

# Micro-local Analysis for the Metropolis Algorithm

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December 7, 2007

## Abstract

We prove sharp rates of convergence to stationarity for a simple case of the Metropolis algorithm: the placement of a single disc of radius  $h$  randomly into the interval  $[-1 - h, 1 + h]$ , with  $h > 0$  small. We find good approximations for the top eigenvalues and eigenvectors. The analysis gives rigorous proof for the careful numerical work in ([DN04]). The micro-local techniques employed offer promise for the analysis of more realistic problems.

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# 1 Introduction

The Metropolis algorithm is a basic tool of modern scientific computation. It was introduced by N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller and E. Teller in 1953 ([MRR<sup>+</sup>53]) as a method for simulating non-overlapping hard discs in a bounded region. A natural extension by W. Hastings ([Has70]) and its popularization as the basic step in simulated annealing result in a very widely used algorithm.

This paper is a contribution to the running time analysis of the Metropolis algorithm. We carry out a careful spectral analysis in perhaps the simplest special case: the placement of a single disc of radius  $h$  randomly into the interval  $I_h = [-1 - h, 1 + h]$ . Here, the Metropolis algorithm is easy to state (informally). Suppose at some stage, the center of the disc (here an interval of length  $2h$ ) is at  $x \in [-1, 1]$ . Choose  $u$  uniformly in  $[-h, h]$  and attempt to slide the disc to  $x + u$ . If the disc is still entirely contained in  $I_h$ , the center moves to  $x + u$ . If part of the disc falls outside  $I_h$ , the center stays at  $x$ . In either case, this is one step of the Metropolis algorithm. Successive steps, iterating the same procedure, result in a uniform placement in the limit.

In this paper we show that order of  $1/h^2$  steps are necessary and sufficient for convergence from an arbitrary start. The main contribution of the paper is the introduction of micro-local techniques to give sharp asymptotics for the relevant eigenvalues and eigenvectors of the associated operator. Such spectral techniques have been important in giving sharp analysis for the Metropolis algorithm in discrete spaces ([DSC98]). Spectral techniques are lacking for continuous state spaces and indeed, even in the present simple problem, there is continuous and imbedded spectrum that is hard to understand. We are able to get around this and our techniques indicate that it is avoidable in many others problems.

Section 2 continues this introduction by giving a formal description of the Metropolis algorithm and a brief review of alternate approaches to getting rates of convergence. Finally, it gives a high level overview of the rather technical proof.

The argument proceeds by a careful analysis of

$$Z_\lambda = \{\zeta \in \mathbb{C}; \hat{\varphi}(\zeta) = \lambda\} \tag{1.1}$$

with  $\varphi$  a fixed, symmetric probability density on  $[-1, 1]$  (taken as uniform above, we allow more general proposals). This is done in section 3. It is followed by an analysis of the spectrum of the random walk generated by  $\varphi$ , restricted to  $[0, \infty[$  in section 4. Finally, the walk, rescaled by  $h$ , is restricted to  $[-1, 1]$  in section 5. In the  $h \rightarrow 0$  limit, we find the discrete spectrum of the Metropolis algorithm in  $[1 - \delta, 1]$  with  $\delta > 0$  independent of  $h$ . Explicit approximations of the associated eigenvectors, with uniform exponential error bounds are given. The final result is summarized in theorem 5.1 of section 5.

These results are harnessed in section 6 to give sharp rates of convergence to stationarity in total variation distance.

This paper suggests a new picture for a formally intractable problem. Roughly, for Metropolis algorithms on a domain, based on small proposed moves, the spectrum near 1 is discrete and well approximated (both eigenvalues and vectors) by the Neumann spectrum on the domain. Further, the continuous spectrum associated to the holding of the Metropolis chain is well isolated from 1 and does not cause trouble in proving sharp total variation convergence rates. This program has been successfully carried out in two other settings. In ([LM07]), a local ball walk on a general compact Riemannian manifold is metropolized to have area measure as stationary distribution. In ([DLM07]) a local ball walk on a domain in  $R^n$  is metropolized to have a prescribed stationary density. In both cases, the picture that emerges from the present paper guides the analysis.

**Acknowledgment:** We thank Joseph Keller, Andras Vasy, Susan Holmes, and especially John Neuberger for their help.

## 2 Metropolis, convergence, and an overview

### A. The Metropolis algorithm

Let  $(X, \mathcal{B}, \mu)$  be a  $\sigma$ -finite measure space. Let  $f(x) > 0$ ,  $\int f(x)d\mu(x) = 1$ , be a probability density on  $X$ . The Metropolis algorithm gives a way of drawing samples from  $f$ . It requires a symmetric proposal density  $p(x, y) = p(y, x) \geq 0$  for all  $x, y$ , and  $\int p(x, y)\mu(dy) = 1$  for all  $x$ . This kernel allows us to define the Metropolis kernel

$$\begin{aligned} m(x, dy) &= m(x)\delta_x + p(x, y)\min\left(\frac{f(y)}{f(x)}, 1\right)\mu(dy) \\ m(x) &= \int_{\{z:f(z)<f(x)\}} \left(1 - \frac{f(z)}{f(x)}\right)p(x, z)\mu(dz) \end{aligned} \tag{2.1}$$

Formula 2.1 has a simple algorithmic interpretation. From  $x$ , choose  $y$  from the density  $p(x, y)$ . If  $f(y) \geq f(x)$ , move to  $y$ . If  $f(y) < f(x)$  flip a coin with probability of heads  $f(y)/f(x)$ . If it comes up heads, move to  $y$ . If it comes up tails, stay at  $x$ . Observe that implementing this does not require knowledge of the normalizing constant for  $f$ . This is a crucial feature in applications where  $f(x)$  is given as  $Z^{-1}e^{-\beta H(x)}$  with  $Z$  unknowable in practice.

The Metropolis algorithm was introduced in ([MRR<sup>+</sup>53]) with important extensions in ([Has70]), ([Pes73]). For a text book treatment and many examples see ([HH64]). For examples in physics see ([BH02]), in biology and statistics see ([Liu01]). A geometrical interpretation is in ([BD01]); it shows that the kernel  $m(x, dy)$  is closest to  $p(x, y)\mu(dy)$  in an  $L^1$  metric on kernels.

The Metropolis algorithm, with many variations, is still widely used to simulate configurations of hard discs in compact regions of  $\mathbb{R}^d$  and for the closely related problem of simulating configurations of particles in potentials such as the Lennard-Jones potentials ([AT87]). A first serious study, giving rigorous rates of convergence for various hard core models, appears in the work of Kannan, Mahoney and Montenegro ([KMM03]). They study several algorithms, local, global and multiple, our scenario corresponds to a local

algorithm: one particle is chosen at random and moved locally. Global algorithms correspond to choosing a particle at random and a position at random, and trying to move the chosen particle to that position. In ([AT87]), useful convergence results are given for global algorithms in low dimensions assuming toroidal boundary conditions. The coupling techniques used in ([AT87]) can surely be adapted to the present problem, presumably with less precise constants. Sharp results are given for a related problem by Randall and Winkler ([RW05]). They study  $N$  particles in the unit interval. Each time, a particle is chosen at random and moved uniformly between the two surrounding particles. Again using coupling, it is shown that order  $N^3 \log(N)$  steps are necessary and sufficient to achieve randomness. Finally, we mention the coupling techniques in ([MT96]) as a potential method of getting rates of convergences.

## B. Convergence

Let  $L^2(f)$  be the space of real valued functions  $g$  which are square integrable with respect to  $f(x)\mu(dx)$ . The Metropolis kernel  $m(x, dy)$  acts on  $L^2(f)$  via

$$Mg(x) = \int g(y)m(x, dy) = m(x)g(x) + \int g(y)p(x, y)\min\left(\frac{f(y)}{f(x)}, 1\right)\mu(dy) \quad (2.2)$$

Note that we use  $m(x, dy)$  for the distribution kernel of the operator, and  $m(x)$  for the multiplier. Elementary arguments show that  $M : L^2(f) \rightarrow L^2(f)$  is a self adjoint contraction. Iterates of  $M$  are defined as usual by

$$M^k g(x) = \int (M^{k-1}g)(z)m(x, dz) = \int g(z)m^k(x, dz) \quad (2.3)$$

In our examples,  $X = \mathbb{R}$ ,  $\mu$  is the Lebesgue measure and  $f \equiv 1/2$  on  $[-1, 1]$  and zero elsewhere. We work throughout with a more general proposal as follows: let  $\tilde{\varphi}(x) = \tilde{\varphi}(-x)$ ,  $x \in [-1, 1]$ , be a symmetric, smooth, non negative function with  $\int_{-1}^1 \tilde{\varphi}(x)dx = 1$  and  $\tilde{\varphi}(\pm 1) > 0$ . Thus  $\tilde{\varphi}(x)dx$  is a probability density on  $[-1, 1]$  with respect to Lebesgue measure. Let  $\varphi(x)$ ,  $x \in \mathbb{R}$  be the extension of  $\tilde{\varphi}$  by 0 outside  $[-1, 1]$ . Re-scale to

$$\varphi_h(x) = \frac{1}{h}\varphi(x/h), \quad -h < x < h \quad (2.4)$$

Set  $p_h(x, y) = \varphi_h(x - y)$ . Thus in our examples

$$\begin{aligned} Mg(x) &= m_h(x)g(x) + \int_{[-1,1]} g(y)\varphi_h(x - y)dy \\ m_h(x) &= \int_{\{y < -1\}} \varphi_h(x - y)dy + \int_{\{y > 1\}} \varphi_h(x - y)dy \end{aligned} \quad (2.5)$$

Returning to the generality of 2.2, under mild conditions on  $p(x, y)$ , met in all our examples

$$\|m_x^k - f\|_{TV} \rightarrow 0 \quad \text{as } k \rightarrow \infty \quad \text{for all } x. \quad (2.6)$$

Here, the total variation distance is defined by

$$\|m_x^k - f\|_{TV} = \sup_A |m^k(x, A) - \int_A f(y)d\mu(y)| \quad (2.7)$$

with the sup over measurable sets  $A$ .

In applications, for example, for the original task of packing discs or for simulation of lattice models such as the Ising model, it is important to have a rate of convergence in 2.6. There are various flavors available. Perhaps weakest is “geometric ergodicity” ([MT93]), ([JH00]), ([RR01]), which asserts

$$\|m_x^k - f\|_{TV} \leq a(x)\gamma^k \quad (2.8)$$

for (usually unspecified)  $a(x) > 0$  and  $|\gamma| < 1$ . Observe that, without some information about  $a(x)$  and  $\gamma$ , 2.8 says little more than 2.6. More refined estimates have been developed for special cases ([JH01]), . These have come to be called ”honest bounds” because specific  $a(x) > 0$  and  $\gamma$  are given. Of course, upper bounds need not be sharp and one may ask about matching lower bounds, at least up to ”good constants”. We call such bounds ”sharp” in the sequel. A survey of sharp bounds for Markov chains on discrete state-spaces is in ([SC97]). This develops analytic techniques (Poincaré, Cheeger, Nash, Sobolev and log-Sobolev inequalities). Applications of these techniques to the Metropolis algorithm on discrete state spaces is in ([DSC98]) which has extensive further references.

