \frac{\partial(p_i)}{\partial s_a} p_l s_j s_k = \frac{\partial(p_i)}{\partial s_a} \lambda p_i = \frac{1}{2} \lambda \cdot \frac{\partial p^2}{\partial s_a} = \frac{1}{2} \lambda \cdot \frac{\partial 1}{\partial s_a} = 0. \tag{5.25}$$

As a conclusion we deduce from (5.17),(5.18) and (5.24) [1] the following important expression for the velocity:

$$v_i = c_{ijkl} p_j p_k s_l / \rho. \tag{5.26}$$

Again we emphasise that in the anisotropic case this velocity is not in general parallel to the normal of the planes of equal phase. We see from the expression for the velocity that it is exactly proportional to the energy flux vector derived in sect. 4.4.

Second, we investigate the change of slowness: Since here neither c_{ijkl} nor ρ are assumed to depend on the spatial variable $\vec{x}$ we get

$$\frac{d\vec{s}}{d\tau} = 0. \tag{5.27}$$

Therefore $\vec{s}$ and hence $\vec{n}$, $\vec{p}$, s and $\vec{v}$ are conserved along the bicharacteristic. The "classical paths" are indeed straight lines! Finally the change of our phase function T is

$$dT = \frac{\partial T}{\partial \vec{x}} \cdot \frac{d\vec{x}}{d\tau} d\tau = \vec{s} \cdot \vec{v} d\tau$$

$$= s\vec{n} \cdot \frac{1}{s} \left(\vec{n} - (\mathbf{1} - \vec{\mathbf{n}}\vec{\mathbf{n}}) \frac{1}{s} \frac{\partial s}{\partial \vec{n}} \right) d\tau = d\tau, \tag{5.28}$$

[1] This derivation is something I could not find in the acoustic literature but it seems natural when one takes a Hamiltonian point of view. The nice thing is that the result is in agreement with the averaged energy flux vector derived in a completely different way.

since the slowness is longitudinal and therefore only projects out the longitudinal part of the velocity. The same result is also found when one uses the second expression for the velocity (5.26):

$$dT = \vec{s} \cdot \vec{v} d\tau = s_i \frac{c_{ijkl}}{\rho} p_j p_k s_l d\tau = 1 \cdot d\tau, \tag{5.29}$$

since the slowness vector fulfils (4.15). Thus the curve parameter is of dimension time and equal to the phase T. Geometrically, we find

$$\Delta T = \Delta \tau = \frac{\Delta x}{v}, \tag{5.30}$$

simply by integrating the velocity equation along the configuration space path. Hereby the function T is the flight-time.

Now let us check with the isotropic case: For the velocity field we found two expressions. The first one (5.22) reduces to

$$\vec{v} = \frac{1}{s} \vec{n}, \tag{5.31}$$

since the size of the slowness vector, s, is independent on the direction. This is because of the isotropy. Thus the slowness surfaces are spheres of constant radius s. But now $\frac{1}{s}$ is the velocity of the phase, either longitudinal $v_{\|} = (\frac{\lambda+2\mu}{\rho})^{1/2}$ or transversal $v_{\perp} = (\frac{\mu}{\rho})^{1/2}$. So we conclude that the velocity on the left-hand-side of the equality sign , the ray-velocity, coincides with the phase-velocity. To check the second expression of the velocity (5.26) we use the isotropic elasticity tensor (3.26):

Consider the case of transversal polarisation: $\vec{e} \cdot \vec{n} = 0$ and $\vec{s} = s\vec{n}$. The velocity is:

$$v_i = c_{ijkl} p_j p_k s_l / \rho = \frac{1}{\rho}(\lambda \cdot 0 + \mu(0 + s_i 1))$$

$$= (v_{\perp}^2 \cdot s) n_i = v_{\perp} n_i. \tag{5.32}$$

So the velocity is directed along the normal as it should. The same result is found for the longitudinal mode.

5.3 Transport equation

Inserting the acoustic mode $\vec{a} = a\vec{p}$ associated with the polarisation $\vec{p}$ in (5.8) we find

$$0 = c_{abcd}(a_{,c}\, s_b + a_{,b}\, s_c) p_d + a(p_{d,c} s_b + p_{d,b} s_d + p_d s_{c,b}). \tag{5.33}$$

Since the velocity

$$v_a = c_{abcd} p_b p_c s_d / \rho,$$

the divergence of the velocity is,

$$v_{a,a} = (c_{abcd}p_{b,a}p_c s_d + c_{abcd}p_b p_{c,a}s_d + c_{abcd}p_b p_c s_{d,a})/\rho, \tag{5.34}$$

because the density ρ is assumed spatially constant.

After contracting the transport equation with p_a, we get

$$c_{abcd}(p_a s_b a_{,c}p_d + p_a a_{,b}s_c p_d + a(p_a s_b p_{d,c} + p_a p_{d,b}s_c + p_a s_{c,b}p_d)) = 0. \tag{5.35}$$

Next we use the symmetries of exchange of the pair (12) with the pair (34) and finally the operation of reversing the indices in each pair:

$$c_{abcd}(2a_{,a}p_b p_c s_d + a(p_{b,a}p_c s_d + p_b p_{c,a}s_d + p_b p_c s_{d,a})) = 0. \tag{5.36}$$

So by division of ρ we indeed get:

$$2\vec{v}\cdot\vec{\nabla}a + a\vec{\nabla}\cdot\vec{v} = 0, \tag{5.37}$$

or

$$\vec{v}\cdot\vec{\nabla}a + a\frac{1}{2}\vec{\nabla}\cdot\vec{v} = 0. \tag{5.38}$$

This equation is exactly of the same form as the one for the scalar Helmholtz equation (2.26). Again we can invoke (1.7) to get rid of the divergence of the velocity and obtain

$$a(\vec{x}(t)) = e^{-\frac{1}{2}\int_0^t \vec{\nabla}\cdot\vec{v}d\tau}a(\vec{x}) = \frac{1}{\sqrt{j^t(x)}}a(\vec{x}). \tag{5.39}$$

Thus we have found the time evolution of the amplitude of one polarisation. The above results for one given mode are summarised as follows:

$$\vec{u}(x(t),t) = \frac{1}{\sqrt{j^t(x)}}e^{i\omega(\int \vec{s}\cdot d\vec{x}-t)}\vec{u}(x), \tag{5.40}$$

where we have re-introduced the original time dependence. But in acoustics the slowness and the wave-vector are related by $\omega\vec{s} = \vec{k}$, so

$$u(\vec{x(t)},t) = \frac{1}{\sqrt{j^t(x)}}e^{i(\int \vec{k}\cdot d\vec{x}-\omega t)}u(x,\vec{t=0}). \tag{5.41}$$

This form appears to be the general WKB-result cf. (2.29),(2.47) and (2.68). For instance also in QM one has the similar expression, when one absorbs the $\hbar$ in the wave vector.

5.4 Acoustic evolution operator

In this chapter we find an evolution operator in the sense of Vattay for isotropic acoustics. We first describe shortly one of the obstacles for constructing an evolution operator in the general case.

