**Lecturas Matemáticas**
*Volumen* **26** *(2005), páginas 145–163*

# Spectral classification in a periodic structure[1]

F. Gherib
Centre universitaire de Mascara, Algérie
B. Messirdi
Université d' Oran Es-senia, Algérie

Abstract. In this paper we consider the Schrödinger operators $P = -\frac{d^2}{dx^2} + V$, where $V$ is a periodic real function. Essentially we show that the spectra of these operators can be determined by a smooth function $\alpha$, the phase of the eigenvalues of a matrix $M(E, x, V)$ expressing the states of a particle in a $L-$ periodical structure. The recurrent spectrum and the transient spectrum of $P$ are also calculated. Such structures are met meet, for example, in solid state physics in the study of a linear molecule formed of regularly spaced atoms.

*Key words and phrases.* Schrödinger operator, periodic potential, absolutely continuous spectrum, transient and recurrent spectrum.

*2000 AMS Classification Subject: 35P15, 35Q20, 35P99, 47A53.*

Resumen. En este trabajo se estudian los operadores de Schrödinger $P = -\frac{d^2}{dx^2} + V$, donde $V$ es una función periódica real. Esencialmente, mostramos que los espectros de estos operadores pueden determinarse con mediante una función suave $\alpha$, que es la fase de los valores propios de una matriz $M(E, x, V)$ que expresa los estados de una partícula en una estructura $L-$periódica. También calculamos los espectos recurrente y transiente de $P$. Estas estructuras se encuentran, por ejemplo, al estudiar en la fíca del estado sólido una molécula lineal formada por átomos regularmente espaciados.

[1]Investigation supported by University of Oran Es-senia, Algeria. Research topics CNEPRU.

## 1. Introduction

We know that the spectral properties of Schrödinger operators $P = -\frac{d^2}{dx^2} + V$ on $L^2(\mathbb{R})$ depend mainly on the behavior of the real potential function $V$ at infinity.

Basically, in spectral theory we distinguish four distinct classes of Schrödinger operators $P$. In the first class $V(x) \to \infty$ as $|x| \to +\infty$, and has empty essential spectrum. The next simplest class consists of Schrödinger operators for which $V(x) \to 0$ as $|x| \to +\infty$. Under fairly general hypotheses these operators have $\sigma_{ess}(P) = [0, +\infty[$ for essential spectrum and empty singular continuous spectrum $\sigma_{sc}(P) = \emptyset$. The essential tools used to establish these results are the min-max principle, Weyl's theorem, perturbation theory of linear operators, etc. (See [ReSi, theorems XIII15, XIII16, and XIII33]; [CyFrKiSi], [Ka] and [DaLi].)

The third class is made up of the $N-$body Schrödinger operators for which $V(x) \to 0$ as $|x| \to +\infty$ in most directions (*e.g.*, Coulombic interactions). Under specialized hypotheses, for these operators we have $\sigma_{ess}(P) = [\alpha, +\infty[$ and $\sigma_{sc}(P) = \emptyset$, where $\alpha \geq 0$. (See [ReSi, theorems XIII17 and XIII36].)

In the fourth and last class one finds Schrödinger operators $P$ where $V$ is a periodic real function. These operators, considered as unbounded and self adjoint on $L^2(\mathbb{R})$, are important in solid state physics. Indeed, periodicity is the property that characterizes the potential to which a particle in a crystal is submitted.

If $V$ is $L-$periodic it has not a limit as $|x| \to +\infty$ , so the spectral analysis of periodic Schrödinger operators is difficult (see *e.g.* [AvSi2], [Ea]). Nevertheless, the property that allows the study of these situations is that $P$ has a large symmetry group

$$[P, U(L)] = 0\,,$$

where $U(L)$ is the unitary operator defined on $L^2(\mathbb{R})$ by $U(L)\varphi(x) = \varphi(x+L)$, and $[P, U(L)]$ is the commutator of $P$ and $U(L)$.

It is known that (see eg. [AvSi2], [Ea], [DaLi]) the study of these operators has been based on the concept of decomposable operators by the direct integral decomposition so far. Also, the classification of the spectrum of these operators is done naturally studying the spectrum of their fibers. It follows that Schrödinger operators with sufficiently smooth potentials and $2\pi$-periodical have purely absolutely continuous spectrum and are unitarily equivalent to the

Hilbertian integral operator

$$\int_{[0,2\pi]}^{\oplus} P(\theta)\frac{d\theta}{2\pi}\,,$$

where the fiber $P(\theta)$ is the operator $P = -\dfrac{d^2}{dx^2}+V$ defined on $L^2\left([0,2\pi],\dfrac{d\theta}{2\pi}\right)$, with boundary conditions:

$$\psi(2\pi) = e^{i\theta}\psi(0)\,,\quad \psi'(2\pi) = e^{i\theta}\psi'(0)\,.$$

For all $\theta \in [0,2\pi]$, $P(\theta)$ has a compact resolvent and a discrete spectrum, which reveals the existence in the spectrum of $P$ continuous bands of energy known as allowed bands, possibly separated by energy bands known as forbidden bands. The spectrum of $P$ on $L^2(\mathbb{R})$ is the union of all the allowed bands.

Several recent papers have treated the localization of bands of energy and the estimation of their width. For this we refer to results obtained by OUTASSOURT in the semi-classical case [Ou].

The main difficulties appear while extending the analysis of the fibers of $P$. For this analysis depends critically on the simplicity of the eigenvalues of $P(\theta)$, simplicity which fails in the multidimentional case since eigenvalues are not necessarily analytic at degeneracy points [Me].

Here we plan to give a new and original spectral analysis of the Schrödinger operators with real and continuous $L-$periodical potentials. Our method is also valid in the degenerate case and will allow us to obtain all the quoted results by using direct and easy proofs. In particular, we obtain in this way a precise refinement of the absolutely continuous spectrum of $P$.

