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Reinhard Lang

# Spectral Theory of Random Schrödinger Operators

## A Genetic Introduction

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Dedicated to Frank Spitzer on the occasion of his sixty fifth birthday.

## Preface

These notes are taken from seminars on the spectral theory of random Schrödinger operators, held at the University of Heidelberg during 1988 and 1989. Addressed to the non-specialist they are intended to provide a brief and elementary introduction to some branches of this field. An attempt is made to show some of the basic ideas *in statu nascendi*, and to follow their evolution from simple beginnings to more advanced results. The term "genetic" in the title refers to this procedure.

The main theme is the interplay between the spectral theory of Schrödinger operators and probabilistic considerations. After developing a general intuitive picture to give the reader some orientation in the field, we elaborate on two topics which in the history of the subject have proved to be of major conceptual importance. We consider on the one hand the Laplacian in a random medium and study its spectrum near the left end, where large fluctuations in the medium play an essential role. Expressed in terms of Wiener measure, this amounts to large deviation problems for Brownian motion. Guided by these questions we show how the notion of *entropy* has undergone mutations, and explain its relation to the spectral theory of the Laplacian. On the other hand we specialize to one-dimensional space and consider there Schrödinger operators with general ergodic potentials. We explain how certain aspects of the Floquet theory can be extended from periodic to general potentials. Based on this extension, the absolutely continuous spectrum of one-dimensional Schrödinger operators is studied. Here the notion of *rotation number* and its relation to Weyl's theory of singular Sturm-Liouville operators play an important role.

An effort is made throughout to give heuristic arguments before going to rigorous proofs. By means of a few characteristic problems and their solution we attempt to explain basic ideas and concepts in the simplest possible setting rather than to collect the most refined results.

These notes are dedicated by a grateful disciple to Frank Spitzer on the occasion of his sixty fifth birthday.

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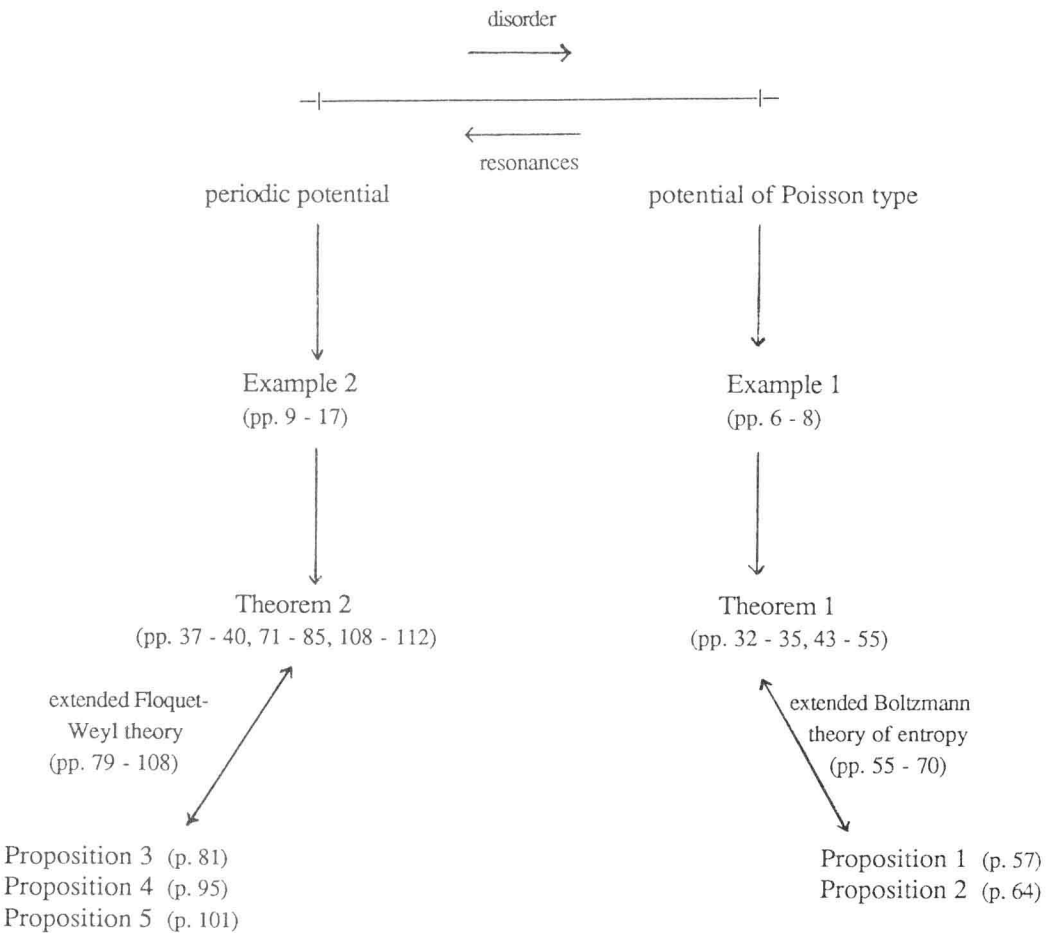
## Structure of the notes