5.4.1 Amplitude evolution and curvature matrix

The "curvature" matrix $\mathbf{M}$ is defined by (2.69). We wish here to point out one of the differences between the anisotropic and the isotropic case (which is equivalent to QM and other scalar equations as well). The curvature matrix was the Hessian of the action function S in QM: $\mathbf{M} = \frac{\partial^2 S}{\partial \vec{q} \partial \vec{q}}$ (in acoustics we should replace the S with our homemade T).

One of the features of this curvature evolution was that the trace of the curvature matrix was related to the divergence of the velocity field - which shows up in the transport equations for the amplitude cf. (2.65):

$$\dot{\kappa} = -\frac{1}{m} \mathrm{Tr}\, \mathbf{M}, \tag{5.42}$$

where $\kappa = \log(a^2)$, since

$$\vec{\nabla} \cdot \vec{v} = \frac{1}{m} \vec{\nabla} \cdot \vec{p} = \frac{1}{m} \vec{\nabla} \cdot \vec{\nabla} S = \frac{1}{m} \mathrm{Tr} \left(\frac{\partial^2 S}{\partial \vec{q} \partial \vec{q}} \right) = \frac{1}{m} \mathrm{Tr}\, \mathbf{M}.$$

The step where we transformed the velocity to momentum seems necessary if one wants to introduce the Hessian of the phase function. This step cannot be done in the general anisotropic case. The reason is the "extra-ordinary " refraction, that the velocity is no longer parallel to the "momentum", the so-called slowness, see (5.26). Thus in the general anisotropic case (5.42) no longer holds.

This is in fact not something particular for acoustics - it is also found in QM when a magnetic field is present. We recall the following fact from ref. [13] that the momentum in that case has the form

$$\vec{p} = m\vec{v} + q\vec{A}/c, \tag{5.43}$$

where $\vec{A}$ is the vector potential.

However, in the isotropic case the velocity is parallel to the momentum, the slowness. For a fixed mode the velocity will always be a constant multiple of the slowness and therefore the situation is just as in QM with its constant of proportionality $1/m$. In the isotropic case we have that the velocity of the ray is the phase-velocity, so here

$$\vec{v} = v^2 \vec{s} = v^2 \frac{\partial T}{\partial \vec{q}}, \tag{5.44}$$

with the constant $v^2 = \frac{\mu}{\rho}$ or $v^2 = \frac{\lambda + 2\mu}{\rho}$. Hence the divergence of the velocity becomes

$$\vec{\nabla} \cdot \vec{v} = v^2 \mathrm{Tr} \left(\frac{\partial^2 T}{\partial \vec{q} \partial \vec{q}} \right), \tag{5.45}$$

which gives us the Hessian of the phase function and thus (5.42) holds.

We shall now only consider the isotropic case since the general anisotropic case does not seem to fit in the scheme of curvature evolution or perhaps the curvature evolution is more complicated than in the isotropic case. To investigate these matters furter seems to be beyond the scope of this thesis.

5.4.2 Isotropic case

Above we saw that the curvature matrix in the isotropic case did describe the amplitude evolution. Thus the arguments of ref. [33] carries over to this case and a construction of an evolution operator is straight forward. Time is here the curve coordinate, so the amplitude $a = a(q(t))$ and the phase $S = S(q(t))$ depend implicitely on t.

The evolution operator acts on densities of the form:

$$\tilde{\vec{u}}(\mathbf{q}, \mathbf{s}, \mathbf{M}) = \vec{u}(\mathbf{q})\delta(\vec{s}\,' - \vec{\nabla}T(\vec{q}\,'))\delta(\mathbf{M}' - \mathbf{D}^2T(\vec{q}\,')), \tag{5.46}$$

Suppose we have a given initial displacement $\vec{u_0}$. We know how one fixed mode will evolve. That is described in the WKB-part. An operator to select the piece of $\vec{u_0}$ that has a given polarisation is a projector $\vec{p}\vec{p}$ (dyadic form), where $\vec{p} = \vec{p}(\partial T/\partial \vec{q})(\vec{q}(t))$ is the polarisation vector of unit length. Similarly we know that when a given mode hits the boundary splits into 3 new outgoing waves. From the plane wave analysis which also holds in the case of oscillatory solutions the amplitudes changes with certain factors which are determined from the free boundary condition (see sect. 4.6.2).

This suggests cf. (2.4) the introduction of the following operators acting on our oscillatory solutions: A flight operator associated with polarisation p:

$$\begin{aligned} F_p^t &= e^{i\omega \int \vec{s}\cdot d\vec{q} + \frac{1}{2}v^2 \int_0^t d\tau\, \mathrm{tr}\,\mathbf{M}^\tau(q', s', \mathbf{M}')} \\ &\quad \times \delta(\vec{q}\,' - \vec{q}'^t)\delta(\vec{s}\,' - \vec{s}'^t)\delta(\mathbf{M}' - \mathbf{M}^t(q, p, \mathbf{M}))\vec{p}\vec{p}. \end{aligned} \tag{5.47}$$

The exponential containing the integral of the trace of the curvature matrix gives us the desired $1/\sqrt{j}$-factor found in the WKB expansion.

Similarly there is a a reflection operator at the boundary which converts one mode to another:

$$\vec{\vec{R}}_{p_2p_1} = \mathcal{F}_{p_2p_1}\vec{p_2}\ \vec{p_1}. \tag{5.48}$$

Here $\mathcal{F}_{p_2p_1}$ is some fraction. Following ref. [26] it is the square root of the ratio of the outgoing energy flux to the incoming flux with a sign s_p equal to the sign of the product of all the amplitude ratios. In that way the displacement field (which is the field we evolve) gets the right sign and the balance of energy at the boundary is maintained. We adopt the same choice. Thus in the isotropic case we use the formulas from sect. 4.6.2.

The accumulated effect of free flight and wave split is now described by the evolution operator:

$$\mathcal{L}^t(\tilde{x}, \tilde{s}, \tilde{\mathbf{M}}|x, s, M) = \sum_{n=0}^{\infty} \sum_{p_0, p_1, \ldots, p_n \in \{1,2,3\}} R_{p_n p_{n-1}} \cdot F_{p_{n-1}} \cdot \ldots \cdot R_{p_1 p_0} \cdot F_{p_0}. \tag{5.49}$$

The sum over n is a sum over possible reflections. For a given fixed time there will sometimes exist orbits with infinitely many reflections, for instance in a corner. That is why we have to sum to infinity and finally the sum over p_i is sum over the

possible modes. If $n = 0$ we just have free flight. If $n = 1$, however, we hit the boundary and the wave is split into three, since we sum over the last polarisation p_1. We remark that the operator is a matrix operator since it has to act on the vectorial displacement field.

5.4.3 Fredholm determinant and zeta function for acoustic wavesplit

The evolution operator for acoustics is basically for free flight equal to Vattay's operator, since also curvature evolution is needed. The interesting things happen at the boundary. What we are interested in is the case of free boundary conditions which lead to mode conversions. Hence the trace of our matrix evolution operator contain orbits consiting of segments with different polarisations.