Our technique is based on the behavior of the eigenfunctions of $P$ at the time of the crossing of the totality of the successive barriers created by the periodic potential $V$. For this, we introduce for $E$ real a matrix of transition $M(E,x,V)$ with eigenvalues $e^{\pm w(E)L}$ such that $w(E) = \gamma(E) + i\alpha(E)$. $M(E,x,V)$ describes the states of a particle in a $L-$periodical structure $V$ at the energy $E$ and the position $x$.

The function $\alpha$ is known as the phase function. We show that $\alpha$ is differentiable and obtain our main result

$$\sigma(P) = \overline{\left\{E \in \mathbb{R}\ ;\ \frac{d\alpha}{dE}(E) \neq 0\right\}}$$

(Here $\sigma$ stands for the spectrum). The function $\gamma(E)$ characterizes the spectrum of the fibers of $P$ and its resolvent set and $\gamma(E)$ vanishes on the allowed bands.

Using the function $\alpha$ it is now possible in this case to deduce the spectral measure and the various components of the absolutely continuous spectrum: the transient spectrum $\sigma_{rac}(P)$ and the recurrent spectrum $\sigma_{tac}(P)$ of $P$. This decomposition is possible thanks to a partition of the positive density of the spectral measure of $P$ in two essential parts: the essential interior and the essential frontier (see. [GhMe],[AvSi1]).

## 2. Behavior of the solutions in a periodic structure

Consider

$$\left[-\frac{d^2}{dx^2} + (V(x) - E)\right]\varphi = 0 \qquad (\mathcal{E})$$

where $V$ is a real continuous function on $\mathbb{R}$ which is constant in the exterior of the compact $[0\,,L]$:

$$V(x) = V_0\,, \quad \forall x \in \mathbb{R} \setminus [0\,,L]\,,$$

$$(V_0 = V(0) = V(L))\,, \quad L,\, E \in \mathbb{R}\,, \quad \text{such that} \quad V_0 < E\,.$$

Let $\varphi_1(E,x)$ and $\varphi_2(E,x)$ be two linearly independant solutions of $(\mathcal{E})$, then $\varphi_i(E,x)$ , $i = 1,2$, is analytic in $E$ and $C^2$ for each $x$ by the standard theory of ordinary differential equations.

In particular,

$$\varphi_1(E,x) = \begin{cases} e^{ikx} & \text{if} \quad x \leq 0 \\ F(E)e^{ikx} + G(E)e^{-ikx} & \text{if} \quad x \geq L \end{cases}$$

$$\varphi_2(E,x) = \begin{cases} e^{-ikx} & \text{if} \quad x \leq 0 \\ F'(E)e^{ikx} + G'(E)e^{-ikx} & \text{if} \quad x \geq L \end{cases}$$

with $k = \sqrt{E - V_0}$. $F(E), G(E), F'(E)$ and $G'(E)$ are coefficients depending on $V$ and analytically on $E$.

Since $V$ is real, we see that if $\varphi$ is solution of $(\mathcal{E})$ its conjugated is also solution. One can take therefore $F'(E) = \overline{G(E)}$ and $G'(E) = \overline{F(E)}$.

All other solutions of $(\mathcal{E})$ are of the form

$$\varphi(E,x) = A_1\varphi_1(E,x) + A_1'\varphi_2(E,x)\ ,\ x \in \mathbb{R}\,.$$

Thus

$$\varphi(E,x) = \begin{cases} A_1 e^{ikx} + A_1' e^{-ikx} & \text{if} \quad x \le 0 \\ \widetilde{A_1} e^{ikx} + \widetilde{A_1'} e^{-ikx} & \text{if} \quad x \ge L \end{cases} \tag{2.1}$$

and

$$\begin{cases} \widetilde{A_1} = F(E) A_1 + \overline{G(E)} A_1' \\ \widetilde{A_1'} = G(E) A_1 + \overline{F(E)} A_1' \end{cases} , \tag{2.2}$$

where $A_1$, $A_1'$, $\widetilde{A_1}$, and $\widetilde{A_1'}$ are some complex constants. The coefficients $F(E)$ and $G(E)$ allow us to know the behavior of the solution $\varphi$ on the left of the potential from its behavior on the right of $V$.

We now want to study the behavior of the solution at the time of the crossing of all the successive barriers, that is to find the solution $\varphi(E,x)$ of the equation $(\mathcal{E})$ where $V$ is a $L-$periodical superposition on $\mathbb{R}$ of functions of the previous type.

By virtue of the previous calculus, the general solution of $(\mathcal{E})$ is given on $\mathbb{R}$ by:

$$\varphi(E,x) = \begin{cases} A_1 \varphi_1(E,x) + A_1' \varphi_2(E,x) \quad \text{if} \quad 0 \le x \le L \\ A_2 \varphi_1(E,x-L) + A_2' \varphi_2(E,x-L) \quad \text{if} \quad L \le x \le 2L \\ \cdots \\ A_{n+1} \varphi_1(E,x-nL) + A_{n+1}' \varphi_2(E,x-nL) \quad \text{if} \\ \qquad nL \le x \le (n+1)L \,, n \in \mathbb{Z} \end{cases}$$

Moreover, it is easy to calculate the values of $\varphi_1(E,x)$ and $\varphi_1(E,x)$, as well as those of their derivatives at the extremities of every period. So, $\varphi(E,x)$ has the same value and the same derivative than the function

$$A_n e^{\,ik(x-(n-1)L)} + A_n' e^{\,-ik(x-(n-1)L)}$$

at the extremity on the left of the $n-$th period. In the same way, on the right, it has the same value and the same derivative than

$$\widetilde{A_n} e^{\,ik(x-(n-1)L)} + \widetilde{A_n'} e^{\,-ik(x-(n-1)L)} \,.$$