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## 1. Introduction

We consider Schrödinger operators

(1.1) $H = -\Delta + q$,

where $\Delta = \frac{\partial^2}{\partial x_1^2} + \ldots + \frac{\partial^2}{\partial x_d^2}$ denotes the Laplacian in $\mathbf{R}^d$, $d \geq 1$, and $q: \mathbf{R}^d \to (-\infty, +\infty]$ is a random potential, and address ourselves to the following general problem:

(1.2) What is the spectrum $\Sigma = \Sigma(q)$ of the operator $H = H(q)$ and what do the solutions $g_\lambda$ to the equation $Hg_\lambda = \lambda \cdot g_\lambda$, $\lambda \in \Sigma$, look like? How does the answer depend on the degree of disorder of the potential q?

A solution $g_\lambda$ to the equation

(1.3) $Hg_\lambda = \lambda \cdot g_\lambda$

is called an eigenfunction corresponding to the eigenvalue $\lambda$, if $g_\lambda \in L^2(\mathbf{R}^d)$. The spectrum $\Sigma$ is the union of the pure point spectrum $\Sigma_{pp}$, which is defined as the closure of the set of eigenvalues, and of the continuous spectrum $\Sigma_c$, the precise definition of which is postponed to the end of this section; roughly speaking, $\lambda$ belongs to $\Sigma_c$, if equation (1.3) has approximate solutions in $L^2(\mathbf{R}^d)$ which are orthogonal to the space spanned by the eigenfunctions. As will be seen later, this notion has still to be refined by splitting $\Sigma_c$ into an absolutely continuous part and a singularly continuous part.

Problem (1.2) has at least two quite different origins coming from (i) solid state physics and (ii) purely mathematical considerations.

(i) In order to see how it arises in solid state physics, we consider a solid whose atoms are located at sites $x_i \in \mathbf{R}^d$, $i \geq 1$, and a pair potential

(1.4) $\Phi: \mathbf{R}^d \to (-\infty, +\infty]$,

describing the interaction between a particle and an atom. In the one-body approximation one considers the Schrödinger operator (1.1) with potential

(1.5) $q(x) = \sum_i \Phi(x - x_i)$ , $x \in \mathbf{R}^d$ .

In the case of a perfect crystal, the $x_i$ are points of a lattice, e.g. of the lattice $\mathbf{Z}^d$, so that q is a deterministic periodic function. In general there are random deviations from the lattice structure and the points $x_i$ are randomly distributed. One is in a case of maximal disorder if the $x_i$ are distributed according to a Poisson point process on $\mathbf{R}^d$. The degree of randomness may range from periodic structures (respectively periodic potentials q) to structures with strong randomness (respectively to strongly mixing potentials q).