Now let us consider the special case of 2-d isotropic acoustics. For classical calculations we use as a boundary factor $f_p = \prod_{i=1}^{n_p} \epsilon_{i+1,i}$ the product of all the flux ratios (see (4.60)) for every hit of the boundary of the orbit. Similar for acoustic calculations we use the square of the flux factor as above with a sign s_p equal to the sign of the product of all the amplitude ratios as in ref. [26]. Finally we get the usual Maslov phase which in the 3 disc case reduces to multiplication by a sign.

In practice we need to calculate the flight time, stability and the reflection coefficients from the boundary. The flight time T_p is the physical flight time, ie. the time calculated with respect to the different velocities of propagation. The stability is found by multiplying all the differentials of the different segments of the orbit in the same cyclic order as the segments. The free flight is given by the differential

$$\begin{bmatrix} 1 & \Delta x \\ 0 & 1 \end{bmatrix} \tag{5.50}$$

and the reflection by

$$-\begin{bmatrix} 1 & 0 \\ \frac{2}{R\cos(\phi_-)} & 1 \end{bmatrix}. \tag{5.51}$$

whereas a refraction from a S- to a P-wave is

$$-\begin{bmatrix} \frac{\cos(\phi_+)}{\cos(\phi_-)} & 0 \\ \frac{1}{R}\left(\frac{\kappa}{\cos(\phi_+)} + \frac{1}{\cos(\phi_-)}\right) & \kappa\frac{\cos(\phi_-)}{\cos(\phi_+)} \end{bmatrix}. \tag{5.52}$$

and similar for P to S (replace κ with $1/\kappa$). The symbols used are Δx flight length, R radius of curvature and ϕ angle of incidence. See the appendix A.3 for a derivation. The flux factor $f_p = \prod_{i=1}^{n_p} \epsilon_{i+1,i}$ is the product of all the flux ratios (see (4.60)) for every hit of the boundary of the orbit.

Classically we find the trace of the evolution operator is cf. (1.11) and (1.16)

$$\mathrm{tr}\,\mathcal{L}(s) = \sum_p T_p \sum_{r=1}^{\infty} f_p^r \frac{e^{sT_p r}}{|\det(\mathbf{1} - \mathbf{J}_p^r)|} z^{n_p r}. \tag{5.53}$$

leading to the Fredholm determinant

$$\det(1-\mathcal{L}) = \exp\left(-\sum_{p,r}\frac{f_p^r}{r|\Lambda_p|^r}\frac{e^{sT_p r}}{(1-1/\Lambda_p^r)^2}\right) \tag{5.54}$$

Expanding the Fredholm determinant to leading order we find the cycle weight

$$t_p = f_p\frac{e^{sT_p}}{|\Lambda_p|}z^{n_p}, \tag{5.55}$$

which looks like the familiar classical orbit weight, however modificated by the flux factor f_p.

In acoustics we find

$$\det(1-\mathcal{L}) = \exp\left(-\sum_{p,r}\frac{s_p^r\sqrt{f_p^r}}{r|\Lambda_p^r|}\frac{e^{(i\omega T_p - im_p\pi/2)r}}{(1-1/\Lambda_p^r)^2}\Delta_{p,r}\right)$$

where

$$\Delta_{p,r} = \frac{|\Lambda_p^r|^{1/2}+|\Lambda_p^r|^{-5/2}}{1-1/\Lambda_p^{2r}}. \tag{5.56}$$

Similarly when expanding the acoustic Fredholm determinant above we find the cycle weight

$$t_p = s_p\sqrt{f_p}\frac{e^{i\omega T_p - im_p\pi/2}}{\sqrt{|\Lambda_p|}}z^{n_p} \tag{5.57}$$

looking just like the Gutzviller weight except for the extra flux factor.

Chapter 6

Numerical results

In this chapter we apply the above theory for acoustics. It should be said that the investigations here are only a very preliminary test of the formalism. Basically we repeat some of the published calculations for classical flows and QM and then carry out the corresponding 2-d acoustic calculation. We specialise the acoustic medium to be isotropic. The ratio $\kappa = 1.429$ is studied, following ref. [26]. In this case the critical angle is $\approx 45°$.). We consider only the 3-disc system as described in ref. [12, 8] and below. The formulas used are given in sect. 5.4.3.

The first part is devoted to "classical" investigations of the escape rate whereas the last part predicts acoustic resonances. The acoustic spectrum we find is related to a (thin) plate experiment where only vibrations in the plate, ie. non-orthogonal displacements, are measured. We compute the spectrum of the 2-d isotropic acoustic wave equation in the high frequency approximation. The code for determining which orbits were allowed was fixed by considering the touching scalar 3-disc system ($R/a = 2.0$) [1] .

6.1 The 3-disc system

This billiard consists of 3 discs of equal size. The radius of a disc is denoted with an a whereas the disc separation (measured from the disc centres) is denoted with an R. We assume that the disc centres are situated in the vertices of an equilateral triangle. Just as in ref. [8] we study the case $R/a = 6$ in order to

[1] In that system the 10 forbidden orbits are

Symbol string	Orbit #
0	1
000011	16
0000001	24
0000011	25
00000001	70
00000011	71
000000001	126
000000011	127
0000000001	225
0000000011	226

as shown in ref. [29].

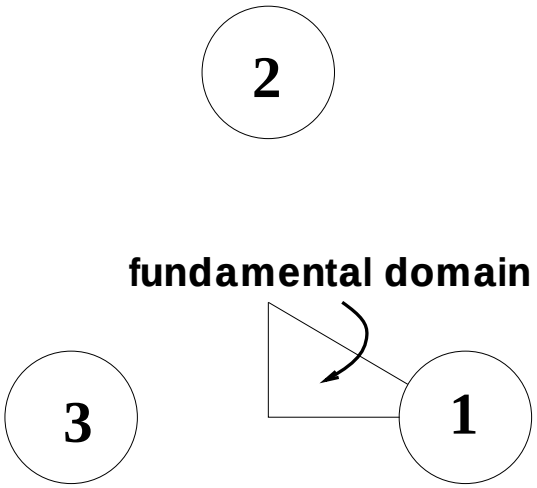


Figure 6.1: The 3-disc system.

compare with the quantum mechanical case. Because of the symmetry of the system the dynamics reduces to the fundamental domain, fig. 6.1.