Then,

$$\widetilde{A_n} e^{\,ik(nL-(n-1)L)} + \widetilde{A_n'} e^{\,-ik(nL-(n-1)L)} = A_{n+1} e^{\,ik(nL-nL)} + A_{n+1}' e^{\,-ik(nL-nL)}$$

and

$$ik[\widetilde{A_n} e^{\,ik(nL-(n-1)L)} - \widetilde{A_n'} e^{\,-ik(nL-(n-1)L)}] \\ = ik[A_{n+1} e^{\,ik(nL-nL)} - A_{n+1}' e^{-ik(nL-nL)}]$$

and therefore, for all $n$ in $\mathbb{N}^*$,

$$\begin{cases} A_{n+1} = e^{ikL}\widetilde{A_n} \\ A'_{n+1} = e^{-ikL}\widetilde{A'_n} \end{cases} .$$

Using (2.2), we obtain

$$\begin{pmatrix} A_{n+1} \\ A'_{n+1} \end{pmatrix} = (Q(E))^n \begin{pmatrix} A_1 \\ A'_1 \end{pmatrix}, \quad \forall n \in \mathbb{N}^*, \tag{2.3}$$

where

$$Q(E) = \begin{pmatrix} e^{ikL}F(E) & e^{ikL}\overline{G(E)} \\ e^{-ikL}G(E) & e^{-ikL}\overline{F(E)} \end{pmatrix} . \tag{2.4}$$

Now the characteristic equation of $Q(E)$ is

$$\lambda^2 - D(E)\lambda + 1 = 0 ,$$

where $D(E) = Tr(Q(E)) = e^{ikL}F(E) + e^{-ikL}\overline{F(E)} = 2\mathrm{Re}\left(e^{ikL}F(E)\right)$.

The calculus of $(Q(E))^n$ will be easy if one changes the basis to get a diagonal form of $Q(E)$. This is the reason why we are going to study the spectrum of $Q(E)$.

Then, the eigenvalues of $Q(E)$ can be expressed in the form $\lambda_{\pm}(E) = e^{\pm w(E)L}$ with $w(E)=\gamma(E) + i\alpha(E)$, $\gamma(E) \geq 0$; such as:

**Propisition 2.1.**

(i) $\gamma(E) = 0 \Leftrightarrow |D(E)| \leq 2$

(ii) $|D(E)| > 2 \Rightarrow \begin{cases} \alpha(E) = \pi/L & \text{if} \quad D(E) > 0 \\ \alpha(E) = 0 & \text{if} \quad D(E) < 0 \end{cases}$

*Proof.* We only prove (ii). Indeed, for $|D(E)| > 2$, the eigenvalues of $Q(E)$ are $\lambda_{\pm}(E) = \varepsilon e^{\pm\gamma(E)L}$, $\varepsilon = \pm 1$.

If

$$\varepsilon = -1, \quad D(E) < 0 , \quad \lambda_{\pm}(E) = e^{\pm\,[\gamma(E)+i(\pi/L)]L} , \quad \text{then} \quad \alpha(E) = \frac{\pi}{L} .$$

If

$$\varepsilon = +1 , \quad D(E) > 0, \quad \lambda_{\pm}(E) = e^{\pm[\gamma(E)]L} , \quad \text{then} \quad \alpha(E) = 0 .$$

## 3. Original calculus of the continuous spectrum

By virtue of Proposition 2.1, we note that there are two types of energy $E$. The energy $E$ such that $|D(E)| \leq 2$ or $|D(E)| > 2$.

We show that:

$$\sigma(P) = \{E \in \mathbb{R}\ ;\ |D(E)| \leq 2\} = \overline{\left\{E \in \mathbb{R}\ ;\ \frac{d\alpha}{dE}(E) \neq 0\right\}}$$

for that we are brought more particularly to study the properties of the function $\alpha(E)$ when $V$ is a real continuous function and periodic on $\mathbb{R}$.

Let $\varphi_1(E,x)$ and $\varphi_2(E,x)$ be two independent solutions of the equation $(\mathcal{E})$, such that

$$\left\{\begin{array}{l} \varphi_1(E,0) = 1 \\ \\ \dfrac{d\varphi_1}{dx}(E,0) = 0 \end{array}\right. \quad \text{and} \quad \left\{\begin{array}{l} \varphi_2(E,0) = 0 \\ \\ \dfrac{d\varphi_2}{dx}(E,0) = 1 \end{array}\right.$$

Consider the matrix $M(E,x,V)$ defined by

$$M(E,x,V) = \begin{pmatrix} \varphi_1(E,x) & \varphi_2(E,x) \\ \\ \dfrac{d\varphi_1}{dx}(E,x) & \dfrac{d\varphi_2}{dx}(E,x) \end{pmatrix} \tag{3.1}$$

then by using (2.1) and (2.2) we have

$$M(E,L,V) = \begin{pmatrix} \text{Re}\left(e^{ikL}F(E)\right) + \text{Re}\left(e^{-ikL}G(E)\right) & \dfrac{1}{k}\text{Im}\left(e^{ikL}F(E)\right) + \dfrac{1}{k}\text{Im}\left(e^{-ikL}G(E)\right) \\ -k\text{Im}\left(e^{ikL}F(E)\right) + k\text{Im}\left(e^{-ikL}G(E)\right) & \text{Re}\left(e^{ikL}F(E)\right) - \text{Re}\left(e^{-ikL}G(E)\right) \end{pmatrix}$$

We observe that $Tr(M(E,L,V)) = Tr(Q(E)) = D(E)$, thus $M(E,L,V)$ and $Q(E)$ have the same characteristic equation and therefore the same eigenvalues.