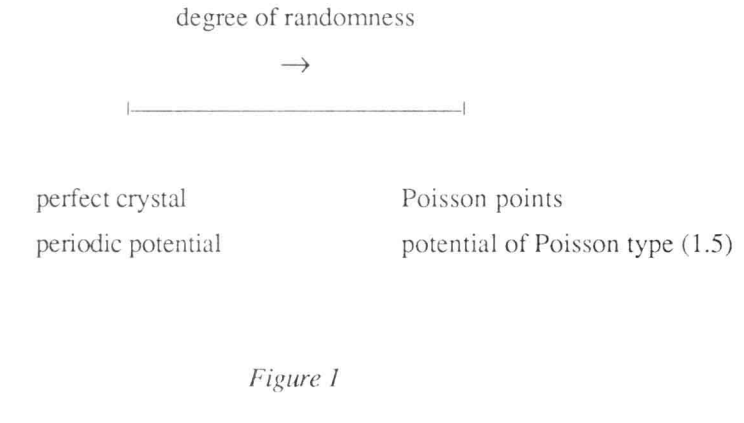


*Figure 1*

The disorder gives rise to qualitatively new properties of the solid state which cannot be understood merely on the basis of perturbations around the case of perfect order. It is a fundamental problem to understand the conditions on the potential q under which the solutions $g_\lambda$ of (1.3) are exponentially decreasing at infinity (localization) or wavelike (extended states). Physically, the transition from extended states to localized states corresponds to the transition from a metal to an insulator (see Anderson (1958)).

(ii) On the mathematical side one tries to understand the spectral properties of the operator (1.1) for a given deterministic potential q. Until the seventies mathematical results existed for three classes of potentials. If $q(x) \to +\infty$ as $|x| \to \infty$, H has purely -

discrete spectrum. A characteristic example is the case of a vibrating membrane D with fixed boundary, which formally corresponds to the potential

$$q(x) = \begin{cases} 0, & x \in D \\ +\infty, & x \notin D \end{cases},$$

where D denotes a bounded open set in $\mathbf{R}^d$. The second class is the class of potentials rapidly decreasing at infinity, which is treated by scattering theory. A characteristic example is given by a non-negative potential with compact support where the spectrum $\sum = [0,\infty)$ is purely continuous and where one has wavelike solutions $g_\lambda$ for $\lambda \in \sum$. Thirdly, in the case of a periodic potential, one has purely continuous spectrum and Bloch waves as eigenstates. In all other cases however, if q is bounded and oscillating but not strictly periodic, very little is known about the spectral properties of H. Since it is difficult to get results for an individual non-periodic bounded q, one randomizes the problem and contents oneself with asking what the spectral behaviour of H is for typical bounded random potentials. A similar probabilistic approach was introduced by Bloch and Pólya (1932) in order to get estimates about the number of real roots of a real polynomial of high degree. This problem serves Kac as a striking example illustrating the nature and power of probabilistic reasoning, see p. 11 in Kac (1959).

From these remarks on the different origins of problem (1.2) it is already clear that it has connections with many fields, ranging, as we will see, from Statistical Mechanics to the theory of integrable Hamiltonian systems. This diversity of the subject makes its beauty but also its difficulty. There exists a rich literature, for example a monograph of encyclopedic character by Carmona and Lacroix (1990), and also several expositions and review papers. A sample of the more recent ones are Spencer (1986), Cycon, Froese, Kirsch and Simon (1987), Martinelli and Scoppola (1987), Bellissard (1989), Pastur (1989). It is the aim of the present paper, to give an elementary introduction to some basic problems and ideas in the field outlined above and to follow their evolution approximately in historical order. The paper assumes no particular background. It is addressed to the general reader and mainly deals with the following questions.

(i) What is the heuristic picture underlying problem (1.2)? What kind of mathematical questions arise from this picture? What are the relations between its several aspects?

(ii) How did ideas evolve from the simple beginnings of spectral theory to more advanced results related to the clarification of (1.2)? How did, conversely, probabilistic considerations lead to a mutation and advancement of classical theories?