The symmetry group is the group of symmetries of an equilateral triangle C_{3v}. This group consist of 2 rotations ($\pm 120^\circ$ C_3 and C_3^2) and 3 reflections (σ_{12}, σ_{23} and σ_{13}) besides the neutral element e. There are 3 irreducible representations of C_{3v} : A_1 (symmetric), A_2 (antisymmetric) and E (2 dimensional). The characters are

C_{3v}	A_1	A_2	E
e	1	1	2
C_3, C_3^2	1	1	-1
σ_v	1	-1	0

A suitable symbolic dynamics has been found to be the following. A "0" indicates that an orbit returns to the disc it started from (e.g. discs 1,2,1 are visited) and "1" that the orbit continues to the third disc (e.g. 1,2,3 are visited). This symbolic dynamics is designed for the case without wave split. However, when dealing with acoustics in 2-d we have 2 kinds of waves: P and S (pressure and shear). Now for every periodic orbit we will have sequence of 0's and 1's like e.g. (01) for 010101... . Similarly there will be a sequence of wave types used e.g. (PPS) for PPSPPS... . We describe such an orbit with the "product" of the 2 alphabets. The orbit considered is therefore ([0P][1P][0S][1P][0P][1S]). Instead of concatenating the 0,1-symbols with the wave type symbols we choose to use the 4 symbols 0,1,2 and 3, where 0=[0P],1=[0S],2=[1P] and 3=[1S]. Thus the orbit considered will be (021203). The primitive orbits are described by the prime words in the above alphabet (here we think modulo cyclic permutation). For 2 symbols the total number of prime words up to length 10 is 226. For 4 symbols, however, this number is largely increased in our calculations: we use 40584 prime words up to symbolic length 9.

The material is assumed to have velocity of the S-wave $v_S = 1$ whereas the P-wave velocity is $v_P = \kappa v_s = 1.429$. The periodic orbits now also contain refracted orbits, ie. orbits with wave split. Because of the difference of velocity it is no longer the law of reflection that holds but rather the law of refraction (Snell's law). To find the orbits we minimise the flight time, following the method of ref. [12]. This method find all the orbits, including the refracted ones.

As the discs get closer some of the free flight parts start to cross, and many orbits cease to exist.

6.2 Calculations

When we do numerics we introduce a cycle expansion (chapter 1.2) and reduction to the fundamental domain (chapter 1.4) as usual. The group C_{3v} was implemented by storing the group multiplication table as a matrix but since we only investigate the fundamental representation A_1 where all characters equals 1 we actually do not need any reference to the group.

Our evolution operators have the form (1.11). When trace is taken all we need to calculate is the flight time, stability and the boundary reflection coefficients. The stability is found by multiplying all the differentials of all the segments along the orbit.

6.3 Classical case

Even though all orbits exist in a geometrical sense (the reflection and the refraction law are fulfilled) some orbits do not contribute. This is because some orbits contain forbidden conversions. If a P-wave bounces at a right angle and changes to a S-wave the corresponding flux ratio is actually zero (see (4.60)). Therefore the short orbit (01) is forbidden. Thus we no longer have maximal shadowing and the convergence is no longer as good in the scalar 3-disc case. Using double precision (64 bits) we find for various cycle lengths:

N	number of orbits	escape rate
2	10	0.442
3	30	0.441
4	90	0.443
5	294	0.444159
6	964	0.44416302
7	3304	0.444163083
8	11464	0.444163086
9	40584	0.4441630859

These numbers should probably only be interpreted to the 6'th digit because of the limited precision (unfortunately the programming language I used did not have quadruple precision). Comparing with the non-splitting case (cf. ref. [8]) we have found that double precision only gives the escape rate found by Rosenquist ref. [12] to 6 significant digits. We estimate the leading eigenvalue (corresponding

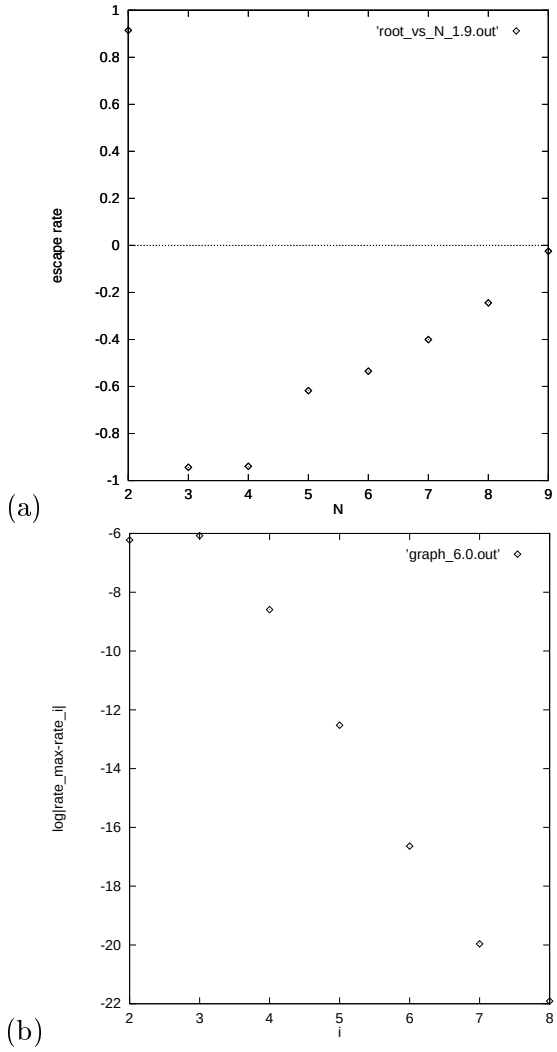


Figure 6.2: (a) Escape rate of the $R/a = 1.9$ wave split 3-disc system and (b) convergence in the open $R/a = 6$ 3-disc system.

to an escape rate) to 0.444163 ± 0.000003, slightly larger than Per Rosenquist's scalar escape rate 0.41033840776934648933846130781 92 (!). Finally a closed billiard ($R/a = 1.9$) was also considered but there we did not find any convergence of the leading eigenvalue. We refer to fig. 6.2. Of the 40584 orbits only 12827 existed geometrically (actually there are even fewer acoustic orbits since some have weight equal to zero).

6.4 Acoustics

Using a plotting program (e.g. GNUPLOT) we draw contour plots of the function $\log|1/\zeta|^2$ resp. $\log|F(\omega)|^2$ for both QM and acoustics. Zeros will then occur as valleys in the plot.

At fig. 6.3(a) we see a part of the quantum resonances for the 3-disc system

together with some acoustic resonances at fig. 6.3(b).

The exact location of the resonances can be found by using a Newton algorithm to find the zeros of the Fredholm determinant. In this thesis we content ourselves by determining the leading resonance by manual interpolation. The leading resonance is determined by the frequency with the smallest imaginary part (corresponding to the longest lifetime). We find approximately for acoustics $\omega = 0.8428 - i0.1295$ in the fundamental representation. This resonance is not so different from the quantum mechanical leading resonance at $0.758 - i0.122$. The next leading acoustic resonance appears to be at $2.5 - i0.22$. It is clear that the frequency scales as 1/length. Thus if the whole 3-disc system is enlarged by a factor 2 the frequencies become half as big. Thus 2 isotropic 3-disc system may be compared if they share the same R/a and $\kappa = v_{||}/v_{\perp}$.