Consequently, we obtain the following corollary:

**Corollary 3.1.** *The following assertions are equivalent:*

(1) $|D(E)| \leq 2$
(2) $\gamma(E) = 0$
(3) $e^{i\alpha(E)L}$ *is an eigenvalue for* $Q(E)$

(4) $e^{i\alpha(E)L}$ *is an eigenvalue for* $M(E,L,V)$*.*

Let us consider $P(\theta)$ the operator $P$ defined on $L^2([0,L])$ with the boundary conditions

$$\begin{cases} \psi(L) = e^{i\theta}\psi(0) \\ \psi'(L) = e^{i\theta}\psi'(0) \end{cases}$$

where $\theta \in [0, 2\pi]$. Then,

**Theorem 3.2.** $\gamma(E) = 0$ *if and only if there exist* $\theta \in [0,\pi]$*, such that* $E$ *is an eigenvalue for* $P(\theta)$*. In this case, we have:*

$$\theta = \alpha(E)L$$

*Proof.* If $\varphi$ is a solution of $(\mathcal{E})$, then

$$\varphi(E,x) = c_1\varphi_1(E,x) + c_2\varphi_2(E,x)\,.$$

Thus,

$$\begin{cases} \varphi(E,L) = c_1\varphi_1(E,L) + c_2\varphi_2(E,L) \\ \dfrac{d\varphi}{dx}(E,L) = c_1\dfrac{d\varphi_1}{dx}(E,L) + c_2\dfrac{d\varphi_2}{dx}(E,L) \\ \varphi(E,0) = c_1 \\ \dfrac{d\varphi}{dx}(E,0) = c_2 \end{cases}$$

and then

$$\begin{pmatrix} \varphi(E,L) \\ \\ \dfrac{d\varphi}{dx}(E,L) \end{pmatrix} = M(E,L,V) \begin{pmatrix} \varphi(E,0) \\ \\ \dfrac{d\varphi}{dx}(E,0) \end{pmatrix}.$$

If $e^{i\alpha(E)L}$ is an eigenvalue for $M(E,L,V)$, there exist $c_1'$ and $c_2'$ such that $(c_1', c_2') \neq (0,0)$ and

$$M(E,L,V)\begin{pmatrix} c_1' \\ c_2' \end{pmatrix} = e^{i\alpha(E)L}\begin{pmatrix} c_1' \\ c_2' \end{pmatrix}.$$

We put

$$\psi(E,x) = c_1'\varphi_1(E,x) + c_2'\varphi_2(E,x)\,.$$

$\psi$ is thus an eigenfunction associated with the eigenvalue $E$ of the operator $P(\alpha(E)L)$. Conversely, if $E$ is an eigenvalue for $P(\theta)$ and $\theta \in [0,\pi]$, then there exist $\Psi(E,.) \neq 0$ solution of $(\mathcal{E})$ such that:

$$\begin{pmatrix} \Psi(E,L) \\ \\ \dfrac{d\Psi}{dx}(E,L) \end{pmatrix} = e^{i\theta} \begin{pmatrix} \Psi(E,0) \\ \\ \dfrac{d\Psi}{dx}(E,0) \end{pmatrix} = M(E,L,V) \begin{pmatrix} \Psi(E,0) \\ \\ \dfrac{d\Psi}{dx}(E,0) \end{pmatrix},$$

which shows that $e^{i\theta}$ is an eigenvalue for $M(E,L,V)$ and $\theta = \alpha(E)L$.

We are thus brought to study the operators $P(\theta)$, $\theta \in [0,\pi]$. We recall some properties of these operators.

**Theorem 3.3.** [See. [GhMe],[ReSi]]

(i) *for all $\theta \in [0,\pi]$, $P(\theta)$ has purely discrete spectrum $(E_n(\theta))_{n\in\mathbb{N}^*}$, such that for any $n$, $E_n(.)$ is analytic on $]0,\pi[$ and continuous at $0$ and $\pi$.*

(ii) *$P(\theta)$ and $P(2\pi-\theta)$ are antiunitarily equivalent under ordinary complex conjugation. In particular, their eigenvalues are identical and their eigenfunctions are complex conjugates.*

(iii *For $n$ odd (respectively, $n$ even) $E_n(.)$ is strictly increasing (respectively, strictly decreasing) as $\theta$ increases from $0$ to $\pi$. In particular,*

$$0 < E_1(0) < E_1(\pi) \leq E_2(\pi) < E_2(0) \leq \cdots$$
$$\leq E_{2n-1}(0) < E_{2n-1}(\pi) \leq E_{2n}(\pi) < E_{2n}(0) \leq \cdots$$

We can now combine Corollary 3.1 and Theorems 3.2 and 3.3 to get:

**Theorem 3.4.** *If $P = -\dfrac{d^2}{dx^2} + V$ is now defined on $L^2(\mathbb{R})$ with domain*

$$H^2(\mathbb{R}) = \left\{ u \in L^2(\mathbb{R})\,;\, \frac{d^2u}{dx^2} \in L^2(\mathbb{R}) \right\}$$

*and $V$ is a continuous real and periodic function on $\mathbb{R}$, we have*

$$\{E \in \mathbb{R}\ ;\ \gamma(E) = 0\} = \bigcup_{n\in\mathbb{N}^*} \bigcup_{\theta\in[0,\pi]} \{E_n(\theta)\}$$

*and, if $\rho$ designates the resolvent set,*

$$\{E\ ;\ \gamma(E) > 0\} \subset \rho(P)\,.$$

*Proof.* Indeed, if $\gamma(E) > 0$, by the standard theory of ordinary differential equations, we obtain two linearly independent functions $\varphi_1(E,.)$ and $\varphi_2(E,.)$ analytic in $E$ and $C^2(\mathbb{R})$ solutions of the equation $(\mathcal{E})$ such that

$$\varphi_1(E,x) = v_1(E,x)e^{+w(E)x} \quad ; \quad \varphi_2(E,x) = v_2(E,x)e^{-w(E)x}\,,$$

where $v_1(E,x)$ and $v_2(E,x)$ are two periodic functions. Moreover, for all $x \in \mathbb{R}$:

$$\varphi_1(E,x)\frac{d\varphi_2}{dx}(E,x) - \varphi_2(E,x)\frac{d\varphi_1}{dx}(E,x) = \text{constant}=c \neq 0\,. \tag{3.2}$$

Let us define the function

$$G_E(x,y) = G_E(y,x) = -\frac{\varphi_1(E,x)\varphi_2(E,y)}{c} \quad , \, x \leq y\,,$$

and consider the integral operator $G_E$ with kernel $G_E(x,y)$ acting on $L^2(\mathbb{R})$ by

$$\begin{aligned}(G_E f)(x) &= \int_{\mathbb{R}} G_E(x,y)f(y)dy \\ &= -\frac{1}{c}[\varphi_2(E,x)\int_{-\infty}^{x} \varphi_1(E,y)f(y)dy + \varphi_1(E,x)\int_{x}^{+\infty} \varphi_2(E,y)f(y)dy].\end{aligned} \tag{3.3}$$