Turning to continuous spaces, we know very few examples of sharp rates of convergence for the Metropolis algorithm. In ([Kie00]), ([MR00]), ([AT87]), ([JY04]), useful spectral gap estimates are derived. They give, for the chain 2.5

$$Ah^2 \leq \text{gap} \leq Bh^2 \quad \text{for specific } A, B. \quad (2.9)$$

In the present problem, we are able to prove (see theorem 5.1, formula 5.11)

$$\text{gap} = \frac{\alpha h^2 \pi^2}{8} + \mathcal{O}(h^3), \quad \alpha = \int_{-1}^1 z^2 \varphi(z) dz \quad (2.10)$$

The proof shows that the gap is achieved at the unique second largest eigenvector  $\psi$

$$\psi(x) = \cos(\eta_{1,h} \frac{x+1}{h}) + \frac{b(\hat{\varphi}(\eta_{1,h}))}{\eta_{1,h}} \sin(\eta_{1,h} \frac{x+1}{h}) + r_h(x) \quad (2.11)$$

where  $\eta_{1,h}$  is defined in theorem 5.1 and the  $b$ - function is defined in theorem 4.3. One has

$$\begin{aligned} \eta_{1,h} &= h\pi/2 + \mathcal{O}(h^2), \quad b(1) = 0 \\ |r_h(x)| &\leq c_1 |\lambda_1(h) - 1| \exp(-\frac{c_2}{h} \text{dist}(x, \{[-1, -1+h] \cup [1-h, 1]\})) \end{aligned} \quad (2.12)$$

for universal  $c_1, c_2 > 0$ . Similar results are given in theorem 5.1 for the (countably many) eigenvalues in  $[1-\delta, 1]$ , with  $\delta$  small, uniformly with respect to  $h$ . We have compared the asymptotic 2.10, 2.11, 2.12, with numerical calculations of a discretization of the operator 2.2 with  $\varphi$  uniform on  $[-1, 1]$  carried out for us by John Neuberger. The theory matched the numerics surprising closely. For example, for  $h = 0.1, 0.05, 0.03$ , successive refinements of the discretized operator stabilized to give the following results for the spectral gap  $1 - \lambda_1$ . Here, theory =  $h^2 \pi^2 / 24$  from 2.10.

true	.004107	.001028	.000457	(2.13)
theory	.004112	.001028	.000457	

Using these results we show in section 6

**Theorem 2.1** *Let  $h_0 > 0$  small. For the Metropolis chain 2.5 on  $[-1, 1]$ , there are universal  $M > 0, C > 0$  and  $A, A'$  such that for all  $h \in ]0, h_0]$  the following holds true :*

$$C \leq \min_{x \in [-1, 1]} \|m_x^n - f\|_{TV} \quad \text{for all } n \leq M/h^2 \quad (2.14)$$

$$A'e^{-\gamma'(h)nh^2} \leq \sup_{x \in [-1, 1]} \|m_x^n - f\|_{TV} \leq Ae^{-\gamma(h)nh^2} \quad \text{for all } n \geq M/h^2 \quad (2.15)$$

Here  $\gamma(h), \gamma'(h)$  are two positive functions such that  $\gamma(h) \simeq \gamma'(h) \simeq \alpha\pi^2/8$  when  $h \rightarrow 0$ , with  $\alpha$  from 2.10. The constants  $M, C, A, A'$  depend mildly on  $\varphi$ .

This is made explicit in section 6.

### C. An overview of the proof and the microlocal tools

Microlocal analysis was created by M.Sato, T.Kawai and M.Kashiwara in their famous paper ([SKK]). Unfortunately, the cohomological techniques used by Sato in the definition of hyperfunctions and the derived category language used by Kashiwara as a basic tool for the study of the sheaf of microfunctions and the algebraic analysis of  $\mathcal{D}$ -modules, has been an obstacle to the popularization of these powerful ideas in the analysis of partial differential equations. These ideas have been translated in a more accessible language and extended to more general problems occurring in the analysis of the singularities of solutions of linear pde's by L.Hörmander and many others, and the reader will find a complete introduction to this point of view on microlocal analysis in ([Hör85]). Soon after, J.Sjöstrand discover a rather simple way to express the ideas of ([SKK]) in a natural analytic language using basic properties of holomorphic functions and the so-called FBI transforms (see ([Sjö82])). Then, it turns out that microlocal analysis, originally used to analyse singularities, was also a powerful tool to understand the semi-classical limit of solutions of the Schrödinger equations, when the Planck constant  $h$  is considered as a small parameter. In fact, this is natural since the original motivation for the work of Sato comes from the mathematical analysis of Quantum mechanics. Then, part of the microlocal community moved to "semi-classical analysis", and the reader will find in the Dimassi-Sjöstrand book ([DS99]) a rather complete exposition of these techniques, and related results concerning spectral asymptotics. An accessible introduction to the microlocal techniques used in the paper is in ([Mar02]).

What we discover is that the Metropolis chain 2.5 can be understood as a "semi-classical-pseudo-differential boundary value problem", and that is why microlocal techniques enter in the proof.

Since here we deal with a 1-dimensional and constant coefficient problem, we can easily explain, at least at a formal level, what we use in our study, and what are the main differences with the very classical study of boundary value problems for pde's, which are just ordinary differential equations in one space dimension.

The study of the tempered solutions of an ode's  $p(D_x)f = 0$  on  $\mathbb{R}$ , where  $p$  is a polynomial, reduces via Fourier transform, to the study of the so called "real characteristic variety", that is to say here, the real roots of the algebraic equation  $p(\xi) = 0$  with  $\xi \in \mathbb{R}$ .

The same holds true at the semi-classical level for the equation  $p(hD_x)f = 0$ , where  $h$  is a small parameter. Assume for simplicity that  $p(\xi) = \xi^2$ , and that one wants to study the spectral theory for the simple self-adjoint Neumann boundary value problem

$$-h^2 f'' = \lambda f \quad \text{in } ]-1, 1[, \quad f'(\pm 1) = 0 \quad (2.16)$$

The spectrum of 2.16 is of course easy to compute, and the  $h$  dependence is trivial: the eigenvalues are  $\lambda_k(h) = p(hk\pi/2) = h^2 k^2 \pi^2 / 4$  for  $k \in \mathbb{N}$ , and the eigenvector associated to the eigenvalue  $\lambda_k(h)$  is proportional to

$$f_{k,h}(x) = \cos(k\pi \frac{x+1}{2}) \quad (2.17)$$

Let us now recall how one can understand the calculation which leads to 2.17 using basic micro-local ideas.

Take  $\lambda \in \mathbb{C}$  and let  $f \in L^2(-1, 1)$  be a tempered in  $h$  (i.e  $\|f\| \leq ch^{-m}$  for some  $c, m$ ) solution of the equation  $h^2 f'' + \lambda f = 0$ . Take  $[a, b] \subset ]-1, 1[$ . Then if  $\lambda \notin [0, \infty[$ ,  $\|f\|_{L^2(a,b)}$  is exponentially small in  $L^2$  norm. In fact, this is the "elliptic regularity" theorem: for  $\lambda \notin [0, \infty[$ , the symbol  $\xi^2 + \lambda$  is elliptic (i.e does not vanish for  $\xi \in \mathbb{R}$ ), thus any local tempered in  $h$  solution of the equation  $h^2 f'' + \lambda f = 0$  must be exponentially small in  $h$ . On the other hand, for  $\lambda \in [0, \infty[$ ,  $f$  is of the form

$$f(x) = a_+ e^{ix\mu_+/h} + a_- e^{ix\mu_-/h} \quad (2.18)$$

where  $\mu_{\pm}$  are the two real solutions of the algebraic equation  $p(\mu) = \mu^2 = \lambda$ .

This is the local theory, and it extends to the equation, with  $\varphi$  as in 2.4,

$$\int \varphi_h(x-y)f(y)dy - \lambda f(x) \in \mathcal{O}(e^{-c/h}) \quad (2.19)$$

since 2.19 is a semi-classical pseudodifferential equation with symbol  $\hat{\varphi}(\xi) - \lambda$ . Elliptic regularity asserts that for  $\lambda \neq 0$  such that  $\hat{\varphi}(\xi) - \lambda \neq 0 \forall \xi \in \mathbb{R}$ , any solution of 2.19 must be exponentially small in  $h$  in  $L^2(a, b)$ , and for  $\lambda \in \hat{\varphi}(\mathbb{R})$  and  $\lambda \neq 0$ ,  $f|_{(a,b)}$  belongs (up to an exponentially small in  $h$  correction) to the vector space spanned by the  $e^{ix\mu/h}$  (up to multiplicity), where  $\mu$  belongs to the finite set of real solutions of the equation  $\hat{\varphi}(\mu) = \lambda$ . Observe that since  $\lim_{\xi \rightarrow \infty} \hat{\varphi}(\xi) = 0$ , the special value  $\lambda = 0$  is highly singular for the problem 2.19. Fortunately, we do not have to understand the spectral theory of the Markov chain 2.5 near  $\lambda = 0$  in order to get results on the rate of convergence.

In particular, the same simple Metropolis example on periodic functions, i.e without the extra difficulty of the cut-off at the end points  $\pm 1$ , is an easy exercise, since by Fourier transform, theorem 2.1 is just a way to express the central limit theorem, for which we do not need any sophisticated analysis.

Then to get 2.17, it remains to understand how the boundary condition  $f'(\pm 1) = 0$  selects the spectral values  $\lambda_k(h)$ , and the values of the constants  $a_{\pm}$  in 2.18. Usually, the analysis of a boundary value problem is done using Calderon projectors. Let us recall

how it works. Let  $f$  be a given solution of 2.16 and let us denote by  $\underline{f}$  the extension of  $f$  by 0 outside  $[-1, 1]$ . Then  $\underline{f}$  satisfies

$$h^2 \underline{f}'' + \lambda \underline{f} = h^2 (f(-1)\delta_{-1} - f(1)\delta_1) \quad \text{on } \mathbb{R} \quad (2.20)$$

Then 2.20 is a local problem near any  $x \in \mathbb{R}$ , and in particular, we can analyze separately the contribution of the end points  $\pm 1$ . Near  $x = -1$ , set  $x = -1 + z$ . Then  $\underline{f}$  satisfies in the open set  $z \in ]-\infty, 1[$  the following equation, with  $a = f(-1)$

$$h^2 \underline{f}'' + \lambda \underline{f} = h^2 a \delta_0 \quad (2.21)$$

For  $\lambda \notin [0, \infty[$ , 2.21 has a unique globally defined tempered in  $h$  solution  $g$ , given for  $z \geq 0$  by

$$g(z) = a(2\pi h)^{-1} \int e^{iz\xi/h} \frac{d\xi}{\lambda - \xi^2} = \frac{a}{2ih\mu} e^{iz\mu/h} \quad (2.22)$$

where  $\mu$  is the unique solution of  $p(\mu) = \mu^2 = \lambda$  such that  $Im(\mu) > 0$ . The Calderon operator for this elementary example is just the map

$$g(0) = \frac{a}{2ih\mu} \mapsto hg'(+0) = \frac{a}{2h} = i\mu g(0) \quad (2.23)$$

Then by the local elliptic regularity theorem, one has  $\underline{f} - g \in \mathcal{O}(e^{-c/h})$  on any compact subset of  $]-\infty, 1[$ . In particular, the boundary condition  $f'(-1) = 0$  implies  $a \in \mathcal{O}(e^{-c/h})$ , which is just the elliptic regularity theorem at the boundary. Therefore, we get that for a solution of 2.16 with norm 1, we must have  $\lambda \in [0, \infty[$ . Of course, this is obvious by integration by parts since 2.16 is a positive self adjoint problem, but 2.22 says more, since it is a local result near the end point which does not use any global information on  $f$ . Then using  $f'(-1) = 0$  and  $\lambda \in [0, \infty[$ , we get that  $f$  has to be equal to

$$f(x) = b \cos(\mu(x+1)/h) + \mathcal{O}(e^{-c/h}) \quad (2.24)$$

on the interval  $x \in [-1, 1/2[$ , with  $\mu^2 = \lambda$ . Finally, one gets the spectral values of the parameter  $\lambda$  by matching the two formulas 2.24 associated to the two end points  $\pm 1$ .