Summary and Conclusion

We have established that a WKB expansion is possible in acoustics. Following the same steps as Vattay in ref. [33] we then construct an evolution operator describing the free propagation of an individual acoustic mode in an isotropic medium. The acoustic wave is refracted when it hits the boundary, and in general will split into 3 different modes. We include these effects following the approach of ref. [26]. When the methods of periodic orbit theory are applied to the hereby constructed evolution operator we find that we only have to introduce minor changes in the formulas for the spectral functions, the trace and the Fredholm determinant in both the classical and the quantum case. The Fredholm determinant of the Vattay operator in the quantum mechanical case contains extraneous zeros, so one can alternatively derive the Gutzwiller zeta function by standard formal manipulations in the periodic orbit theory. These steps are also possible in acoustics, where we basically find the same zeta function with Gutzwiller's orbit weights. The weights are modified by energy flux factors coming from the boundary reflections. The acoustic isotropic evolution operator does not seem to be derived elsewhere in the literature (to the best knowledge of the author). This leads to a determinant formula for the spectrum:

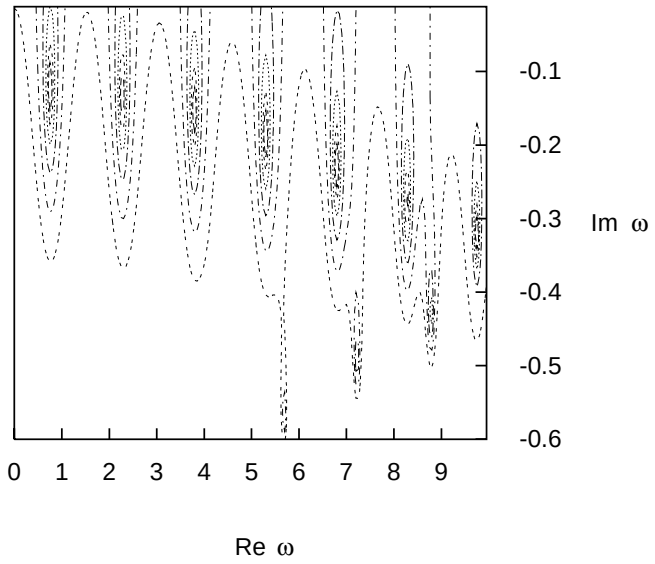
$$\det(1-\mathcal{L}) = \exp\left(-\sum_{p,r}\frac{s_p^r\sqrt{f_p^r}}{r|\Lambda_p^r|}\frac{e^{(i\omega T_p - im_p\pi/2)r}}{(1-1/\Lambda_p^r)^2}\Delta_{p,r}\right)$$

where

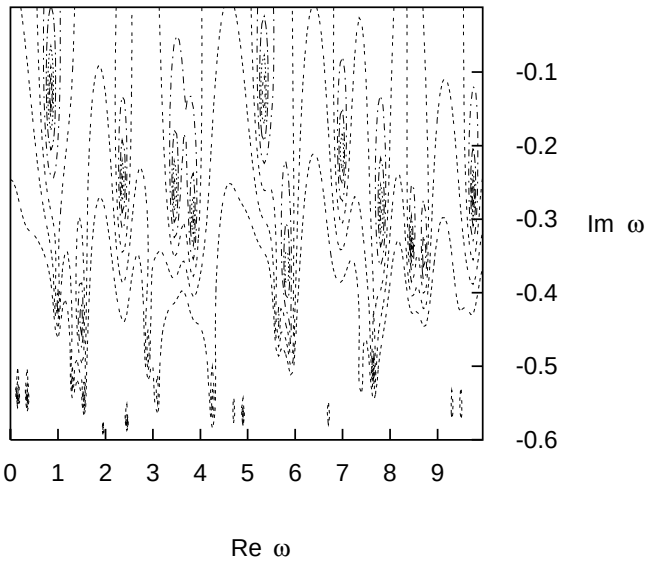
$$\Delta_{p,r} = \frac{|\Lambda_p^r|^{1/2} + |\Lambda_p^r|^{-5/2}}{1-1/\Lambda_p^{2r}}.$$

implying a cycle weight of the form

$$t_p = s_p\sqrt{f_p}\frac{e^{i\omega T_p - im_p\pi/2}}{\sqrt{|\Lambda_p|}}.$$



(a)



(b)

Figure 6.3: (a) Quantum resonances. $\log|1/\zeta|^2$ versus frequency ω. (b) Acoustic resonances. $\log|F|^2$ versus frequency ω.

Here the difference from Gutzwiller's weight is f_p (resp. s_p) square root of the product of all the energy flux ratios (resp. of the sign of all the amplitude ratios) for every hit at the boundary.

The numerical tests in chapter 6 of these formulas are only preliminary and need further work, beyond scope of a master's thesis.

In a larger perspective the obtained results suggest that orbit weights for linear partial differential equations should have the following asymptotic form

$$t_p = \frac{e^{i\omega T_p - i m_p \frac{\pi}{2}}}{\sqrt{|\Lambda_p|}},$$

more or less modified by boundary factors. Here the orbits are found for the corresponding Hamiltonian system given by the so-called principal symbol of the partial differential operator, T_p is the cycle time, m_p the Maslov index and $|\Lambda_p|$ the stability of the orbit (i.e. the product of its expanding eigenvalues).

In crystal acoustics wave splitting and anisotropy play a role. This leads to many more orbits. In closed systems we expect large orbit "pruning" effects. We have checked the closed 3-disc system ($R/a = 1.9$) and found that a lot of orbits are actually forbidden, in comarison to the open 3-disc system ($R/a = 6$). Furthermore the convergence is poorer than in the scalar case because some orbits contain forbidden mode conversions and thus carry no weight. Hence the shadowing of the longer orbits is suppressed. But the shadowing is absolutely necessary when we have much more orbits as in our case, since the cycle expansion is the scheme used here for organising the periodic orbits. If for acoustics one could find a better symbolic dynamics with less pruning one might succeed in constructing more effective cycle expansions.

In order to investigate a theory which focuses on periodic orbits, it therefore pays to first concentrate on scattering problems where most orbits have a non-zero weight. One should compare with the exact spectra calculated by other methods and spectra found in scattering experiments. Then one could start to incorporate diffraction, evanescent/creeping orbits (listening behind a corner) and higher terms in the perturbation series. Surface waves and free plate/membrane vibrations (cf. ref. [18]) and anisotropic media should also be considered. Next electromagnetics and redoing the calculations in crystal optics and piezo-electricity would be of interest.

But at the moment the greatest experimental interest (at least at CATS) in acoustics appears to be in closed systems. Thus one is concerned about the acoustic spectra of blocks, spheres etc. For the time being there is no satisfactory theory of such systems. The best method (if the corresponding classical dynamics is chaotic) right now for acoustics of closed systems is probably the transfer matrix method as described in ref. [31]. But still from a theoretical point of view we would prefer a working theory of periodic orbits to this latter statistical theory of transfer matrices, because the periodic orbits presumably contain much more information about the system. Therefore a theory of acoustic chaos would certainly benefit from developments in the general understanding of closed, pseudo-integrable and mixed systems. That information will hopefully

come from the many ongoing investigations all over the world of closed billiards in quantum chaos and from experiments in microwave cavities.