Now $G_E$ is a bounded operator on $L^2(\mathbb{R})$. Indeed, since there exist $k_1$, $k_2 > 0$ such that for all $x$ in $\mathbb{R}$,

$$|\varphi_1(E,x)| \leq k_1 e^{\gamma(E)x} \quad ; \quad |\varphi_2(E,x)| \leq k_2 e^{-\gamma(E)x}\,,$$

it suffices to establish that the operators

$$K_- f(x) = \int_{-\infty}^{x} e^{-\gamma(E)(x-y)}\,|f(y)|\,dy \;\; ; \; K_+ f(x) = \int_{x}^{+\infty} e^{-\gamma(E)(y-x)}\,|f(y)|\,dy$$

map continuously on $L^2(\mathbb{R})$.

In particular, we see that $K_\pm$ are well defined on $L^2(\mathbb{R})$. By partial integration and Schwarz' inequality we see that, for any $T > 0$,

$$\begin{aligned}
\int_{-T}^{T} |K_- f(x)|^2\, dx &= \int_{-T}^{T} e^{-2\gamma(E)x}[\int_{-\infty}^{x} e^{\gamma(E)y}\, |f(y)|\, dy]^2 dx \\
&= \left\{ -\frac{1}{2\gamma(E)} e^{-2\gamma(E)x} \left[ \int_{-\infty}^{x} e^{\gamma(E)y}\, |f(y)|\, dy \right]^2 \right\}_{x=-T}^{x=T} \\
&\qquad + \frac{1}{\gamma(E)} \int_{-T}^{T} e^{-\gamma(E)x}\, |f(x)| \left( \int_{-\infty}^{x} e^{\gamma(E)y}\, |f(y)|\, dy \right) dx \\
&\leq \frac{1}{2\gamma(E)} (K_- f(-T))^2 + \frac{1}{\gamma(E)} \int_{-T}^{T} |K_- f(x)|\, |f(x)|\, dx \\
&\leq \frac{1}{2\gamma(E)} (K_- f(-T))^2 \\
&\qquad + \frac{1}{\gamma(E)} \left( \int_{-T}^{T} |K_- f(x)|^2\, dx \right)^{1/2} \left( \int_{-T}^{T} |f(x)|^2\, dx \right)^{1/2} .
\end{aligned}$$

However, $\lim_{T \to +\infty} K_- f(-T) = 0$, so that

$$\|K_- f\|_{L^2(\mathbb{R})} \leq \frac{1}{\gamma(E)} \|f\|_{L^2(\mathbb{R})} .$$

We obtain the same estimation for $K_+$. Consequently, for arbitrary $f,\ g \in L^2(\mathbb{R})$, we have

$$\|K_\pm f - K_\pm g\|_{L^2(\mathbb{R})} \leq \frac{1}{\gamma(E)} \|f - g\|_{L^2(\mathbb{R})} . \tag{3.4}$$

Then the $K_\pm$ are continuous. This is so since $G_E$ is the inverse operator of $(P - E)$ and then $E \in \rho(P)$. Indeed,

(i) For all $f$ in $H^2(\mathbb{R})$ we have (by using derivatives in the generalized sense)

$$(P-E)G_E f(x) = -\frac{1}{c}\left[-\frac{d^2\varphi_2}{dx^2}(E,x)\int_{-\infty}^{x}\varphi_1(E,y)f(y)dy - \frac{d\varphi_2}{dx}(E,x)\varphi_1(E,x)f(x) + \frac{d\varphi_1}{dx}(E,x)\varphi_2(E,x)f(x) - \frac{d^2\varphi_1}{dx^2}(E,x)\int_{x}^{+\infty}\varphi_2(E,y)f(y)dy + (V(x)-E)\varphi_2(E,x)\int_{-\infty}^{x}\varphi_1(E,y)f(y)dy + (V(x)-E)\varphi_1(E,x)\int_{x}^{+\infty}\varphi_2(E,y)f(y)dy\right] = f(x)$$

(ii) After two partial integrations we obtain

$$\begin{aligned}(G_E(P-E)f)(x) &= \int_{-\infty}^{+\infty} G_E(x,y)(P-E)f(y)dy \\ &= -\frac{1}{c}\left[\varphi_2(E,x)\frac{d\varphi_1}{dx}(E,x) - \varphi_1(E,x)\frac{d\varphi_2}{dx}(E,x)\right]f(x) + \\ &\quad (G_E(P-E)\varphi_1(E,x)f)(x) + (G_E(P-E)\varphi_2(E,x)f)(x) = f(x)\end{aligned}$$

for all $f \in H^2(\mathbb{R})$

Now, consider the bijective mappings

$$E_n : [0,\pi] \to [E_n(0), E_n(\pi)]\ , \quad \theta \mapsto E_n(\theta)$$

if $n$ is odd, and

$$E_n : [0,\pi] \to [E_n(\pi),\ E_n(0)] \quad \theta \mapsto E_n(\theta)$$

if $n$ is even.