For the Markov chain 2.5, the boundary condition  $f'(\pm 1) = 0$  is replaced by the function  $m_h(x)$  which has support in the boundary layer  $[-1, -1+h] \cup [1-h, 1]$ . This already indicates that the 2-dimensional space of boundary data  $f(-1), f'(-1)$  is, in our problem, replaced by the infinite dimensional Hilbert space  $L^2(-1, -1+h)$ . Obviously, this is not a straightforward generalization, and it explains why the proof of our result seems technical: it is in the very nature of the problem. The analysis of pseudo-differential boundary value problem has been done by L. Boutet de Monvel in ([BdM71]). Here, we are working with a "semi-classical-pseudo-differential boundary value problem", a different situation, since the "boundary" is no longer a subvariety, but is replaced by a boundary layer of size  $h$ . Observe also that the function  $m_h(x)$  is not smooth, but only Lipschitz at  $x = -1+h$  and  $x = 1-h$ . Thus we have to work with weakly singular coefficients. The fact that the probability of staying in the boundary layer after  $n$  steps of the walk decays exponentially has the following analytical counterpart: pseudodifferential operators of variable order are used in section 3 for the study of the spaces  $W_\lambda^c$ .

The study of the characteristic variety 1.1 is done in section 3. Observe that complex solutions of  $\hat{\varphi}(\zeta) = \lambda$  always occur in the study of a boundary value problem since formulas like 2.22 are crucial. We have to do here a careful study:  $\hat{\varphi}(\zeta) = \lambda$  is not an algebraic equation and admits an infinite number of solutions in the complex plane.

Then in our work, the Calderon operator 2.23 is replaced by the map  $S_\lambda^c$  introduced in 4.8. Here the notation  $S$  has been chosen in reference to a "Scattering operator": it connects information at the "boundary" to global properties, and so does formula 2.22. The analysis of the map  $S_\lambda^c$  is done in section 4.

Finally, the matching condition, which for a 1-dimensional problem is just a Bohr-Sommerfeld quantization formula, and which select the spectral values, is performed in section 5.

From this, we get that near  $\lambda = 1$ , the spectral analysis of the Markov chain 2.5 is close to the spectral analysis of the simple Neumann boundary value problem 2.16, a fact already obvious in the numerical simulations of [DN04].

### 3 The convolution on the line $\mathbb{R}$ and the space $W_\lambda^c$

Let  $\tilde{\varphi} \in C^\infty[-1, 1]$  be a non negative function such that

$$\tilde{\varphi}(-z) = \tilde{\varphi}(z), \quad \int_{-1}^1 \tilde{\varphi}(z) dz = 1, \quad \tilde{\varphi}(\pm 1) > 0 \quad (3.1)$$

Let  $\varphi$  be the function on  $\mathbb{R}$ ,

$$\varphi(z) = 1_{[-1,1]}(z) \tilde{\varphi}(z) \quad (3.2)$$

Let  $\hat{\varphi}(\zeta) = \int e^{-iz\zeta} \varphi(z) dz$  be the Fourier transform of  $\varphi$ . Then  $\hat{\varphi}(\zeta)$  is a holomorphic function of  $\zeta \in \mathbb{C}$  such that for all  $\zeta$  one has

$$\hat{\varphi}(\zeta) = \hat{\varphi}(-\zeta), \quad \overline{\hat{\varphi}(\zeta)} = \hat{\varphi}(\bar{\zeta}), \quad |\hat{\varphi}(\zeta)| \leq e^{|\text{Im}(\zeta)|} \quad (3.3)$$

For any  $\zeta \in \mathbb{C} \setminus 0$ , one gets by integration by parts

$$\hat{\varphi}(\zeta) = 2\tilde{\varphi}(1) \frac{\sin \zeta}{\zeta} + \int_{-1}^1 \frac{e^{-iz\zeta}}{i\zeta} \tilde{\varphi}'(z) dz \quad (3.4)$$

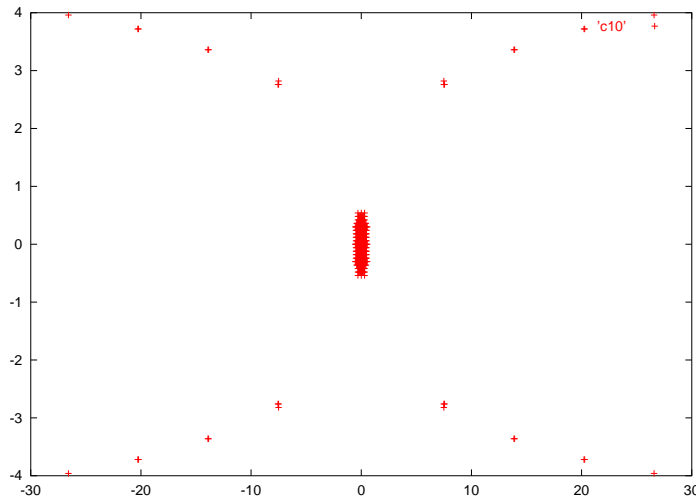
For any real  $\xi$ , one has  $\hat{\varphi}(\xi) = \hat{\varphi}(-\xi) \in \mathbb{R}$ ,  $|\hat{\varphi}(\xi)| \leq 1$ ,  $\lim_{|\xi| \rightarrow \infty} \hat{\varphi}(\xi) = 0$ . Moreover, from the continuity of  $\varphi$  and  $1 \pm \hat{\varphi}(\xi) = \int_{-1}^1 (1 \pm \cos(x\xi)) \varphi(x) dx$ , one gets  $\hat{\varphi}(\xi) = 1$  iff  $\xi = 0$  and that there exists  $\nu_0 \in ]0, 1[$  such that

$$\hat{\varphi}(\mathbb{R}) = [-\nu_0, 1] \quad (3.5)$$

For any  $\lambda \in \mathbb{C}$ , we denote by  $Z_\lambda$  the set

$$Z_\lambda = \{\zeta \in \mathbb{C}, \quad \hat{\varphi}(\zeta) = \lambda\} \quad (3.6)$$

Then one has, for any  $\zeta \in Z_\lambda$ ,  $-\zeta \in Z_\lambda$  and  $\bar{\zeta} \in Z_{\bar{\lambda}}$ . The following lemma determines the asymptotic behavior of the set  $Z_\lambda$  for any  $\lambda \in \mathbb{C} \setminus 0$ . Roughly, it shows that  $Z_\lambda$

Figure 3.1: The set of zeros  $Z_1$ .

appears as in figure 1. For the special case where  $\varphi = 1$  on  $[-1, 1]$ , the Fourier transform is  $\hat{\varphi}(\zeta) = \sin(\zeta)/\zeta$  and lemma 3.1 determines the behavior of the complex solutions of  $\sin(\zeta) = \lambda\zeta$ . The asymptotic results 3.9 were first derived by Hardy ([Har02]) in this case. These results are refined and applied in materials science analysis of the stress field of a thin plate in ([BS73]). In the following figures, we draw the set  $\{z \in \mathbb{C}, |\frac{\sin(z)}{z} - \lambda| \leq 0.05\}$ . Figure 1 is in the case  $\lambda = 1$ : one sees the effect of the double zero at  $z = 0$  and the others zeros on the logarithmic curves. Figure 2 is the superposition of these sets for the values  $\lambda = e^{i\theta}$ ,  $\theta = 0, 45, 90, 180, 270$  degrees: one sees the monodromie structure of the set  $Z_\lambda$  when  $\lambda$  moves, and the splitting of the double zero for  $\theta \simeq 0$ .

Thus, there are four symmetrically placed ends which are asymptotically evenly spaced, on logarithmic curves. Near zero, the points in  $Z_\lambda$  need not be so regular, but this involves only finitely many points. The following lemma makes this precise.

**Lemma 3.1** *Let  $0 < \rho_0 < \rho_1$ . There exists  $M > 0$  such that for all  $\zeta = a + ib$  one has*

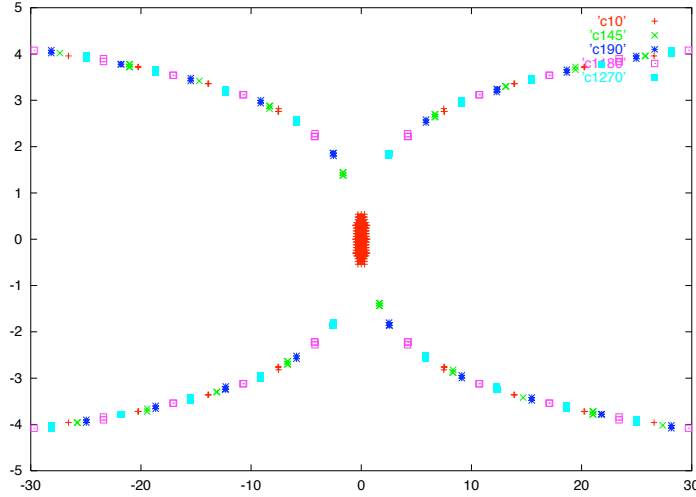
$$\begin{aligned} |a| \geq Me^{|b|} &\Rightarrow |\hat{\varphi}(\zeta)| \leq \rho_0/2 \\ |a| \leq \frac{1}{M}e^{|b|} - 1 &\Rightarrow |\hat{\varphi}(\zeta)| \geq 2\rho_1 \end{aligned} \quad (3.7)$$

*For any  $\lambda_0 \in \mathbb{C}$  in the annulus  $\rho_0 \leq |\lambda_0| \leq \rho_1$ , there exists  $R > 0, l_0 > 0, \tau_0 > 0, r_0 > 0$ , with  $2l_0\pi + \pi/2 > \tau_0$  and a symbol  $\Theta(\tau, \lambda)$  defined for  $\tau \geq \tau_0$ , holomorphic in  $|\lambda - \lambda_0| \leq r_0$ , satisfying the estimates (hereafter, we choose a determination of  $\log(\lambda)$  in  $|\lambda - \lambda_0| \leq r_0$ )*

$$\begin{aligned} \Theta(\tau, \lambda) &= \frac{i}{\tau} \left( \log\left(\frac{\tau}{\tilde{\varphi}(1)}\right) + \log\lambda + \frac{\tilde{\varphi}'(1)}{\tilde{\varphi}(1)} \right) + \Theta_1(\tau, \lambda) \\ \forall k \quad \exists C_k \quad |\partial_\tau^k \Theta_1(\tau, \lambda)| &\leq C_k \tau^{-k} \left( \frac{\log\tau}{\tau} \right)^2 \end{aligned} \quad (3.8)$$

*such that for all  $\zeta = a + ib$  with  $|\zeta| \geq R, a > 0, b > 0$ , one has  $\zeta \in Z_\lambda$  iff there exists an integer  $l \geq l_0$  such that  $\zeta = \zeta_l$  with*

$$\zeta_l = \tau_l + i \log(\lambda) + i \log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + i \Theta(\tau_l, \lambda), \quad \tau_l = 2l\pi + \pi/2 \quad (3.9)$$

Figure 3.2: The monodromy of the set  $Z_\lambda$ .