Sections 2 - 4 are devoted to question (i). Here a general heuristic picture is drawn which suggests, roughly speaking, a tendency to localization with increasing disorder. In sections 5 and 6 we deal with question (ii) by way of two characteristic problems. Along with their solution, we try to explain how the classical notions of entropy and of Floquet exponent were extended to general concepts of wide applicability.

In section 2 we begin with two quite elementary examples. The first, which is located at the right end point on the scale of disorder in Figure 1, deals with one-dimensional potentials of Poisson type. The second example is located at the left end point on the scale in Figure 1 and concerns one-dimensional periodic potentials. Guided by these examples we sketch in section 3 some heuristic ideas concerning localization and the asymptotic behaviour of the density of states near to the bottom of the spectrum (so called Lifschitz tails). Section 4 contains a discussion about the present mathematical status of these ideas and some of the main open problems are mentioned. In order to illustrate question (ii), we have chosen two key results by Donsker and Varadhan (1975a,b,c) and by Kotani (1984) respectively, whose proofs are conceptually significant and basic for many other work too, and we try to explain their contents in detail in sections 5 and 6. Theorem 1, which can be seen as generalization of example 1 to higher dimensions, deals with Lifschitz tails in a Poisson model. Along with a sketch of its proof in section 5, an extension of the Boltzmann theory of entropy is given. Theorem 2 is inspired by example 2. It says, roughly speaking, that randomness implies the absence of the absolutely continuous spectrum, if the dimension is one. Its proof requires a far reaching extension of the Floquet theory as will be explained in section 6. Section 5 and 6 are formally independent of each other. Parallel reading however could help the reader to get a balanced picture of probabilistic and deterministic aspects of the theory: on the random side of Figure 1 large fluctuations in the medium and

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correspondingly the theory of large deviations are relevant, whereas on the deterministic side conserved quantities and the notion of a generalized Floquet exponent play an essential role. In the final section we reflect the meaning of what has been done in the previous sections and we reconsider the development from the simple vibrating string to the spectral theory of infinitely many randomly coupled vibrating membranes.

Before we begin with the discussion of the two examples let us give some definitions. We denote by $L^2(\mathbf{R}^d)$ the space of measurable functions $u: \mathbf{R}^d \to \mathbf{C}$ with finite norm $\|u\| = (\int |u(x)|^2 \, dx)^{1/2}$ and by $\mathcal{H}_{pp}$ the subspace of $L^2(\mathbf{R}^d)$ spanned by the eigenfunctions of H. The continuous spectrum $\Sigma_c$ is defined as follows. A number $\lambda \in \mathbf{R}$ belongs to $\Sigma_c$ if and only if there exists a sequence $u_n \in L^2(\mathbf{R}^d)$ such that $u_n$ is orthogonal to $\mathcal{H}_{pp}$, $\|u_n\| = 1$ for all $n \in \mathbf{N}$, and $\|(H - \lambda)u_n\| \to 0$ as $n \to \infty$.

The following general probabilistic framework is used. We denote by $\Omega$ a subspace (which has to be specified according to the context in which we are working) of the space of measurable functions $q: \mathbf{R}^d \to (-\infty, +\infty]$ and by $(\Omega, \mathcal{F}, P)$ a probability space. The shift operator $\theta_x: \Omega \to \Omega$ is defined by $\theta_x q(y) = q(x + y)$ for $x, y \in \mathbf{R}^d$.

We assume that P satisfies

(1.6) $P(\theta_x A) = P(A)$ for $A \in \mathcal{F}$, $x \in \mathbf{R}^d$ (shift invariance)

and

(1.7) if $A \in \mathcal{F}$ and $P((\theta_x A) \Delta A) = 0$ for all $x \in \mathbf{R}^d$,
then $P(A) = 0$ or $P(A) = 1$ (ergodicity).

The ergodicity of P implies that many quantities are selfaveraging, see for example (2.6) below. We say a property holds almost everywhere with respect to P (abbreviated by P-a.e.), if the set of potentials with this property has P-measure 1.