Appendix A

Appendices

A.1 Regular representation

Here follows a little introduction to the theory related to the regular representation. For references see ref. [16]. The regular representation is defined as follows: Let the group G have the elements $g_1, ..., g_{|G|}$. Define a vector space by the basis $|g_i>, i = 1, ..., |G|$. Let G act in the obvious way

$$D(h)|g>=|hg>=\sum_{l\in G}\delta_{hg,l}|l>, \tag{A.1}$$

corresponding to a $|G| \times |G|$ matrix representation with $D(h)_{lg} = \delta_{hg,l}$. We see that the trace in the regular representation is nothing but:

$$\mathrm{tr}\,(D(h)) = \sum_g D(h)_{gg} = \sum_g \delta_{hg,g} = \sum_g \delta_{h,e} = |G|\delta_{h,e}. \tag{A.2}$$

The decomposition of the regular representation into its irreducible components follows the standard procedure: Since $D = \oplus n_\alpha D_\alpha$, where n_α is the number the representation α occurs in the regular, we get $\mathrm{tr}\,(D(h)) = \oplus n_\alpha \chi_\alpha(h)$. By orthonormality of characters:

$$n_\alpha =< \mathrm{tr}\, D, \chi_\alpha >\equiv \sum_i \chi_\alpha^{*i}\chi_{(Reg)i}\cdot\frac{n_i}{|G|}. \tag{A.3}$$

Here we sum over all the different conjugacy classes i (the character only depends on the conjugacy class) and n_i is the number of elements in the class. Now the elements conjugated to the neutral element (e ie. the identity) is only the neutral element itself:

$$e \sim x \Leftrightarrow \exists g \in G : g\cdot e\cdot g^{-1} = x \Leftrightarrow \exists g \in G : e = x. \tag{A.4}$$

So since the regular character only is non-zero on the neutral element we get:

$$n_\alpha = \frac{1}{|G|}\chi_\alpha^{*i=e}\cdot|G|. \tag{A.5}$$

But the character of the neutral element is the dimension of the representation:

$$n_\alpha = d_\alpha. \tag{A.6}$$

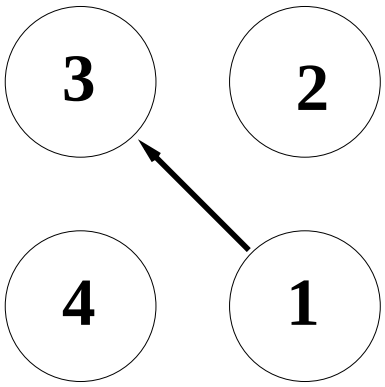


Figure A.1: The 4-disc system and one of its boundary orbits (13).

We therefore conclude

$$D_{reg} = \bigoplus_{\alpha} d_\alpha D_\alpha. \tag{A.7}$$

A.2 Boundary orbit

To describe boundary orbits we choose to consider the 4-disc system (4 equally sized discs with the centers in the vertices of a square) with the symmetry group C_{4v}.

We classify the orbits by using the disc labels: 1,2,3 and 4 or use a symmetry reduced alphabet (ie. an alphabet in which the "words" are invariant under the symmetry operations) using only 3 letters 0,1,2 ; see ref. [10]. For the 4-disc system which is the system considered here we only have one orbit in the fundamental domain where the sum over group elements above have more than 1 term, namely the orbits corresponding to (13) and (24). These orbits run along the 2 "diagonals " which are symmetry lines. In the fundamental domain these orbits become the orbit called (2) in the symmetry reduced alphabet. The 2 group elements are C_2 and σ_{13}. This boundary orbit requires special treatment. The two orbits of the form $\overline{2}$, (13) and (24), run on the boundaries of the tiles that constitute the whole 4-disc billiard. The purpose of this section is first by careful inspection to see what group element one should use in the particular case of the 4-disc system:

$$\frac{C_2 + \sigma_{13}}{2}. \tag{A.8}$$

Second we will give plausible arguments for general boundary orbits that the corresponding "element" is of the form

$$g_{close}\frac{\sum_{h\in\mathcal{H}_p} h}{|\mathcal{H}_p|}, \tag{A.9}$$

where $\mathcal{H}_p$ is the invariance group of the orbit.

The path that goes from disc 1 to 3 corresponds to the primitive orbit in the fundamental domain. This orbit does not close in the physical domain. For odd

repetitions the group elements that bring us back to the fundamental domain are C_4 and σ_{13}, for even repetions the elements are e and σ_{24}. For the path from disc 2 to disc 4 we find the same, just with σ_{13} replaced by σ_{24}. When summing over orbits one should also consider the orbits going from disc 3 to 1 resp. 4 to 2. All these orbits in fact give the same characters in the trace. That the character related to the orbit (24) is the same as the one related to (13) comes from the fact that the corresponding group elements that bring the orbit back to the fundamental domain are just conjugated to the group elements from (13): Suppose we have two points a and b and $h \in G$ is the element such that $h^{-1} \cdot b = a$ and similarly two points $a' = g \cdot a$ and $b' = g \cdot b$ where g is some group element (in the 4-disc case it could be C_4 which relates the orbit (24) to (13)). We then see that $h' = g \cdot h \cdot g^{-1}$ is the group element that brings us back from b' to a'. But now $\chi(h) = \chi(h')$ for any character χ.

Ignoring $|\det(\mathbf{1} - (h_{p,r}\mathbf{J}_p)^r)|$ for a moment we get a factor $\chi_\alpha((\frac{C_2+\sigma_{13}}{2})^r)$ in the trace when one includes all these periodic orbits (in the fundamental domain) (since $(\frac{C_2+\sigma_{13}}{2})^2 = \frac{e+\sigma_{24}}{2}$ and in fact $\frac{C_2+\sigma_{13}}{2} \cdot \frac{e+\sigma_{24}}{2} = \frac{C_2+\sigma_{13}}{2}$). Thus it is possible to actually resum the Fredholm determinant and find to leading order the zeta function, now however with this more general group element: $\frac{C_2+\sigma_{13}}{2}$.

This factor is not an element of the group but rather an element in the more abstract group algebra which is simply described as all finite sums of group elements with coefficients in some field e.g. the complex numbers:

$$c_1 g_1 + ... + c_n g_n, n \ \in \mathcal{N}. \tag{A.10}$$

Addition and multiplication of such elements is defined in the obvious way (think of the group elements as matrices). [1]

Thus we have found that we should replace the closing group element in the case of boundary orbits by a closing element in the group algebra. This element has the form

$$g_{close} \frac{\sum_{h \in \mathcal{H}_p} h}{|\mathcal{H}_p|}, \tag{A.11}$$

where $\mathcal{H}_p$ is the invariance group of the orbit (for the 2-orbit above this subgroup of C_{4v} is e, σ_{24}) and as a closing element we can choose any of the closing elements the boundary orbit may posses (C_2 or σ_{13}).

The reason for this form is the following fact which is not hard to prove:

All the closing elements=$g_{close}\mathcal{H}_p$,

where g_{close} is some closing element. This expression also holds for non-boundary orbits. It does not matter which closing element we use (a different element would have the form $g'_{close} = g_{close}h'$ with $h' \in \mathcal{H}_p$). All the elements which do not leave the orbit invariant must belong to $G/\mathcal{H}_p$ giving us the multiplicity of the orbit as

$$m_p = |G|/|\mathcal{H}_p|. \tag{A.12}$$

[1] This formal definition can also be formulated by saying that the group algebra over the field $\mathcal{F}$ is all functions $f : G \to \mathcal{F}$ such that $f(g) \neq 0$ only for a finite number of group elements $g \in G$. This last condition is of course fulfilled for finite groups. Addition now becomes point-wise addition whereas multiplication becomes convolution.