For all  $c_0 > 0$ , there exists  $C > 0$  such that if  $\zeta$  is such that  $|\zeta|$  is large and  $|\zeta - \zeta_l| \geq c_0$  for all  $l$ , then one has

$$|\hat{\varphi}(\zeta) - \lambda| \geq C \frac{e^{Im(\zeta)}}{|\zeta|} \quad (3.10)$$

*Proof.* Set for  $\zeta \neq 0$

$$R(\zeta) = \int_{-1}^1 \frac{e^{-iz\zeta}}{i\zeta} \tilde{\varphi}'(z) dz = \frac{e^{-i\zeta}}{i\zeta} \int_0^2 e^{it\zeta} \tilde{\varphi}'(1-t) dt \quad (3.11)$$

For any  $g \in C^\infty([0, 2])$ , the holomorphic function  $F_g(\zeta) = \int_0^2 e^{it\zeta} g(t) dt$  is bounded in the upper half plane  $Im(\zeta) \geq 0$ , and by integration by parts, one has for any  $N \geq 1$

$$F_g(\zeta) = \sum_{j=0}^{N-1} (i/\zeta)^{1+j} \left( g^{(j)}(0) - e^{2i\zeta} g^{(j)}(2) \right) + (i/\zeta)^N F_{g^{(N)}}(\zeta) \quad (3.12)$$

From  $\partial_\zeta^k F_{g^{(N)}}(\zeta) = F_{(it)^k g^{(N)}}(\zeta)$  and  $|\int_0^2 e^{it\zeta} (it)^k g^{(N)}(t) dt| \leq C(k, N)/|\zeta|$ , we get that for all  $k, N$  there exists  $C_{k,N}$  such that for all  $\zeta \neq 0$ ,  $Im(\zeta) \geq 0$  one has

$$|\partial_\zeta^k \left( F_g(\zeta) - \sum_{j=0}^{N-1} (i/\zeta)^{1+j} (g^{(j)}(0) - e^{2i\zeta} g^{(j)}(2)) \right)| \leq C_{k,N} |\zeta|^{-1-N} \quad (3.13)$$

Thus, from 3.13, we get that for all  $k, N$  there exists a constant  $C_{k,N}$  such that for all  $\zeta \neq 0$  in the upper half plane  $Im(\zeta) \geq 0$  one has with  $R(\zeta) = \frac{e^{-i\zeta}}{i\zeta} S(\zeta)$

$$|\partial_\zeta^k \left( S(\zeta) - \sum_{j=0}^{N-1} (i/\zeta)^{1+j} (-1)^j (\tilde{\varphi}^{(1+j)}(1) - e^{2i\zeta} \tilde{\varphi}^{(1+j)}(-1)) \right)| \leq C_{k,N} |\zeta|^{-1-N} \quad (3.14)$$

In order to prove 3.7, we may assume  $\zeta \neq 0$ , and  $\zeta = a + ib$  with  $a \geq 0, b \geq 0$ . By 3.4, 3.14 and  $|\frac{\sin(\zeta)}{\zeta}| \leq \frac{2}{|\zeta|}e^b$ , one has

$$\begin{aligned} |\hat{\varphi}(\zeta)| &\leq \frac{C}{|\zeta|}e^b \\ |\hat{\varphi}(\zeta) - 2\tilde{\varphi}(1)\frac{\sin \zeta}{\zeta}| &\leq \frac{C}{|\zeta|^2}e^b \end{aligned} \quad (3.15)$$

There exists  $c' > 0$  such that for all  $b \geq 1$  one has  $|\frac{\sin(\zeta)}{\zeta}| \geq \frac{c'}{|\zeta|}e^b$ , and therefore, 3.7 follows easily from 3.15.

In order to prove 3.8 and 3.9, we may assume  $\lambda = |\lambda|e^{i\theta}$  with  $\log(\lambda) = \log(|\lambda|) + i\theta$ , and  $\zeta = a + ib$ ,  $\frac{e^b}{M} - 1 \leq a \leq Me^b$  with  $b \geq b_0$  and  $b_0$  large. In particular,  $|\zeta| = a + \mathcal{O}((\log(a))^2/a)$  and  $|e^{i\zeta}| = \mathcal{O}(1/a)$ . By 3.4, the equation  $\hat{\varphi}(\zeta) = \lambda$  is equivalent to

$$\zeta e^{i\zeta} \lambda = i\tilde{\varphi}(1)(1 - e^{2i\zeta}) - iS(\zeta) \quad (3.16)$$

which implies by 3.14

$$\zeta e^{i\zeta} \lambda = i\tilde{\varphi}(1)(1 + \mathcal{O}(1/a)) \quad (3.17)$$

Thus there must exist an integer  $l > 0$  such that

$$\zeta - i\log(\zeta) = 2l\pi + \pi/2 + i\log(\lambda) - i\log(\tilde{\varphi}(1)) + \mathcal{O}(1/a) \quad (3.18)$$

The equation  $\zeta - i\log(\zeta) = s$  is equivalent to  $\zeta = \psi(s)$  with  $\psi(s) = s + i\log(s) + \mathcal{O}((\log(s))/s)$ . Thus 3.18 implies, with  $\tau_l = 2l\pi + \pi/2$

$$\zeta = \tau_l + i\log(\lambda) + i\log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + i\mu, \quad \mu \in \mathcal{O}((\log(l))/l) \quad (3.19)$$

Set

$$\beta = \frac{1}{\tau_l}(\log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + \log(\lambda) + \mu) \quad (3.20)$$

so that  $\zeta = \tau_l(1 + i\beta)$ ,  $\zeta e^{i\zeta} \lambda = i\tilde{\varphi}(1)e^{-\mu}(1 + i\beta)$  and  $e^{2i\zeta} = -\frac{\tilde{\varphi}(1)^2 e^{-2\mu}}{\lambda^2 \tau_l^2}$ . Then 3.16 is now equivalent to

$$e^{-\mu}(1 + i\beta) = 1 + \frac{\tilde{\varphi}(1)^2 e^{-2\mu}}{\lambda^2 \tau_l^2} - \frac{S(\zeta)}{\tilde{\varphi}(1)} \quad (3.21)$$

By 3.14, the right hand side of 3.21 is equal to  $1 - i\frac{\tilde{\varphi}'(1)}{\zeta\tilde{\varphi}(1)} + \mathcal{O}(1/l^2)$ , thus we get  $\mu = i\beta + i\frac{\tilde{\varphi}'(1)}{\zeta\tilde{\varphi}(1)} + \mathcal{O}((\log(l))/l^2)$ , and therefore by 3.20

$$\mu = \frac{i}{\tau_l}(\log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + \log(\lambda) + \mu) + i\frac{\tilde{\varphi}'(1)}{\zeta\tilde{\varphi}(1)} + \mathcal{O}((\log(l))/l^2) \quad (3.22)$$

and using 3.19 we get

$$\mu = \frac{i}{\tau_l}(\log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + \log(\lambda) + \frac{\tilde{\varphi}'(1)}{\tilde{\varphi}(1)}) + \mathcal{O}((\log(l))/l^2) \quad (3.23)$$

From 3.19 we get that 3.9 holds true with  $\Theta(\tau, \lambda) = \mu$ , where  $\mu$  is the solution of the equation 3.21 with  $\zeta$  defined by 3.19 and  $\tau = \tau_l$ . More precisely,  $\mu$  is the solution close to 0 of the equation, where  $\tau$  is large

$$\begin{aligned} e^{-\mu}(1 + i\beta) &= 1 + \frac{\tilde{\varphi}(1)^2 e^{-2\mu}}{\lambda^2 \tau^2} - G(\lambda, \tau, \mu) \\ \beta &= \frac{1}{\tau} (\log(\frac{\tau}{\tilde{\varphi}(1)}) + \log(\lambda) + \mu) \\ G(\lambda, \tau, \mu) &= \frac{1}{\tilde{\varphi}(1)} \int_0^2 e^{it(\tau + i \log(\frac{\tau}{\tilde{\varphi}(1)}))} e^{-t \log(\lambda)} e^{-t\mu} \tilde{\varphi}'(1-t) dt \end{aligned} \quad (3.24)$$

For  $r_0 > 0$  small, the function  $G(\lambda, \tau, \mu)$  is holomorphic in  $\lambda, \mu$  in  $|\lambda - \lambda_0| \leq r_0, |\mu| \leq r_0$  and satisfies in this set for  $\tau \geq \tau_0$  large

$$|\partial_\tau^k G(\lambda, \tau, \mu)| \leq C_k \tau^{-1-k} \quad (3.25)$$

Thus, with  $\gamma = \frac{1}{\tau} (\log(\frac{\tau}{\tilde{\varphi}(1)}) + \log(\lambda))$ , so that  $\beta = \gamma + \mu/\tau$ , the solution of the equation 3.24 is of the form  $\mu = H(\lambda, \gamma, \tau)$  where  $H$  is holomorphic in  $\lambda, \gamma$  in  $|\lambda - \lambda_0| \leq r_0, |\gamma| \leq r_0$  and satisfies in this set for  $\tau \geq \tau_0$  large

$$|\partial_\tau^k (H(\lambda, \gamma, \tau) - \log(1 + i\gamma))| \leq C_k \tau^{-1-k} \quad (3.26)$$

Then 3.8 follows from 3.26 and 3.23.

Finally, let us show that 3.10 holds true. By 3.16, it is equivalent to prove

$$|i\tilde{\varphi}(1)(1 - e^{2i\zeta}) - iS(\zeta) - \lambda\zeta e^{i\zeta}| \geq C \quad (3.27)$$

and by 3.15 we may assume as before  $\zeta = a + ib$ ,  $\frac{e^b}{M} - 1 \leq a \leq Me^b$  with  $b \geq b_0$  and  $b_0$  large. In fact, by 3.7, one has for  $a \geq Me^b$ ,  $|\hat{\varphi}(\zeta) - \lambda| \geq \rho_0/2 \geq \frac{Ce^b}{|\zeta|}$  and by 3.15, one has for  $\frac{e^b}{M} - 1 \geq a$ ,  $|\hat{\varphi}(\zeta)| \geq \frac{C}{|\zeta|} e^b$ , and so  $|\hat{\varphi}(\zeta) - \lambda| \geq \frac{Ce^b}{|\zeta|} - |\lambda| \geq \frac{C'e^b}{|\zeta|}$  for  $M$  large. Then, by 3.14 one has  $S(\zeta) \in \mathcal{O}(1/|\zeta|)$ , and also  $|\zeta| = a + \mathcal{O}((\log(a))^2/a)$ ,  $|e^{i\zeta}| = \mathcal{O}(1/a)$ , so that 3.27 reduces to showing

$$|i\tilde{\varphi}(1) - \lambda\zeta e^{i\zeta}| \geq C \quad (3.28)$$

Then 3.28 is an obvious consequence of 3.9 and  $\Theta(\tau, \lambda) \in \mathcal{O}(\frac{\log(\tau)}{\tau})$  since if one has  $|i\tilde{\varphi}(1) - \lambda\zeta e^{i\zeta}| \leq C$  with  $C > 0$  small, there must exist an  $l$  and a  $\mu$  small such that 3.19 holds true. The proof of lemma 3.1 is complete.  $\square$