In the following we do not enter into questions about the selfadjointness of the operator H or into measurability questions, and refer instead to the literature, e.g. to Carmona and Lacroix (1990).

## 2. Two simple examples

In order to get a feeling for problem (1.2) we begin with two quite elementary one-dimensional examples, which are chosen as extreme cases on the scale of disorder in Figure 1.

### *2.1. Example 1*

In the first example we consider the one-dimensional potential of Poisson type

$$q(x) = \sum_{i \in Z} \Phi(x - x_i) , \tag{2.1}$$

where $x_i$, $i \in \mathbf{Z}$, are the points of a Poisson process on $\mathbf{R}^1$, say with average density 1, and where

$$\Phi(x) = \begin{cases} +\infty , & |x| \leq R \\ 0 , & |x| > R \end{cases} \tag{2.2}$$

is a hard core potential of a given radius $R > 0$. The corresponding operator $H = H(q)$ is just the operator $-\frac{d^2}{dx^2}$ in the random region $\mathbf{R} \setminus \bigcup_{i \in Z} [x_i - R, x_i + R] = \bigcup_{i \in Z} D_i$ with Dirichlet boundary conditions, see Figure 2.

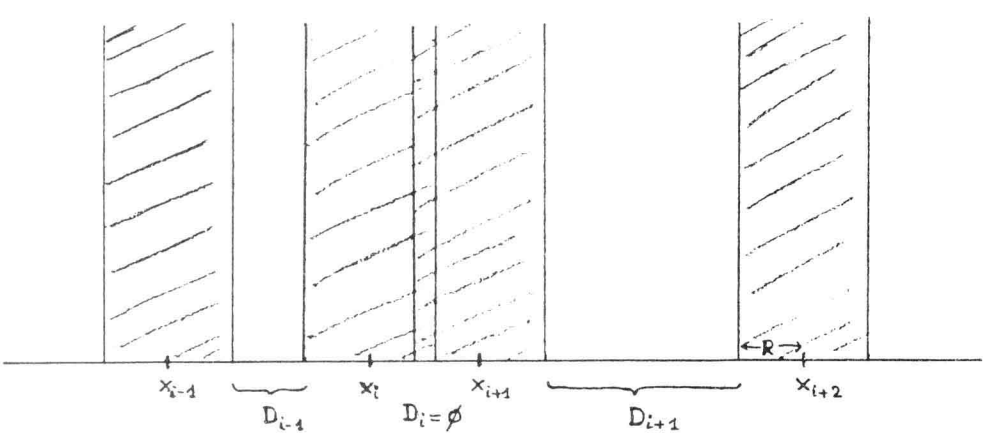


*Figure 2*

The spectral behaviour of H is the following:

(2.3) $\Sigma = \Sigma_{pp} = [0,\infty)$, the eigenvalues are P – a.e. dense in $\Sigma$

and

(2.4) the eigenfunctions have compact supports P – a.e..

This is obvious since the $D_i$, $i \in \mathbf{Z}$, can be viewed as strings of random length $|D_i|$ which vibrate *independently* of each other. The eigenvalues corresponding to a string $D_i$ with $D_i \neq \emptyset$ are given by

(2.5) $$\lambda_{i,j} = \frac{\pi^2 \cdot j^2}{|D_i|^2} \quad , \qquad j \geq 1 \quad .$$

The numbers $\{ |D_i| , i \in \mathbf{Z} \}$ and therefore the eigenvalues $\{\lambda_{i,j}, (i,j) \in \mathbf{Z} \times \mathbf{N}$ with $D_i \neq \emptyset \}$ are P – a.e. dense in $[0,\infty)$ and the corresponding eigenfunctions are localized in the intervals $D_i$. This shows (2.3) and (2.4).