If for instance $n$ is odd and $E \in [E_n(0),\ E_n(\pi)]$ then there is a unique $\theta \in [0,\pi]$ such that $E = E_n(\theta)$, and $e^{i\theta}$is an eigenvalue for $M(E,L,V)$. Consequently $\alpha(E)L = \theta$ according to Theorem 3.2. While using Theorem 3.3, we obtain that

$$\alpha(\,.\,)L : [E_n(0),\ E_n(\pi)] \to [0,\pi]\ , \quad E \mapsto \alpha(E)L\,,$$

is the inverse mapping of

$$E_n : [0,\pi] \to [E_n(0),\ E_n(\pi)]\ , \quad \theta \mapsto E_n(\theta)\,.$$

It is then continuous and strictly monotone, and thus strictly increasing on $]0,\pi[$, because $E_n$ is analytic

$$\begin{cases} \alpha(E_n(0))L = 0 \\ \alpha(E_n(\pi))L = \pi\,. \end{cases}$$

Therefore, $\alpha$ is differentiable on the interval $]E_n(0),\ E_n(\pi)[$. By the same method, we show that for $n$ even the application

$$\alpha(\,.\,)L : [E_n(\pi)\,, E_n(0)] \to [0,\pi]\ , \quad E \mapsto \alpha(E)L\,,$$

is the inverse of

$$E_n : [0,\pi] \to [E_n(\pi),\ E_n(0)]\ , \quad \theta \mapsto E_n(\theta)\,.$$

It is continuous and strictly decreasing on $]\,0\,,\pi[$, so it is differentiable on this interval.

Put

$$\alpha_n = \begin{cases} E_n(0) & \text{if } n \text{ is odd} \\ E_n(\pi) & \text{if } n \text{ is even} \end{cases} \quad , \quad \beta_n = \begin{cases} E_n(\pi) & \text{if } n \text{ is odd} \\ E_n(0) & \text{if } n \text{ is even} \end{cases}$$

We have obtained the following result:

**Lemma 3.5.** *The phase $\alpha$ is possibly constant on the intervals $]\,\beta_n, \alpha_{n+1}[$. Or it is strictly increasing for $n$ odd and strictly decreasing for $n$ even on $]\,\alpha_n, \beta_n[$.*

Let

$$f(E) = \begin{cases} 0 \quad \text{if} \quad E \in \,]\,\beta_n, \alpha_{n+1}[ \\ \\ (-1)^{n-1}\dfrac{d\alpha}{dE}(E) \quad \text{if} \quad E \in \,]\,\alpha_n, \beta_n[ \end{cases} \tag{3.5}$$

According to Lemma **3.5**, $f$ is $dE-$almost everywhere defined on $\mathbb{R}$. Moreover it is locally integrable because it is bounded, so the corresponding absolutely continuous measure $d\nu = f(E)dE$ is then well defined (where $dE$ is the Lebesgue measure in $\mathbb{R}$ denoted by $|\,.\,|$ in section 4).

**Theorem 3.6.** *If $V$ is a continuous real and periodic function on $\mathbb{R}$ , then the spectrum of the operator $P$ on $L^2(\mathbb{R})$ is purely absolutely continuous.*

*Proof.* Let us define for all $n$ in $\mathbb{N}^*$

$$\mathcal{H}_n = \left\{ \Psi \in L^2(\mathbb{R}, dx) ;\ \exists g \in L^2\left([0, 2\pi], \frac{d\theta}{2\pi}\right),\quad \Psi(x+kL) = \int_0^{2\pi} e^{ik\theta} g(\theta) \Psi_n(\theta, x) \frac{d\theta}{2\pi},\ 0 \leq x \leq L,\ k \in \mathbb{Z} \right\}$$

where $\{\Psi_n(\theta, .)\}_{n\in\mathbb{N}^*}$ is an orthonormal basis of eigenfunctions associated with the discrete spectrum $(E_n(\theta))_{n\in\mathbb{N}^*}$ of $P(\theta)$. $\mathcal{H}_n$ is a closed subspace of $L^2(\mathbb{R}, dx)$ and $L^2(\mathbb{R}, dx) = \bigoplus_{n=1}^{n=+\infty} \mathcal{H}_n$. On the other hand, $P$ preserves all the spaces $\mathcal{H}_n$, $n \in \mathbb{N}^*$. Indeed, for all $\Psi \in \mathcal{H}_n \cap H^2(\mathbb{R})$, we have:

$$(P\Psi)(x+kL) = \int_0^{2\pi} e^{ik\theta} g(\theta) E_n(\theta) \Psi_n(\theta, x) \frac{d\theta}{2\pi}\ ;\ \forall k \in \mathbb{Z}$$

and since $E_n(\,.\,)$ is analytic on $[0, 2\pi]$ then $g(\,.\,)E_n(\,.\,) \in L^2\left([0, 2\pi], \frac{d\theta}{2\pi}\right)$. Consequently,

$$\sigma(P) = \bigcup_{n=1}^{n=+\infty} \sigma(P_{|\mathcal{H}_n}) \tag{3.6}$$

In particular, if we set for all $n$ in $\mathbb{N}^*$

$$\mathcal{U}_n : \mathcal{H}_n \to L^2\left([0, 2\pi], \frac{d\theta}{2\pi}\right),\quad \Psi \to g$$

such that

$$\Psi(x+jL) = \int_0^{2\pi} e^{ij\theta} g(\theta) \Psi_n(\theta, x) \frac{d\theta}{2\pi},$$

we then see that $\mathcal{U}_\backslash$ is unitary. We get $P_n = \mathcal{U}_n P \mathcal{U}_n^{-1}$, then $P_n(g(\,.\,)) = E_n(\,.\,)g(\,.\,)$, for all $n \in \mathbb{N}^*$. Furthermore,

$$L^2\left([0, 2\pi], \frac{d\theta}{2\pi}\right) = L^2\left([0, \pi], \frac{d\theta}{2\pi}\right) \bigoplus L^2\left([\pi, 2\pi], \frac{d\theta}{2\pi}\right)$$

and $P_n$ preserves these two spaces. If for instance $n$ is odd,

$$\alpha(\,.\,)L : [E_n(0),\ E_n(\pi)] \to [0, \pi],\quad E \mapsto \alpha(E)L = E_n^{-1}(E),$$

$\alpha$ is a $C^1$ function and $d\alpha$ is absolutely continuous with respect to the Lebesgue measure.