For  $\zeta \in \mathbb{C}$ , we set  $\langle \zeta \rangle = \sqrt{1 + |\zeta|^2}$ . We shall say that a function  $\zeta \in \mathbb{C} \rightarrow d(\zeta) \in \mathbb{C}$  is moderate if it satisfies for some  $A, B > 0$  an estimate

$$|d(\zeta)| \leq A \langle \zeta \rangle^B \quad (3.29)$$

For all  $\zeta \in \mathbb{C}$ , and since  $\varphi$  is compactly supported, the following formula holds true

$$\varphi * e^{iz\zeta} = \hat{\varphi}(\zeta) e^{iz\zeta} \quad (3.30)$$

This suggests looking at sums of exponentials, for a given  $\lambda \in \mathbb{C} \setminus 0$ ,

$$f(z) = \sum_{\zeta \in Z_\lambda} d(\zeta) e^{iz\zeta} \quad (3.31)$$

Lemma 3.1 implies that for any moderate function  $d$ , the formula 3.31 defines a distribution  $f \in \mathcal{D}'(\mathbb{R})$ . Here and in the sequel, we shall always use the following convention : If  $\zeta \in Z_\lambda$  is a multiple root of order  $m$  of the equation  $\hat{\varphi}(\zeta) = \lambda$ , then  $d(\zeta)e^{iz\zeta}$  denotes any function of the form  $\sum_0^{m-1} d_j z^j e^{iz\zeta}$ . By lemma 3.1, multiple roots may only occurs for  $\zeta$  in a compact subset of  $\mathbb{C}$  which depends on  $\lambda$ , but remains in a fixed compact set for  $0 < \rho_0 \leq |\lambda| \leq \rho_1 < \infty$ .

Observe that by lemma 3.1, there exist  $c_0 > 0$  such that for all  $\zeta \in Z_\lambda$ , one has  $|Im(\zeta)| \leq c_0 \log(1 + |\zeta|)$ . Thus, for  $z \in [-R, R]$  and  $k > B + 2 + c_0 R$ , the series, where  $Q$  is a compact neighbourhood of 0 in  $\mathbb{C}$ ,

$$g(z) = \sum_{\zeta \in Z_\lambda \setminus Q} \frac{d(\zeta)}{(i\zeta)^k} e^{iz\zeta} \quad (3.32)$$

is uniformly convergent in the interval  $z \in [-R, R]$ , and thus defines a continuous function  $g$  on the interval  $[-R, R]$ . Then

$$f = \partial_z^k g + \sum_{\zeta \in Z_\lambda \cap Q} d(\zeta) e^{iz\zeta}$$

is a well defined distribution on  $] - R, R[$ . We shall denote by  $\mathcal{D}'_\lambda$  the vector space of distributions on  $\mathbb{R}$  of the form 3.31. Observe that, by 3.30, any  $f \in \mathcal{D}'_\lambda$  satisfies the convolution equation

$$\forall f \in \mathcal{D}'_\lambda \quad \varphi * f - \lambda f = 0 \quad (3.33)$$

since  $f$  is defined by a convergent series in  $\mathcal{D}'$ . For  $c \in \mathbb{R}$ , let  $Z_\lambda^c$  be the subset of  $Z_\lambda$

$$Z_\lambda^c = \{\zeta \in Z_\lambda, \quad Im(\zeta) > c\} \quad (3.34)$$

We denote by  $\mathcal{D}'_{\lambda,c}$  the subspace of  $\mathcal{D}'_\lambda$  of distribution on  $\mathbb{R}$  of the form, with  $d$  moderate

$$f(z) = \sum_{\zeta \in Z_\lambda^c} d(\zeta) e^{iz\zeta} \quad (3.35)$$

Let  $L_c^2$  be the following Hilbert space of locally square integrable functions on  $]0, \infty[$

$$L_c^2 = \{f \in L_{loc}^2(]0, \infty[), \quad \int_0^\infty e^{2cz} |f(z)|^2 dz < \infty\} \quad (3.36)$$

Let  $W_\lambda^c$  be the following vector space of distributions on the half line  $]0, \infty[$

$$W_\lambda^c = \{f \in \mathcal{D}'(]0, \infty[), \exists g \in \mathcal{D}'_{\lambda,c} \text{ such that } g|_{]0, \infty[} = f \quad \text{and} \quad f|_{]0, 2[} \in L^2\} \quad (3.37)$$

The following crucial definition is a careful way of saying that a family  $F_\lambda$  of subspaces of an Hilbert space  $H$  depends analytically on the complex parameter  $\lambda$ . The analyticity of  $\lambda \rightarrow W_\lambda^c$  stated in proposition 3.3 will be one of the main essential point in the proof of our results on the rate of convergence of the Metropolis algorithm.

**Definition 3.2** *If  $H$  is a Hilbert space and  $F_\lambda$  a family of closed subspaces of  $H$  defined for  $\lambda$  in an open subset  $U$  of  $\mathbb{C}$ , we shall say that  $\lambda \rightarrow F_\lambda$  is analytic if for any  $\lambda_0 \in U$ , there exists  $r > 0$  and a holomorphic map  $A_\lambda$  from the disc  $|\lambda - \lambda_0| < r$  into the space of bounded linear operators from  $F_{\lambda_0}$  into its orthogonal complement  $F_{\lambda_0}^\perp$  such that*

$$F_\lambda = \{x : x = y + A_\lambda(y), \text{ for some } y \in F_{\lambda_0}\} \quad \text{for} \quad |\lambda - \lambda_0| < r \quad (3.38)$$

**Proposition 3.3** For  $\lambda \in \mathbb{C} \setminus 0$  and  $c \in \mathbb{R}$ ,  $W_\lambda^c$  is a closed subspace of  $L_c^2$ , and

$$\bigcap_{c \in \mathbb{R}} W_\lambda^c = \{0\} \quad (3.39)$$

Moreover, for any fixed  $c$  and  $\lambda_0 \in \mathbb{C} \setminus 0$ , there exists  $r > 0$  such that  $\lambda \rightarrow W_\lambda^c \subset L_c^2$  is analytic for  $|\lambda - \lambda_0| < r$ .

For any  $\lambda \in \mathbb{C} \setminus [-\nu_0, 1]$ , and any  $g \in L^2(\mathbb{R})$  with support in  $[-1, 1]$ , the unique solution  $f \in L^2(\mathbb{R})$  of the convolution equation  $\varphi * f - \lambda f = g$  satisfies

$$f|_{]0, \infty[} \in W_\lambda^0 \quad (3.40)$$

*Proof.* Let  $\lambda_0 \in \mathbb{C} \setminus 0$  and  $D_0 = \{\lambda, |\lambda - \lambda_0| \leq |\lambda_0|/2\}$ . We fix a determination of  $\log(\lambda)$  for  $\lambda \in D_0$ . For  $\bar{\lambda} \in \overline{D_0}$ , we set  $\log(\bar{\lambda}) = \overline{\log(\lambda)}$ . Let  $\tau_0 > 0$  be such that the symbol  $\Theta(\tau, \lambda)$  of lemma 3.1 is well defined for  $\tau \geq \tau_0$  and  $\lambda \in D_0 \cup \overline{D_0}$ . Then there exists  $R > 0$  such that for  $\lambda \in D_0$  and  $\zeta \in Z_\lambda$  with  $|\operatorname{Re}(\zeta)| \geq R$  and  $\operatorname{Im}(\zeta) > 0$ , one has (by 3.9) for some  $l \in \mathbb{Z}$  (we use  $\zeta \in Z_\lambda \Rightarrow -\bar{\zeta} \in Z_{\bar{\lambda}}$  to get the second line of 3.41 from 3.9)

$$\begin{aligned} \zeta &= \tau_l + i \log(\lambda) + i \log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + i \Theta(\tau_l, \lambda), & \tau_l &= 2l\pi + \pi/2, \quad l > 0, \quad \text{if } \operatorname{Re}(\zeta) > 0 \\ \zeta &= -\tau_l + i \log(\lambda) + i \log\left(\frac{\tau_l}{\tilde{\varphi}(1)}\right) + i \overline{\Theta}(\tau_l, \lambda), & \tau_l &= 2|l|\pi + \pi/2, \quad l < 0, \quad \text{if } \operatorname{Re}(\zeta) < 0 \end{aligned} \quad (3.41)$$

where  $\overline{\Theta}(\tau_l, \lambda) = \overline{\Theta(\tau_l, \bar{\lambda})}$ .

Let us define the set of indices

$$L(\lambda, c) \subset \mathbb{Z} \quad (3.42)$$

such that for  $\zeta \in Z_\lambda$ , one has  $\operatorname{Im}(\zeta) > c$  iff  $l \notin L(\lambda, c)$  in 3.41. Then there exists  $c_0 > 0$  such that  $L(\lambda, c)$  is well defined for  $c \geq c_0$ , and all  $\lambda \in D_0$ , and is an interval  $L(\lambda, c) = [-l_1(\lambda, c), l_2(\lambda, c)]$ . One has by 3.41 for  $c$  large

$$2\pi l_{1,2}(\lambda, c) \simeq \frac{e^c \tilde{\varphi}(1)}{|\lambda|} \quad (3.43)$$

Take  $\tau_0$  as in lemma 3.1, and large enough so that for all  $|\xi| \geq \tau_0$  and all  $\lambda \in D_0 \cup \overline{D_0}$ , the following inequality holds true

$$\frac{|\lambda|(|\xi| + \pi/2)}{\tilde{\varphi}(1)} + \operatorname{Re}(\Theta(|\xi| + \pi/2, \lambda)) \geq 1$$

For  $z \in \mathbb{R}$ ,  $\xi \in \mathbb{R}$ ,  $|\xi| \geq \tau_0$  and  $\lambda \in D_0$ , set  $\tau(\xi) = |\xi| + \pi/2$ , and  $\theta(\xi, \lambda) = \Theta(\tau(\xi), \lambda)$  for  $\xi > 0$ ,  $\theta(\xi, \lambda) = \overline{\Theta}(\tau(\xi), \lambda)$  for  $\xi < 0$ . let  $q(z, \xi, \lambda)$  be the function

$$q(z, \xi, \lambda) = e^{iz \operatorname{sign}(\xi) \pi/2} \lambda^{-z} \left(\frac{\tau(\xi)}{\tilde{\varphi}(1)}\right)^{-z} e^{-z \theta(\xi, \lambda)} \quad (3.44)$$

Let  $\chi \in C^\infty(\mathbb{R})$  be equal to 0 in  $|\xi| \leq \tau_0$ , and equal to 1 in  $|\xi| \geq \tau_0 + 1$ . Let  $Q(z, D_z, \lambda)$  be the pseudodifferential operator of variable order

$$Q(z, D_z, \lambda) f = \frac{1}{2\pi} \int e^{iz\xi} q(z, \xi, \lambda) \chi(\xi) \hat{f}(\xi) d\xi \quad (3.45)$$

Let us describe briefly the action of  $Q(z, D_z, \lambda)$  on  $\mathcal{S}'$ , the Schwartz space of tempered distributions on  $\mathbb{R}$ . One has

$$Q(z, D_z, \lambda)f = \int k_\lambda(z, z')f(z')dz' \quad (3.46)$$

where  $k_\lambda(z, z')$  is the distribution kernel defined by the oscillatory integral

$$k_\lambda(z, z') = \frac{1}{2\pi} \int e^{i(z-z')\xi} q(z, \xi, \lambda) \chi(\xi) d\xi \quad (3.47)$$