The solutions $g_\lambda$ to (1.3) and the eigenvalues are random. For general ergodic potentials they are no longer computable explicitly. It is therefore appropriate to introduce another notion, which is defined via an averaging procedure, and hence non-random. This so-called integrated density of states N gives information about "the number of eigenvalues per unit interval", and is defined as follows. For $L > 0$ we denote by $H^{(L)}$ the operator $-\frac{d^2}{dx^2} + q$ in the interval $(-L, +L)$ with Dirichlet boundary conditions. Then

(2.6) $$N = \lim_{L \to \infty} N^{(L)}$$

is the limit of the empirical distributions

(2.7) $$N^{(L)}(\lambda) = \frac{1}{2L} \# \{ i \in \mathbf{N} : \lambda_i^{(L)} < \lambda \} , \quad \lambda \in \mathbf{R} ,$$

where $\lambda_i^{(L)}$, $i \geq 1$, are the eigenvalues of the operator $H^{(L)}$. In the case of the Poisson potential (2.1), it is easy to show the existence of the limit (2.6) and to compute, for $\lambda \geq 0$,

$$(2.8)\qquad N(\lambda) = \lim_{L\to\infty} \frac{1}{2L} \# \left\{ (i,j)\in \mathbf{Z}\times\mathbf{N}:\ D_i \subset (-L,+L),\ j \le \frac{\sqrt{\lambda}}{\pi} |D_i| \right\} =$$

$$= E\left[ \frac{1}{\pi} \sqrt{\lambda}\, |D_1| \right] ,$$

where [x] denotes the greatest integer which is $\le x$. In particular, one gets from (2.8) the following asymptotic behaviour of N near the boundaries of the spectrum:

$$(2.9)\qquad N(\lambda) \sim \begin{cases} e^{-\pi/\sqrt{\lambda}} & , \lambda \to 0 \\ e^{-2R} \frac{1}{\pi} \sqrt{\lambda} & , \lambda \to \infty , \end{cases}$$

which more precisely means

$$(2.10)\qquad \lim_{\lambda\to 0} \sqrt{\lambda}\, \log N(\lambda) = -\pi ,$$

respectively

$$(2.11)\qquad \lim_{\lambda\to\infty} \pi\, e^{2R} \frac{1}{\sqrt{\lambda}}\ N(\lambda) = 1 .$$

The asymptotic behaviour of N as $\lambda \to \infty$ is, up to a constant factor, clearly the same as in the free case $q \equiv 0$, where the integrated density of states is $N_0(\lambda) = \frac{1}{\pi} (\max\{0,\lambda\})^{1/2}$. To see the probabilistic meaning of the asymptotic behaviour of N as $\lambda \to 0$ we denote by D(r) the open ball of radius r, which in the present one-dimensional case is just an interval of length 2r, and to a given $\lambda > 0$ we determine the radius $r(\lambda) = \frac{\pi}{2\sqrt{\lambda}}$ so that the lowest Dirichlet eigenvalue of the operator $-\frac{d^2}{dx^2}$ in the interval $D(r(\lambda))$ is $\lambda$. Then we have

$$(2.12)\qquad N(\lambda) \sim e^{-\pi/\sqrt{\lambda}} = P(D(r(\lambda)) \text{ is free of Poisson points}),\ \lambda\to 0.$$

That is, near to the bottom of the spectrum, the essential contribution to $N(\lambda)$ comes from large intervals $D_i$ which have approximately $\lambda$ as lowest Dirichlet eigenvalue and which are free of Poisson points (see Figure 2 above).