For the operator $\mathcal{U}$ from $L^2\left([0,\pi]\,, \dfrac{d\theta}{2\pi}\right)$ into $L^2([E_n(0),\ E_n(\pi)]\,, dx)$, defined by

$$(\mathcal{U}g)(E) = \left(\frac{d\alpha}{dE}\right)^{1/2} g(\alpha(E)) = \left[\left(\frac{dE_n}{d\theta}\right)_{\theta=\alpha(E)}\right]^{-1/2} g(\alpha(E))\,,$$

we have

$$\begin{aligned}\|(\mathcal{U}g)\|^2_{L^2([E_n(0),\ E_n(\pi)],dx)} &= \int_{E_n(0)}^{E_n(\pi)} |g(\alpha(E))|^2 \left[(\frac{dE_n}{d\theta})_{\theta=\alpha(E)}\right]^{-1} dE \\ &= \int_0^{\pi} |g(x)|^2\, dx\end{aligned}$$

We see that $\mathcal{U}$ is a surjective isometry, i.e. unitary. Moreover,

$$\left(\mathcal{U}P_n\mathcal{U}^{-1}\right) g(E) = Eg(E)\,; \tag{3.7}$$

then each $P_n$ has an absolutely continuous spectrum, and so does $P$ according (3.6).

**Theorem 3.7.** *If $V$ is a continuous real and periodic function on $\mathbb{R}$ and $\mu$ the spectral measure associated with the operator $P$, then $\mu$ is equivalent to $\nu$.*

In order to show this theorem we are going to need the following fundamental results:

**Lemma 3.7.** [See. [Is],[Pa],[JoMo], [Ko],[Ri]]

(1) *In the general case $\gamma$ can be extended to continuous potentials, not necessary periodic, using the expression*

$$\gamma(E) = \lim_{|x|\to+\infty} \frac{1}{|x|} \log\|M(E,x,V)\|\ . \tag{3.8}$$

(2) *Let $d\mu_{ac}(E) = g(E)dE$ the absolutely continuous part of the spectral measure $\mu$ with respect to the Lebesgue measure $dE$, then for all Borel sets $B$ of $\mathbb{R}$, we have $\gamma(E) = 0$, $dE-$almost everywhere on $B \Rightarrow g(E) \neq 0$ $dE-$almost everywhere on $B$.*

*Proof of theorem 3.7* Let $B$ be a Borel set of $\mathbb{R}$. Then, we have

$$\begin{aligned}\nu(B) &= 0 \Rightarrow f(E)=0\ ,\ dE\text{- almost everywhere on } B\\ &\Rightarrow \frac{d\alpha}{dE}(E)=0\ ,\ dE\text{- almost everywhere on } B\\ &\Rightarrow \gamma(E)>0\ ,\ dE\text{- almost everywhere on } B\,.\end{aligned}$$

Now thanks to Lemma 3.4, we know that $E \in \rho(P)$ if $\gamma(E) > 0$. Thus

$$\nu(B)=0 \Rightarrow E\in\rho(E) \Rightarrow \mu_{ac}(B)=0\,.$$

Moreover, $\nu(B) \neq 0 \Rightarrow f(E) \neq 0$, $dE-$almost everywhere on $B \Rightarrow \frac{d\alpha}{dE}(E) \neq 0$, $dE-$almost everywhere on $B \Rightarrow \gamma(E) = 0$.

According to Lemma 3.8, we also have $\gamma(E) = 0$, $dE-$almost everywhere on $B \Rightarrow f(E) > 0$, $dE-$almost everywhere on $B$. Then $\nu(B) \neq 0 \Rightarrow \mu_{ac}(B) \neq 0$, and

$$\begin{aligned}\sigma_{ac}(P) &= \operatorname{supp}\mu_{ac} = \operatorname{supp} f\\ &= \overline{\left\{E\in\mathbb{R}\ ;\ \frac{d\alpha}{dE}(E)\neq 0\right\}} = \{E\in\mathbb{R}\ ;\ \gamma(E)=0\}\end{aligned}$$

According to Lemma 3-4,

$$\sigma_{ac}(P)=\sigma(P)=\{E\in\mathbb{R}\ ;\ \gamma(E)=0\}=\bigcup_{n=1}^{+\infty}[\alpha_n,\beta_n]$$

and $d\nu(E) = d\mu_{ac}(E) = f(E)dE$.

## 4. Decomposition of the absolutely continuous spectrum

In this section we give a refinement of absolutely continuous spectrum of the operator $P$ on $L^2(\mathbb{R})$, when $V$ is continuous real and periodic function on $\mathbb{R}$.

Now, using results from the articles of Avron-Simon [AvSi1] and Gherib-Messirdi [GhMe], it is easy to establish that $\sigma(P)$ is decomposed into two disjoint sets called respectivelly the transient $\sigma_{tac}(P)$ and reccurent $\sigma_{rac}(P)$ absolutely continuous spectrum of $P$.

Set

$$B=\bigcup_{n=1}^{+\infty}[\alpha_n,\beta_n]=\{E\in\mathbb{R}\ ;\ \gamma(E)=0\} \tag{4.1}$$

For that it is enough to determine the event $\left[\overset{oes}{B}\right]$ of the essential interior of the $[B]$ and the event $[C]$ of the essential frontier of the event $[B]$. Where the event of the borelian set $B$ is

$$[B] = \left\{A \text{ borelian set of } \mathbb{R}\,;\ \left|A\Delta B\right| = 0\right\}\ ;$$

its essential interior noted $\overset{oes}{B}$ is defined by

$$\left\{x \in \mathbb{R}\,;\ \exists\, t > 0 \text{ such that } \left|\,]x-t, x+t[\cap B\,\right| = 2t\right\}$$

and the essential frontier of $B$ is the event $[C]$, where $C$ is a borelian set of $\mathbb{R}$ satisfying $\left|C\Delta(B\setminus \overset{oes}{B})\right| = 0$, $\Delta$ denotes the symmetric difference between subsets of $\mathbb{R}$.