Let  $\varepsilon_0 > 0$  small and  $R_0 > 0$  large be given. Then, by integration by parts in 3.47 and using the definition 3.44 of  $q(z, \xi, \lambda)$  and the estimate 3.8, one gets that for all  $\alpha, \beta$ , there exists  $C_{\alpha, \beta}$  such that the following inequality holds true for all  $z, z'$  such that  $z \geq -R_0$ ,  $|z - z'| \geq \varepsilon_0$

$$|(z - z')^\alpha \partial_{z, z'}^\beta k_\lambda(z, z')| \leq C_{\alpha, \beta} \quad (3.48)$$

Take  $\psi \in C_0^\infty(\mathbb{R})$  equal to 1 near 0. Then

$$\begin{aligned} Q(z, D_z, \lambda)f &= Q_\psi(z, D_z, \lambda)f + Q_{1-\psi}(z, D_z, \lambda)f \\ &= \int k_\lambda(z, z')\psi(z - z')f(z')dz' + \int k_\lambda(z, z')(1 - \psi)(z - z')f(z')dz' \end{aligned} \quad (3.49)$$

By 3.48, for any  $f \in \mathcal{S}'$ ,  $Q_{1-\psi}(z, D_z, \lambda)f(z)$  is a smooth function of  $z \geq -R_0$ . Moreover,  $Q_\psi(z, D_z, \lambda)$  is a properly supported pseudodifferential operator. This shows that  $Q(z, D_z, \lambda)f$  is a well defined distribution on  $\mathbb{R}$ , and is equal to  $Q_\psi(z, D_z, \lambda)f$  modulo a smooth function.

Let  $\mathcal{D}'_{per} \subset \mathcal{S}'$  be the vector space of distribution on  $\mathbb{R}$  which are periodic of period 1. Then any  $g \in \mathcal{D}'_{per}$  is of the form

$$g(z) = \sum_{l \in \mathbb{Z}} g_l e^{2i\pi lz} \quad (3.50)$$

with  $g_l$  temperate in  $l$ . By definition of  $W_\lambda^c$ , for  $c \geq c_0$  and  $\lambda \in D_0$ , one has

$$W_\lambda^c = \left\{ f = \left( Q(z, D_z, \lambda) \left( \sum_{l \in \mathbb{Z}} g_l e^{2i\pi lz} \right) \right) \Big|_{]0, \infty[}, g_l \text{ temperate and } f \Big|_{]0, 2[} \in L^2(]0, 2[) \right\} \quad (3.51)$$

We shall denote by  $\mathcal{H}$  the subspace of  $\mathcal{D}'_{per}$

$$\mathcal{H} = \left\{ g = \sum_{|l| \neq 0} g_l e^{2i\pi lz}, \text{ such that } \sum_{|l| \neq 0} g_l e^{iz \text{sign}(l)\pi/2} \tau_l^{-z(1+i/\tau_l)} e^{2i\pi lz} \in L^2(]0, 2[) \right\} \quad (3.52)$$

Here, as in 3.41,  $\tau_l = 2|l|\pi + \pi/2$ . If  $q_0(z, \xi) = e^{iz \text{sign}(\xi)\pi/2} \tau(\xi)^{-z(1+i/\tau(\xi))}$ , and with

$$Q_0(z, D_z)f = \frac{1}{2\pi} \int e^{iz\xi} q_0(z, \xi) \hat{f}(\xi) d\xi \quad (3.53)$$

one has

$$\mathcal{H} = \left\{ g = \sum_{|l| \neq 0} g_l e^{2i\pi lz}, \text{ such that } Q_0(z, D_z)g \in L^2(]0, 2[) \right\} \quad (3.54)$$

For  $g = \sum_{|l| \neq 0} g_l e^{2i\pi lz} \in \mathcal{H} \subset \mathcal{D}'_{per}$ , let  $f(z) = \sum_{|l| \neq 0} g_l e^{iz \operatorname{sign}(l) \pi/2 \tau_l^{-z(1+i/\tau_l)}} e^{2i\pi lz}$ . Then  $f = Q_0(z, D_z)g$  is a well defined distribution on  $\mathbb{R}$ . Since  $Q_0(z, D_z)$  is an elliptic operator at  $z$  of order  $-z$ , one has for all  $\alpha > 0$  and all  $z_0 \in ]0, 2[$ ,  $g \in H_{z_0}^{-z_0-\alpha}$  where  $H_{z_0}^s$  denotes the space of distributions which belongs to the Sobolev space  $H^s$  near  $z_0$ . In particular, since  $g$  is periodic of period 1, one has  $g \in H^{-1-\alpha}$  for all  $\alpha > 0$ , and its Fourier coefficients satisfy

$$\forall \alpha > 0, \exists C_\alpha \quad \sum |g_l|^2 |l|^{-2-2\alpha} \leq C_\alpha \|Q_0(z, D_z)g\|_{L^2(]0,2])} \quad (3.55)$$

This shows that  $\|Q_0(z, D_z)g\|_{L^2(]0,2])}$  is a norm on  $\mathcal{H}$ , and that equipped with this norm,  $\mathcal{H}$  is a Hilbert space. Moreover,  $\mathcal{H}$  imbeds continuously in the Sobolev space  $H^{-1-\alpha}(\mathbb{R}/\mathbb{Z})$  for all  $\alpha > 0$ .

Next observe that by 3.55, for all  $z > 3/2$ , the series  $\sum_{|l| \neq 0} g_l e^{iz \operatorname{sign}(l) \pi/2 \tau_l^{-z(1+i/\tau_l)}} e^{2i\pi lz}$  is convergent, and thus one has

$$f(z) = \sum_{|l| \neq 0} g_l e^{iz \operatorname{sign}(l) \pi/2 \tau_l^{-z(1+i/\tau_l)}} e^{2i\pi lz} \quad \forall z > 3/2 \quad (3.56)$$

In particular, one has for  $z \geq 2$ , with  $\alpha \in ]0, 1/2[$  small

$$|f(z)| \leq \sum_{|l| \neq 0} |g_l| \tau_l^{-z} \leq (2\pi)^{-z} \sum_{|l| \neq 0} \frac{|g_l|}{|l|^{1+\alpha}} |l|^{-z+1+\alpha} \quad (3.57)$$

and thus we get from 3.55

$$\|f\|_{L^2([2, \infty))} \leq C \|Q_0(z, D_z)g\|_{L^2(]0,2])} \quad (3.58)$$

Thus we get the equivalence of norms on  $\mathcal{H}$

$$\|Q_0(z, D_z)g\|_{L^2(]0,2])} \leq \|Q_0(z, D_z)g\|_{L^2(]0, \infty))} \leq C \|Q_0(z, D_z)g\|_{L^2(]0,2])} \quad (3.59)$$

The following lemma, where  $L(\lambda, c)$  is defined in 3.42, gives a convenient description of the space  $W_\lambda^c$  for  $c$  large.

**Lemma 3.4** *There exists  $c_0 > 0$  such that for  $c \geq c_0$  and  $\lambda \in D_0$ , one has*

$$W_\lambda^c = \left\{ f = \left( Q(z, D_z, \lambda)g \right) \Big|_{]0, \infty[}, \quad g \in \mathcal{H}, \quad g = \sum_{l \notin L(\lambda, c)} g_l e^{2i\pi lz} \right\} \quad (3.60)$$

Moreover, the map

$$g = \sum_{l \notin L(\lambda, c)} g_l e^{2i\pi lz} \in \mathcal{H} \rightarrow f = \left( Q(z, D_z, \lambda)g \right) \Big|_{]0, \infty[} \in W_\lambda^c \quad (3.61)$$

is injective.

*Proof.* By 3.44 and 3.8, one has

$$q(z, \xi, \lambda) = \left( \frac{\lambda}{\tilde{\varphi}(1)} \right)^{-z} q_0(z, \xi) (1 + q_{-1}(z, \xi, \lambda)) \quad (3.62)$$

where  $q_{-1}(z, \xi, \lambda)$  is analytic in  $\lambda \in D_0$  with values in symbols of degree  $-1$ . By the rules of composition of pseudodifferential operators, one thus gets

$$Q(z, D_z, \lambda) = \left( \frac{\lambda}{\tilde{\varphi}(1)} \right)^{-z} \left( (1 + R_{-1}(z, D_z, \lambda))Q_0(z, D_z) + R_{-\infty}(z, D_z, \lambda) \right) \quad (3.63)$$

where  $R_{-1}(z, D_z, \lambda)$  is analytic in  $\lambda \in D_0$  with values in pseudodifferential operators of degree  $-1$  and  $R_{-\infty}(z, D_z, \lambda)$  is of order  $-\infty$  on any compact subset of  $\mathbb{R}$ . Thus for  $f = \left( Q(z, D_z, \lambda)g \right)|_{]0, \infty[} \in W_\lambda^c$ , the condition  $f|_{]0, 2[} \in L^2$  is equivalent to

$$(1 + R_{-1}(z, D_z, \lambda))Q_0(z, D_z)g|_{]0, 2[} \in L^2 \quad (3.64)$$

Near  $z = 1$ , by the definition of  $Q_0(z, D_z)$ , 3.64 is equivalent to  $|D_z|^{-z}g \in L^2$ , and since  $g$  is periodic of period 1, this implies near  $z = 0$ ,  $|D_z|^{-z}g \in H^{-1}$ , or equivalently,  $Q_0(z, D_z)g \in H^{-1}$  near  $z = 0$ . Thus one has  $R_{-1}(z, D_z, \lambda)Q_0(z, D_z)g \in L^2$  near  $z = 0$ , and 3.64 is equivalent to

$$Q_0(z, D_z)g|_{]0, 2[} \in L^2 \quad (3.65)$$

which is equivalent to  $g \in \mathcal{H}$ . Thus 3.60 holds true.