When we perform the sum over orbits we therefore get a factor $1/|\mathcal{H}_p|$ since the $|G|$-factor is canceled. The element that emerges is therefore g_{close} times the projection operator

$$\mathcal{P} = \frac{\sum_{h\in\mathcal{H}_p} h}{|\mathcal{H}_p|} \tag{A.13}$$

($\mathcal{P}^2 = \mathcal{P}$) of the invariance group. It is not hard to see that

$$g_{close}h = hg_{close},\ h \in \mathcal{H}_p \tag{A.14}$$

so the n'th power of the closing element is just

$$g^n_{close}\frac{\sum_{h\in\mathcal{H}_p} h}{|\mathcal{H}_p|}. \tag{A.15}$$

This is in agreement with the above 4-disc case since the closing element may be written as

$$C_2 \cdot \frac{e+\sigma_{24}}{2}, \tag{A.16}$$

since $\sigma_{13} = C_2\sigma_{24}$

We remark that for a boundary orbit in a system with only C_2 symmetry the closing element reduces to the projector of the orbit:

$$\frac{e+C}{2}, \tag{A.17}$$

where C is the reflection, $C^2 = e$.

Consider now a non-boundary orbit like (1), (1234) in the physical domain. It has multiplicity equal to 8 (4 edges in a square each with 2 directions) so the number of group elements in the invariance group is 8/8=1: e. The closing element C_4 therefore agrees with the above more general group algebra expression. For further discussioins of the role of the stability matrix see ref. [20].

A.3 Stability differentials

In this section we calculate the differentials related to refraction, reflection and free flight related to 2-d billiards. Thus velocities are conserved and the laws of reflection and refraction fulfilled. We recall that the differentials are the linearized transversal flow.

A.3.1 Refraction differential

Consider a ray incident on a surface. The outgoing ray has in general a different angle of incidence, as described by Snell' s law (4.41). We investigate the result of a variation of the ingoing wave in order to find the corresponding differential. For definiteness we think of an incoming S-wave refracting to a P-wave. Some notation: We use the subscript "$-$" to describe the incoming wave and "$+$" the outgoing. The direction of the waves are given by a unit vector $\vec{e}$ and the normal

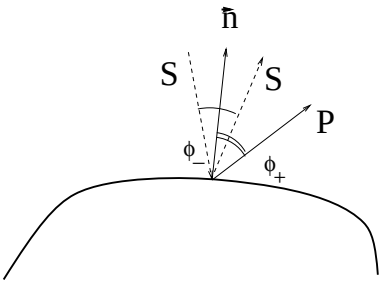


Figure A.2: Wave split

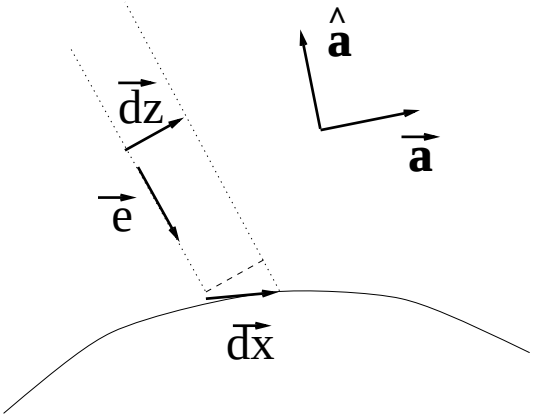


Figure A.3: The shadow of the transverse displacement on the boundary

of the surface is given by a unit vector $\vec{n}$. The linear operation of rotating 90° counter-clockwise vectors is denoted by a "hat" , eg. $\hat{n}$ is now a vector lying in the tangent plane of the surface. The direction of the wave is now parametrized by some angle, ie.

$$\vec{e} = \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix} \tag{A.18}$$

and therefore a variation of the direction is

$$d\vec{e} = \begin{bmatrix} -\sin(\theta) \\ \cos(\theta) \end{bmatrix} d\theta = \hat{e} d\theta. \tag{A.19}$$

A variation in the transverse direction of the ray will be described by the vector

$$d\vec{z} = dz\hat{e}. \tag{A.20}$$

By considering fig. A.3 it is clear that this variation is related to a variation of the point of incidence on the boundary (ie. a tangent vector) $d\vec{x}$ in the following way (dyadic notation):

$$\hat{e}\hat{e} \cdot d\vec{x} = d\vec{z}. \tag{A.21}$$

Thus $dz = \hat{e} \cdot d\vec{x}$. Since $d\vec{x}$ is a tangent vector we have

$$d\vec{x} = \hat{n}(\hat{n} \cdot d\vec{x}) \tag{A.22}$$

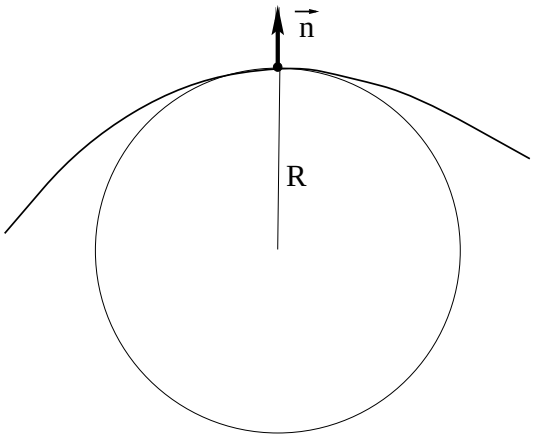


Figure A.4: Local curvature

implying

$$dz = \hat{e} \cdot \hat{n}(\hat{n} \cdot d\vec{x}) = (\vec{e} \cdot \vec{n})(\hat{n} \cdot d\vec{x}). \tag{A.23}$$

Thus

$$d\vec{x} = \hat{n}\frac{dz}{(\vec{n} \cdot \vec{e})}. \tag{A.24}$$

The change in the normal vector is given by

$$d\vec{n} = \frac{d\vec{x}}{R}, \tag{A.25}$$

where R is the local radius of curvature :

Therefore

$$d\vec{n} = \hat{n}\frac{dz}{(\vec{n} \cdot \vec{e})R}. \tag{A.26}$$

This gives

$$dz_+ = \frac{(\vec{n} \cdot \vec{e}_+)}{(\vec{n} \cdot \vec{e}_-)}dz_- = -\frac{\cos(\phi_+)}{\cos(\phi_-)}dz_-. \tag{A.27}$$

Furthermore

$$d\hat{n} = -\vec{n}\frac{dz}{(\vec{n} \cdot \vec{e})R}, \tag{A.28}$$

since $\hat{\hat{a}} = -\vec{a}$ for any vector $\vec{a}$.