Since the essential interior contains the topological interior, then

$$\bigcup_{n=1}^{+\infty} ]\alpha_n, \beta_n[\, \subset \overset{oes}{B}\ .$$

In the other hand if $\alpha_n$ is a degenerate point for $P(\pi)$ if $n$ is even and for $P(0)$ if $n$ is odd, then there exists $t > 0$ such that :

$$\left|\,]\,\alpha_n - t\,,\ \alpha_n + t[\,\cap\,\sigma(P)\right| = 2t$$

Thus $\alpha_n \in \overset{oes}{B}$. Now, if $\alpha_n$ is a nondegenerate point for $P(\pi)$, if $n$ is even ($n$ is taken to be odd for the case $P(0)$), then for all $t > 0$:

$$\left|\,]\,\alpha_n - t\,,\ \alpha_n + t[\,\cap\,\sigma(P)\right| < 2t$$

and $\alpha_n$ must belong to $C$. In the other hand, if $\beta_n$ is a nondegenerate point for $P(\pi)$, if $n$ is odd ($n$ is taken to be even for the case $P(0)$), then for all $t > 0$:

$$\left|\,]\,\beta_n - t\,,\ \beta_n + t[\,\cap\,\sigma(P)\right| < 2t$$

Consequently, $\beta_n$ must belong to $C$ and

$$\overset{oes}{B} = \bigcup_{n=1}^{+\infty} ]\alpha_n, \beta_n[\, \cup \{\alpha_n; \alpha_n \text{ is a degenerate point for } P(\pi) \text{ if } n \text{ is even and for } P(0) \text{ if } n \text{ is odd}\}$$

$$C = \{\alpha_n \; ; \; \alpha_n \text{ is a nondegenerate point for} P(\pi) \text{if } n \text{ is even and for } P(0) \text{ if n is odd}\} \cup \{\beta_n \; ; \; \beta_n \text{ is a nondegenerate point for } P(0) \text{ if n is even and for } P(\pi) \text{ if n is odd}\}$$

Since

$$L^2_{tac} = p(\overset{oes}{B})L^2_{ac} \quad \text{and} \quad L^2_{rac} = p\,(C)\,L^2_{ac} \tag{4.2}$$

where $p\,(\overset{oes}{B})$ and $p\,(C)$ are respectively the orthogonal projections on $\overset{oes}{B}$ and $C$ and $L^2_{ac}$ is the absolutely continuous space associated with the operator $P$ on $L^2(\mathbb{R})$, then

$$\sigma_{tac}\,(P) = \sigma\left(P_{|L^2_{tac}}\right) \subset \overset{oes}{B}$$

and

$$\sigma_{rac}(P) = \sigma\left(P_{|L^2_{rac}}\right) \subset C$$

In addition $\overset{oes}{B}$ and $C$ are a partition of $\sigma_{ac}$, then

$$\sigma_{tac}(P) = \overset{oes}{B} \quad \text{and} \quad \sigma_{rac}(P) = C \tag{4.3}$$

## References


[AvSi1] J. Avron, B. Simon. *Transient and reccurent spectrum*. J. Func. Anal. **43** (1981), 1–31.

[AvSi2] J. Avron, B. Simon. *Almost periodic Schrödinger operators, I. Limit periodic potentials*. Commun. Math. Phys. °bf 82 (1982), 101–120.

[CyFrKiSi] H. L. Cycon, R. G. Froese, W. Kirsh, B. Simon. *Schrödinger operators, with applications to quantum mechanics and global geometry*. Springer–Verlag, New York, 1986.

[DaLi] R. Dautry, J. -L. Lions. *Analyse mathématique et calcul numérique. Spectre des opérateurs* (tome 5). Masson, Paris, 1988.

[Ea] M. S. P. Eastham. *The spectral theory of periodic differential equations*. Hainer, New York, 1974.

[GhMe] F. Gherib, B. Messirdi. *Various classification of the continuous spectrum of a selft-adjoint operator*. Research topics CNEPRU, B3101/13/00, 2002.

[Is] K. Ishii. *Localization of eigenstates and transport phenomena in one-dimentional disordered systems*. Suppl. Prog. theor. phys. **53**, 1973, 77–183.

[JoMo] R. Johnson, J. Moser. *The rotation number for almost periodic potentials*. Commun. Math. Phys. Erratum, Commun. Math. **84**, (1982), 403–438.

[Ka] T. Kato. *Perturbation theory for linear operators*. Springer–Verlag, Heidelberg, New York, 1976.

[Ko] S. Kotani. *Ljaponov indices determine absolutely continuous spectra of stationary random one-dimentional Schrödinger operators*. In: *Pro. Taniguchi Symp.*

*Stocastic Analysis, Katata(1982)*, 225–247. Edited by K. ITO. North Holland, Ameterdam, 1984.

[Me] B. MESSIRDI. *Asymptotique de Born-Oppenheimer pour la prédissociation moléulaire(cas de potentiels réguliers)*. Annales de l'Institut Henri Poincare, **61** (1994), 255–292.

[Ou] A. OUTASSOURT. *Comportement semi-classique pour l'opérateur de Schrödinger à potentiel périodique*. Journal of Functional Analysis **72** (1987), 65–93.

[Pa] L. PASTUR. *Spectral theory of random selft-adjoint operators". Journal of soviet Mathematics* **46** (1989), xxx.

[ReSi] M. REED, B. SIMON. *Methods of modern mathematical physics. Analysis operators*, Vol. 4. Academic Press, New York, 1979.

[Ri] L. RIENARD. *Spectral theory of Random Schrödinger operators*. Springer–Verlag, New York. 1990.

(Recibido en diciembre de 2003; la versión revisada en octubre de 2005)

FATIHA GHERIB
LABORATOIRE DE PHYSIQUE QUANTIQUE DE LA MATIÈRE
ET MODÉLISATIONS MATHÉMATIQUES
CENTRE UNIVERSITAIRE DE MASCARA, ALGERIA
*e-mail:* GFBB@caramail.com, fatiha_gherib@yahoo.fr
BEKKAI MESSIRDI
FACULTY OF SCIENCES, DEPARTMENT OF MATHEMATICS
UNIVERSITY OF ORAN, ALGERIA
*e-mail:* bmessirdi@univ-oran.dz, bmessirdi@yahoo.fr