Let  $c \geq c_0$  with  $c_0$  large and let  $\zeta_l \in Z_\lambda^c$  be defined by 3.41. For any  $g = \sum_{l \notin L(\lambda, c)} g_l e^{2i\pi l z} \in \mathcal{H}$  and  $f(z) = Q(z, D_z, \lambda)g = \sum_{l \notin L(\lambda, c)} g_l e^{iz\zeta_l}$ , one has  $f|_{]0, 2[} \in L^2$ , and so there exists a unique distribution  $f_+(z)$  with support in  $[0, \infty[$ , equal to  $f$  on  $]0, \infty[$ , such that  $f_+|_{]-2, 2[} \in L^2(]-2, 2[)$ . From 3.55 and  $|\zeta_l| \simeq 2|l|\pi$ , we get that the series

$$f_2(z) = \sum_{l \notin L(\lambda, c)} \frac{g_l}{\zeta_l^2} e^{iz\zeta_l} \quad (3.66)$$

is convergent for all  $z > -1/2$  and defines a continuous function  $f_2(z)$  on  $] -1/2, \infty[$ . One has  $f(z) = -\partial_z^2 f_2(z)$  in  $\mathcal{D}'(]-1/2, \infty[)$ . Set  $f_{+,2}(z) = 1_{z \geq 0} f^2(z)$ . Since  $f_{+,2}$  belongs to  $L^2$  near  $z = 0$ , there must exist  $a_0, a_1$  such that

$$f_+ = -\partial_z^2 f_{+,2} + a_0 \delta_0 + a_1 \delta'_0 \quad (3.67)$$

Since  $Im(\zeta_l) > 0$ ,  $f_2$  is bounded on  $[0, \infty[$ , thus  $f_{+,2}$  is a tempered distribution with support in  $[0, \infty[$ , and so is  $f_+$  by 3.67. Their Fourier-Laplace transforms  $\hat{f}_+(\zeta), \hat{f}_{+,2}(\zeta)$  are thus holomorphic in  $Im(\zeta) < 0$ , and we get from 3.67 for all  $\zeta \in \mathbb{C}, Im(\zeta) < 0$

$$\hat{f}_+(\zeta) = \zeta^2 \sum_{l \notin L(\lambda, c)} \frac{g_l}{i\zeta_l^2} \frac{1}{\zeta - \zeta_l} + a_0 + i\zeta a_1 \quad (3.68)$$

Observe that the  $\zeta_l$  are distinct for  $l \notin L(\lambda, c)$  and  $c \geq c_0$ . Thus by 3.68 and 3.55,  $\hat{f}_+(\zeta)$  extends as a meromorphic function on the complex plane  $\mathbb{C}$ , with poles at the  $\zeta_l$ , with residus  $g_l/i$ . Thus, if  $Q(z, D_z, \lambda)g|_{]0, \infty[} = 0$ , one has  $f_+ = 0$ , and thus  $g_l = 0$  for all  $l$ . Thus the map 3.61 is injective. The proof of lemma 3.4 is complete.  $\square$

Let  $c_0$  large and  $c \geq c_0$ . For  $f \in W_\lambda^c$ , one has by the preceding lemma  $f(z) = Q(z, D_z, \lambda)g|_{]0, \infty[} = \sum_{l \notin L(\lambda, c)} g_l e^{iz\zeta_l}$ , and the coefficients  $g_l$  are uniquely determined by 3.68. Since  $\cup_c L(\lambda, c) = \mathbb{Z}$ , we get that 3.39 holds true. One has also

$$e^{cz} f(z) = \sum_{l \notin L(\lambda, c)} g_l e^{iz(\zeta_l - ic)} \quad (3.69)$$

Observe that if  $\lambda, c$  are given, there exists  $\varepsilon > 0, \nu > 0$  such that for all  $\zeta_l \in Z_\lambda^c$

$$\operatorname{Im}(\zeta_l) \geq c + \varepsilon + \nu \log|l| \quad (3.70)$$

From 3.69 and 3.70, we get using 3.55 for  $M > 0$  such that  $M\nu - 1 - \alpha \geq 1$

$$\begin{aligned} |e^{cz} f(z)| &\leq e^{-\varepsilon z} \sum_{l \notin L(\lambda, c)} \frac{|g_l|}{|l|^{1+\alpha}} |l|^{1+\alpha-z\nu} \\ \int_M^\infty |e^{cz} f(z)|^2 dz &\leq C \|g\|_{H^{-1-\alpha}}^2 \int_M^\infty e^{-2\varepsilon z} dz \end{aligned} \quad (3.71)$$

Since  $Q(z, D_z, \lambda)$  is of order  $-z$  at  $z$  and  $g$  belongs to  $H^{-1-\alpha}$  for any  $\alpha > 0$ , one has  $f(z) = Q(z, D_z, \lambda)g|_{]0, \infty[} \in H^{z-1-\alpha} \subset L^2$  near any  $z > 1$ , therefore for any  $M > 0$   $f|_{]0, M[} \in L^2$ . Thus 3.71 shows that  $W_\lambda^c$  is a subspace of  $L_c^2$ . Since  $\mathcal{H}$  is a Hilbert space and since the map  $g = \sum_{l \notin L(\lambda, c)} g_l e^{2i\pi lz} \rightarrow f = Q(z, D_z, \lambda)g|_{]0, \infty[}$  is continuous from  $\mathcal{H}$  into  $\mathcal{D}'(]0, \infty[)$  and takes values in  $L_c^2$ , we get by the closed graph theorem

$$\|f(z)\|_{L_c^2} \leq C \|g\|_{\mathcal{H}} \quad (3.72)$$

Moreover, since  $Q(z, D_z, \lambda)$  is elliptic of order  $-z$  at  $z$ , one has also

$$\forall \alpha > 0, \exists C_\alpha \sum |g_l|^2 |l|^{-2-2\alpha} \leq C_\alpha \|Q(z, D_z, \lambda)g\|_{L^2(]0, 2])} \quad (3.73)$$

Thus, if  $f_n(z) = Q(z, D_z, \lambda)g_n|_{]0, \infty[}$  is a sequence in  $W_\lambda^c$  which converges to  $f$  in  $L_c^2$ , by 3.73, the sequence  $g_n \in \mathcal{H}$  converges to some  $g$  in  $H^{-1-\alpha}$ , and therefore  $f = Q(z, D_z, \lambda)g$  in  $\mathcal{D}'(]0, \infty[)$ . Since  $f|_{]0, 2[} \in L^2$ , by 3.51 one has  $f \in W_\lambda^c$ . Thus  $W_\lambda^c$  is a closed subspace of  $L_c^2$  for  $c \geq c_0$ . To get the general case, we just observe that for  $c' \geq c_0, c' \geq c$ , one has

$$\begin{aligned} W_\lambda^c &= W_\lambda^{c'} \oplus W_{\lambda, A} \\ W_{\lambda, A} &= \operatorname{span}(e^{iz\zeta}; \quad \zeta \in Z_\lambda, \quad c < \operatorname{Im}(\zeta) \leq c') \end{aligned} \quad (3.74)$$

and  $W_{\lambda, A} \subset L_c^2$  has finite dimension by lemma 3.1.

Let  $c \geq c_0$  be given. Then by lemma 3.1, there exists  $r > 0$  such that all the maps  $\lambda \rightarrow \zeta_l(\lambda)$  are analytic in the complex disc  $D_r = \{|\lambda - \lambda_0| \leq r\}$  with values in  $\operatorname{Im}(\zeta) > c$  for  $l \notin L(\lambda_0, c)$ , and  $L(\lambda, c) = L(\lambda_0, c)$  for all  $\lambda \in D_r$ . Let  $J_\lambda$  be the map from  $\mathcal{H}$  into  $L_c^2$

$$J_\lambda(g) = \sum_{l \notin L(\lambda_0, c)} g_l e^{iz\zeta_l(\lambda)} \quad (3.75)$$

By the above discussion,  $J_\lambda$  is bounded, injective, and its range  $W_\lambda^c$  is closed. Therefore,  $J_\lambda$  induces an isomorphism from  $\mathcal{H}$  onto  $W_\lambda^c$  for all  $\lambda \in D_r$ . Moreover, one has by the proof of 3.72  $\|J_\lambda\| \leq C_0$  with  $C_0$  independent of  $\lambda \in D_r$ . It is now easy to get the analyticity of  $\lambda \rightarrow W_\lambda^c$ . Since  $J_\lambda(g)$  is given by a convergent series in  $\mathcal{D}'(]0, \infty[)$ , and all the  $\zeta_l(\lambda)$  are analytic in  $\lambda \in D_r$ , one has  $\bar{\partial}_\lambda J_\lambda(g) = 0$  for all  $g \in \mathcal{H}$ . Thus by the Cauchy formula, one has the equality in  $\mathcal{D}'(]0, \infty[)$

$$J_\lambda(g) = \frac{1}{2i\pi} \int_{|\mu - \lambda_0| = r} \frac{J_\mu(g)}{\mu - \lambda} d\mu \quad \forall \lambda, |\lambda - \lambda_0| < r \quad (3.76)$$

and since both sides of 3.76 belongs to  $L_c^2$ , this equality holds true in  $L_c^2$ . This shows that  $\lambda \rightarrow J_\lambda$  is analytic from  $|\lambda - \lambda_0| < r$  into the Banach space of bounded linear operator from  $\mathcal{H}$  into  $L_c^2$ . Then the map from  $W_{\lambda_0}^c$  into  $L_c^2$ ,  $J_\lambda J_{\lambda_0}^{-1}$  is analytic in  $\lambda$ , and an isomorphism of  $W_{\lambda_0}^c$  onto  $W_\lambda^c$ . Let  $\pi_0$  be the orthogonal projector onto  $W_{\lambda_0}^c$  in  $L_c^2$ . Then the bounded linear operator on  $W_{\lambda_0}^c$ ,  $B_\lambda = \pi_0 J_\lambda J_{\lambda_0}^{-1}$ , depends analytically on  $\lambda$ , is equal to  $Id$  at  $\lambda_0$ , thus is invertible for  $|\lambda - \lambda_0| \leq r_1 < r$  with  $r_1$  small enough. Hence, for  $|\lambda - \lambda_0| \leq r_1$ , one has

$$W_{\lambda_0}^c = \{u = v + A_\lambda(v), v \in \mathcal{H}\}, \quad A_\lambda = (1 - \pi_0)J_\lambda J_{\lambda_0}^{-1} B_\lambda^{-1} \quad (3.77)$$

Thus  $\lambda \rightarrow W_\lambda^c$  is analytic for  $c \geq c_0$ , and one gets easily that it is analytic for all  $c$  using 3.74.

Finally, let us prove that 3.40 holds true. Let  $\lambda \in \mathbb{C} \setminus [-\nu_0, 1]$ , and  $g \in L^2(\mathbb{R})$  with support in  $[-1, 1]$ . Let  $f \in L^2(\mathbb{R})$  be the unique solution of the convolution equation  $\varphi * f - \lambda f = g$ . Then one has  $(\hat{\varphi}(\zeta) - \lambda)\hat{f}(\zeta) = \hat{g}(\zeta)$ . Therefore by the Fourier inversion formula in  $L^2(\mathbb{R})$ , one gets.

$$f(z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{iz\zeta} \frac{\hat{g}(\zeta)}{\hat{\varphi}(\zeta) - \lambda} d\zeta \quad (3.78)$$

Take  $0 < \rho_0 < |\lambda| < \rho_1$ . For  $c > 0$  large, let  $\gamma_c$  be a contour in the complex plane which is the union of 4 pieces,  $\gamma_{c,3}, \gamma_{c,+}, \gamma_{c,-}, \gamma_{c,1}$ , as follows. First,  $\gamma_{c,3} = \{\zeta = a + ic, |a| \geq Me^c\}$ , where  $M$  is given by 3.7, so  $\gamma_{c,3}$  is the union of two half lines. Second  $\gamma_{c,1} = \{\zeta = a + ib, |a| \leq \frac{1}{M}e^b - 1\}$ , where  $b > c$  is at our disposal. Finally,  $\gamma_{c,+}$  and  $\gamma_{c,-}$  connects  $\gamma_{c,3}$  to  $\gamma_{c,1}$  respectively in  $\pm Re(\zeta) > 0$ , and does not intersect  $Z_\lambda^c$ , and such that  $Z_\lambda^c$  is the set of  $\zeta \in Z_\lambda$  above the contour  $\gamma_c$ .

Set  $\langle \zeta \rangle = \sqrt{1 + |\zeta|^2}$ . Since  $g$  has support in  $[-1, 1]$ , one has  $|\hat{g}(\zeta)| \leq Ce^{Im(\zeta)}$ .