*2.2. Example 2*

In the second example we consider a potential which is a continuous periodic function $q: \mathbf{R}^1 \to \mathbf{R}^1$, say with period L. Formally this case can be subsumed under the general framework indicated at the end of the introduction as follows. One chooses a point $\omega$ equidistributed in the interval [0,L] and deals with the random potential $\theta_\omega q$ instead of q. For the purpose of this section such a randomization is not needed, and we consider here the deterministic operator

$$H = -\frac{d^2}{dx^2} + q \ , \qquad -\infty < x < +\infty \ , \tag{2.13}$$

and the corresponding equation

$$Hg_\lambda = \lambda \cdot g_\lambda \ , \qquad \lambda \in \mathbf{C} \ . \tag{2.14}$$

The following result holds true. There exist real numbers $a_i$, $i \geq 0$, with $-\infty < a_0 < a_1 \leq a_2 < a_3 \leq a_4 < \dots$, such that

$$\Sigma = \Sigma_c = \bigcup_{i \geq 0} [a_{2i} , a_{2i+1}] \ , \tag{2.15}$$

and for $\lambda \in \bigcup_{i \geq 0} (a_{2i} , a_{2i+1})$ there exist two linearly independent solutions of (2.14) of the form

$$g_\pm(\lambda;x) = p_\pm(\lambda;x)\, e^{\pm i \alpha(\lambda) x} \ , \ x \in \mathbf{R}, \tag{2.16}$$

where $p_\pm(\lambda; \cdot)$ is a complex valued function with period L and the phase $\alpha(\lambda)$ is a real number. The intervals $[a_{2i}, a_{2i+1}]$ are the allowed energy bands and the $(a_{2i-1}, a_{2i})$ are (possibly empty) gaps in the spectrum; the solutions (2.16) are called Bloch waves.

We indicate the four main steps of the proof of (2.15) and (2.16) with a view towards extensions in later sections. Details can be found for example in the booklet by Magnus and Winkler (1979).

**Step 1.** Transformation of equation (2.14) into a dynamical system.

This step does not rely on the periodicity of q, it can be performed for arbitrary one-dimensional potentials. One can write (2.14) in the form

$$\begin{pmatrix} g_\lambda(x) \\ g_\lambda'(x) \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ q(x)-\lambda & 0 \end{pmatrix} \begin{pmatrix} g_\lambda(x) \\ g_\lambda'(x) \end{pmatrix}, \tag{2.17}$$

with $g_\lambda'(x) = \frac{d}{dx} g_\lambda(x)$. We denote by $\begin{pmatrix} \varphi_\lambda(x) \\ \varphi_\lambda'(x) \end{pmatrix}$ and $\begin{pmatrix} \psi_\lambda(x) \\ \psi_\lambda'(x) \end{pmatrix}$ the solutions of (2.17) with $\begin{pmatrix} \varphi_\lambda(0) \\ \varphi_\lambda'(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} \psi_\lambda(0) \\ \psi_\lambda'(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ respectively, and by

$$Y_\lambda(x) = Y_\lambda(x;q) = \begin{pmatrix} \varphi_\lambda(x) & \psi_\lambda(x) \\ \varphi_\lambda'(x) & \psi_\lambda'(x) \end{pmatrix} \tag{2.18}$$

the fundamental matrix of equation (2.17). The following conservation law is basic and has important consequences as we will later see. The Wronski determinant

$$[f_\lambda, g_\lambda](x) = \det \begin{pmatrix} f_\lambda(x) & g_\lambda(x) \\ f_\lambda'(x) & g_\lambda'(x) \end{pmatrix} \tag{2.19}$$

of two solutions $f_\lambda, g_\lambda$ of (2.17) is constant. This can easily be seen by differentiation of the determinant. In particular one has

$$\det Y_\lambda(x) = [\varphi_\lambda, \psi_\lambda](x) \equiv 1, \quad x \in \mathbf{R}. \tag{2.20}$$

**Step 2.** Floquet theory.

In order to find out for which $\lambda \in \mathbf{C}$ equation (2.14) has wavelike solutions, one tries to understand the stability behaviour of the dynamical system (2.17). To this end one takes advantage of the periodicity of q and asks for solutions $g_\lambda$ which, after turning one period, only change by a (in general complex) factor, i.e. for solutions $g_\lambda$ and factors $\mu(\lambda) \in \mathbf{C}$ such that

$$g_\lambda(x+L) = \mu(\lambda) \cdot g_\lambda(x), \quad x \in \mathbf{R}. \tag{2.21}$$

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