Let us derive Snell's law (4.41). The projected slowness on the border has to be conserved, ie.

$$\hat{n}\hat{n} \cdot \vec{s}_- = \hat{n}\hat{n} \cdot \vec{s}_+, \tag{A.29}$$

where the slowness vector is

$$\vec{s} = s\vec{e}. \tag{A.30}$$

Thus

$$(\hat{n}\cdot\vec{e}_-)s_- = (\hat{n}\cdot\vec{e}_+)s_+ \tag{A.31}$$

or when expressed in terms of angles

$$\frac{\sin(\phi_+)}{\sin(\phi_-)} = \frac{v_+}{v_-}, \tag{A.32}$$

where $v_\pm$ is the velocity.

Varying the projected slowness and using the expression for $d\hat{n}$ we find

$$d((\hat{n}\cdot\vec{e})s) = (-\frac{dz}{R} + (\vec{n}\cdot\vec{e})d\theta)s. \tag{A.33}$$

This differential (1-form) is conserved allowing us to solve for the end angular variation $d\theta_+$. Defining $\kappa = \frac{v_+}{v_-}$ we get

$$d\theta_+ = -(\frac{\kappa}{\cos(\phi_+)} + \frac{1}{\cos(\phi_-)})\frac{dz_-}{R} - \kappa\frac{\cos(\phi_-)}{\cos(\phi_+)}d\theta_-. \tag{A.34}$$

The differential therefore becomes

$$-\begin{bmatrix} \frac{\cos(\phi_+)}{\cos(\phi_-)} & 0 \\ \frac{1}{R}(\frac{\kappa}{\cos(\phi_+)} + \frac{1}{\cos(\phi_-)}) & \kappa\frac{\cos(\phi_-)}{\cos(\phi_+)} \end{bmatrix}. \tag{A.35}$$

This differential is the familiar reflection differential (cf. ref. [8]), when $\kappa = 1$:

$$-\begin{bmatrix} 1 & 0 \\ \frac{2}{R\cos(\phi_-)} & 1 \end{bmatrix}. \tag{A.36}$$

To find the refraction differential when we have the opposite conversion, ie. from P-wave to S-wave, we just have to change the velocity ratio κ to $1/\kappa$. With wave split the refraction differential has determinant κ respectively $1/\kappa$ (ref. [26] find a similar result but in other coordinates). In a closed orbit however every time we have a conversion from S to P we also has to have the opposite, so the product of the differentials for the orbit will still have a determinant equal to 1.

A.3.2 The flight differential

An initial phase space point $(\vec{x}_-, \vec{v}_-)$ evolves during the time t to the point

$$(\vec{x}_+, \vec{v}_+) = (\vec{x}_- + \vec{v}_- t, \vec{v}_-). \tag{A.37}$$

Then it is not hard to find the differential

$$\begin{bmatrix} 1 & \Delta x \\ 0 & 1 \end{bmatrix}, \tag{A.38}$$

when we consider transverse displacements of the ray and angular variations of the velocity as above. Here Δx is the total flight length.

Bibliography

[1] V.I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer, Berlin 1978)

[2] B.A. Auld, *Acoustic Fields and Waves in Solids I,II* (John Wiley and Sons, New York 1973).

[3] R. Artuso, E. Aurell and P. Cvitanović, *Nonlinearity* **3**, 325 (1990).

[4] R. Artuso, E. Aurell and P. Cvitanović, *Nonlinearity* **3**, 361 (1990).

[5] H. Cartan, *Formes différentielles* (Hermann, Paris 1967).

[6] P. Cvitanović, *Phys. Rev. Lett.* **61**, 2729 (1988).

[7] P. Cvitanović, *Physica* **D 51**, 138 (1991).

[8] Cvitanovi et al. (1996) Cvitanović P., et al., (1996): *Classical and Quantum Chaos: A Cyclist Treatise*,
`http://www.nbi.dk/~predrag/QCcourse/`

[9] P. Cvitanović, *CHAOS* **2**, 1 (1992).

[10] P. Cvitanović and B. Eckhardt, *Nonlinearity* **6**, 277 (1993).

[11] Y.V. Egorov and M.A. Shubin (Eds.), *Partial Differential Equations I,II, IV* (Springer; Berlin, Heidelberg, New York 91, 92, 92).

[12] Per Rosenquist, "Periodic orbit theory beyond semiclassics: convergence, diffraction and h-bar corrections", *Ph.D. Thesis*, University of Copenhagen (1995).

[13] H. Goldstein, *Classical Mechanics*, 2. edition (Addison Wesley, Reading Mass. 1980).

[14] V.Guillemin and S. Sternberg, *Geometric Asymptotics, Mathematical Surveys nr.* **14**, Amer. Math. Soc. 1977.

[15] Martin C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, New York 1990).

[16] M. Hamermesh, *Group theory and its application to physical problems* (Addison Wesley, Reading Mass. 1962)

[17] M. H Holmes, *Introduction to Perturbation Methods* (Springer, New York 1995).

[18] L.D. Landau and E.M. Lifshitz, *Theory of Elasticity* (Pergamon, England 1959).

[19] L.D. Landau and E.M. Lifshitz, *Quantum Mechanics, 3.edition* (Pergamon, England 1977).

[20] B. Lauritsen, *Phys. Rev.* **A** 43, 603 (1991).

[21] R. G. Littlejohn, "the Van Vleck Formula, Maslov Theory, and Phase Space Geometry" *J.Stat. Phys.,* **68:** 7 (1992).

[22] A. E. H. Love, *A Treatise on the Mathematical thory of Elasticity, 4. ed.* (Cambridge at the Univ. Press, USA 1952).

[23] J.E. Marsden and T. S. Ratiu, *Introducion to mechanics and symmetry* (Springer, New York 1994)

[24] V.P. Maslov and M.V. Fedoriuk, *Semi-Classical Approximation in Quntum Mechanics* (D.Reidel Publ. Company, Dordrecht 1981).

[25] M.J.P. Musgrave, *Crystal Acoustics* (Holden-Day, San Fransisco 1970).

[26] L. Couchman, E. Ott and T. M. Antonsen, Jr., "Quantum chaos in systems with ray splitting" *Phys. Review A vol. 46, number* **10**, 6193 (1992).

[27] L.E. Reichl, *The Transition to Chaos* (Springer, New York 1992).

[28] D. Ruelle, *Statistical Mechanics, Thermodynamic Formalism*, (Addison-Wesley, Reading MA, 1978).

[29] Peter Scherer, "Quantenzustände eines Klassisch chaotischen Billards" *Ph. D Thesis, Jülich-2554* Nov. 1991 ISSN 0336-0885.

[30] Synge, J. L., *Proc. Roy. Irish Acad.*, **58**, 13 (1956).

[31] G. Tanner & D. Wientgen, "Classical and Semiclassical Zeta Functions in Terms of Transiontion Probabilities" *Chaos, Solitons & Fractals, vol. 5 no.* **7**, pp. 1325-1336 (1995).

[32] P. Cvitanović and B. Eckhardt, "Periodic orbit expansions for classical smooth flows", *J. Phys.* **A 24**, L237 (1991).

[33] Gabor Vattay, "An Entire Spectral Determinant for Semiclassical Quantization" *Progr. of Theor. Ph., Supplement No.* **116**, 251 (1994).