**Lemma 3.5** *There exists  $c_0, C$ , and for all  $c \geq c_0$  a contour  $\gamma_c$  like above such that*

$$\forall \zeta \in \gamma_c \quad \left| \frac{\hat{g}(\zeta)}{\hat{\varphi}(\zeta) - \lambda} \right| \leq C \langle \zeta \rangle \quad (3.79)$$

*Proof.* This lemma is an easy consequence of lemma 3.1, formula 3.10. □

From 3.78, we get for any  $z > 0$  and all  $c \geq c_0$  the equality in  $\mathcal{D}'(]0, \infty[)$

$$\begin{aligned} f(z) &= f_{(0,c)}(z) + f_c(z) \\ f_{(0,c)}(z) &= \frac{1}{2i\pi} \int_{\gamma_{0,c}} e^{iz\zeta} \frac{\hat{g}(\zeta)}{\hat{\varphi}(\zeta) - \lambda} d\zeta \\ f_c(z) &= \frac{1}{2i\pi} \int_{\gamma_c} e^{iz\zeta} \frac{\hat{g}(\zeta)}{\hat{\varphi}(\zeta) - \lambda} d\zeta \end{aligned} \quad (3.80)$$

where  $\gamma_{0,c}$  is a closed contour around the finite set  $\zeta \in Z_\lambda^0, Im(\zeta) \leq c$ . By the residue theorem,  $f_{(0,c)} \in W_\lambda^0$ . By lemma 3.5, one has  $\lim_{c \rightarrow \infty} f_c = 0$  in  $\mathcal{D}'(]0, \infty[)$ , and this implies the equality in  $\mathcal{D}'(]0, \infty[)$

$$f_c(z) = \sum_{\zeta \in Z_\lambda^c} g_l e^{iz\zeta} \quad , \quad g_l = \frac{\hat{g}(\zeta_l)}{\hat{\varphi}'(\zeta_l)} \quad (3.81)$$

Since  $f_{(0,c)} \in L_0^2 = L^2(]0, \infty[)$ , one has  $f_c|_{]0,2[} \in L^2$ , and since by 3.4 and 3.11, for  $\zeta_l = a + ib$ ,  $a > 0, b > 0$  large, one has  $\hat{\varphi}'(\zeta_l) \simeq \tilde{\varphi}(1)e^{-i\zeta_l}/\zeta_l$ , one gets  $|g_l| \leq C < \zeta_l$ , so  $g_l$  is temperate. Thus  $f_c \in W_\lambda^0$ .

The proof of proposition 3.3 is complete.  $\square$

**Remark 3.6** By 3.68 one has  $W_\lambda^c \cap W_{\lambda'}^c = \{0\}$  for  $\lambda \neq \lambda'$ , since the poles of  $\hat{f}_+$  are the  $\zeta_l$  and  $\hat{\varphi}(\zeta_l) = \lambda$ .

By the above proposition,  $W_\lambda^c$ , equipped with the norm of  $L_c^2$ , is a Hilbert space.

**Lemma 3.7** For any  $\lambda \in \mathbb{C} \setminus 0$  and any  $c' \geq c$ ,  $W_\lambda^{c'}$  is a closed subspace of  $W_\lambda^c$ . More precisely, there exists a constant  $M_{\lambda,c,c'}$  such that

$$\|f\|_{L_c^2} \leq \|f\|_{L_{c'}^2} \leq M_{\lambda,c,c'} \|f\|_{L_c^2}, \quad \forall f \in W_\lambda^{c'} \quad (3.82)$$

Further for any given  $c, \lambda_0 \in \mathbb{C} \setminus 0$ , there exists  $r > 0, B, B'$  and for all  $c' \geq c$  a constant  $N_{c,c'}$  such that

$$M_{\lambda,c,c'} \leq N_{c,c'} + B' \inf_{\zeta_l \in Z_\lambda^{c'}} (Im(\zeta_l) - c')^{-B}, \quad \forall \lambda, |\lambda - \lambda_0| \leq r \quad (3.83)$$

*Proof.* The inequality  $\|f\|_{L_c^2} \leq \|f\|_{L_{c'}^2}$  is obviously true for any  $f \in L_{c'}^2$ . Let us prove that 3.82 holds true with a constant  $M_{\lambda,c,c'}$  bounded by the right hand side of 3.83. Let  $c, \lambda_0 \in \mathbb{C} \setminus 0$  be given, and take  $r > 0$  small enough such that  $Im(\zeta_l) - c \geq c_0 > 0$  for all  $|\lambda - \lambda_0| \leq r$  and all  $\zeta_l \in Z_\lambda^c$ . Let  $D(\lambda_0, r) = \{\lambda \in \mathbb{C}, |\lambda - \lambda_0| \leq r\}$ .

Take  $C > 0$  large and  $c' > c$ . For  $f \in W_\lambda^{c'}$ , set  $f = f_1 + f_2$ , with, like in 3.74,

$$\begin{aligned} f &= f_1 + f_2, \quad f_1 \in W_\lambda^{c'+C}, \quad f_2 \in W_{\lambda,A} \\ W_{\lambda,A} &= \text{span}(e^{iz\zeta}; \quad \zeta \in Z_\lambda, \quad c' < Im(\zeta) \leq c' + C) \end{aligned} \quad (3.84)$$

Let us first prove that

$$\|f_1\|_{L_{c'}^2} \leq N_{c,c'} \|f\|_{L_c^2}, \quad \forall \lambda \in D(\lambda_0, r), \forall f \in W_\lambda^{c'} \quad (3.85)$$

For all  $M > 0$ , one has

$$\int_0^M |e^{c'z} f(z)|^2 dz \leq e^{2M(c'-c)} \int_0^M |e^{cz} f(z)|^2 dz \quad (3.86)$$

Take  $\alpha$  such that for all  $f = \sum_{\zeta_l \in Z_\lambda^c} g_l e^{iz\zeta_l}$  and all  $\lambda \in D(\lambda_0, r)$ , one has with  $g = \sum g_l e^{2i\pi lz}$ ,

$$\|g\|_{H^{-1-\alpha}} \leq C' \|f\|_{L^2(]0,2[)} \leq C \|f\|_{L_c^2} \quad (3.87)$$

Set

$$x_l = g_l e^{iM\zeta_l} \quad (3.88)$$

Then by 3.9, one has for  $M$  large,

$$\begin{aligned} |x_l| &\leq \frac{|g_l|}{|l|^{1+\alpha}} |l|^{1+\alpha} e^{-MIm(\zeta_l)} \\ \sum |x_l| &\leq C'' \|g\|_{H^{-1-\alpha}} \leq C \|f\|_{L_c^2} \end{aligned} \quad (3.89)$$

For  $C$  large, all the roots  $\zeta_l \in Z_\lambda^c$  with  $Im(\zeta) \geq c' + C$  are simple, and thus, for  $f_1 = \sum_{\zeta_l \in Z_\lambda^{c'+C}} g_l e^{iz\zeta_l}$

$$\int_M^\infty |e^{c'z} f_1(z)|^2 dz = \sum_{\zeta_l, \zeta_m \in Z_\lambda^{c'+C}} g_l \bar{g}_m \int_M^\infty e^{-z(i(\bar{\zeta}_m - \zeta_l) - 2c')} dz \quad (3.90)$$

Then, from 3.90, we get

$$\begin{aligned} \int_M^\infty |e^{c'z} f_1(z)|^2 dz &= \sum_{\zeta_l, \zeta_m \in Z_\lambda^{c'+C}} g_l \bar{g}_m e^{-M(i(\bar{\zeta}_m - \zeta_l) - 2c')} \frac{1}{i(\bar{\zeta}_m - \zeta_l) - 2c'} \\ &= \sum_{\zeta_l, \zeta_m \in Z_\lambda^{c'+C}} x_l \bar{x}_m e^{2c'M} \frac{1}{i(\bar{\zeta}_m - \zeta_l) - 2c'} \\ &\leq e^{2c'M} \sum_{\zeta_l, \zeta_m \in Z_\lambda^{c'+C}} |x_l| |x_m| \frac{1}{2C} \end{aligned} \quad (3.91)$$

Thus, from 3.86, 3.89 and 3.91, we get that 3.85 holds true.

Observe that the space  $W_{\lambda,A}$  takes care of the fact that a root  $\zeta_l \in Z_\lambda^c$  may cross the line  $Im(\zeta_l) - c'$  for some value of  $\lambda \in D(\lambda_0, r)$ . It is a finite dimensional vector space, uniformly in  $\lambda \in D(\lambda_0, r)$  and  $c' > c$ , and one gets easily, for some  $B, B'$ , using the above estimates,

$$\|f_2\|_{L_c^2} \leq B' \inf_{\zeta_l \in Z_\lambda^{c'}} (Im(\zeta_l) - c')^{-B} \|f\|_{L_c^2}, \quad \forall \lambda \in D(\lambda_0, r), \forall f \in W_\lambda^{c'} \quad (3.92)$$

From 3.85 and 3.92, we get that 3.82 and 3.83 holds true. The proof of lemma 3.7 is complete.  $\square$

Let  $1_+$  be the characteristic function of the half line  $[0, \infty[$ . For  $f \in L_{loc}^1([0, \infty[)$ , we denote by  $1_+ f$  the function on  $\mathbb{R}$  equal to  $f$  in  $z \geq 0$  and equal to 0 in  $z < 0$ .

**Lemma 3.8** For  $\lambda \in \mathbb{C} \setminus 0$  and  $c \in \mathbb{R}$ , the map

$$\begin{aligned} W_\lambda^c &\longrightarrow L_c^2 \\ f &\longrightarrow (\varphi * 1_+ f)|_{]0, \infty[} \end{aligned} \quad (3.93)$$

is compact.

*Proof.* Let  $T$  be the operator given by 3.93, and for  $f \in W_\lambda^c$ ,  $T_M(f) = (\varphi * 1_+ f)|_{]0, M[} \in L_c^2$ . Then by 3.71 and 3.73, one has  $\lim_{M \rightarrow \infty} \|T - T_M\| = 0$ . For any  $M$ , the operator on  $L_c^2$ ,  $f \rightarrow (\varphi * 1_+ f)|_{]0, M[}$  is obviously compact. Hence,  $T$  is compact.  $\square$

## 4 The Kernel $K$ on the half line $[0, \infty[$

Let  $\varphi$  be as in section 3 and let  $m$  be the function defined for  $z \geq 0$  by

$$m(z) = \int_0^\infty \varphi(z+t)dt \quad (4.1)$$

Then  $m$  is a continuous non increasing function with support in  $[0, 1]$  such that  $m(0) = 1/2$ . For any  $f \in L^1_{\text{loc}}([0, \infty[)$ , set for  $z \geq 0$

$$K(f)(z) = m(z)f(z) + (\varphi * 1_+ f)(z) = m(z)f(z) + \int_0^\infty \varphi(z-t)f(t)dt \quad (4.2)$$

Then  $K$  maps  $L^1_{\text{loc}}([0, \infty[)$  into itself.

Since  $(\varphi * 1_+ e^{iz\zeta})(z) = (\varphi * e^{iz\zeta})(z) - \int_0^\infty \varphi(z+t)e^{-it\zeta}dt$ , for any  $\zeta \in \mathbb{C}$ , one has the formula

$$K(1_+ e^{iz\zeta})(z) = \hat{\varphi}(\zeta)e^{iz\zeta} + \int_0^\infty \varphi(z+t)(e^{iz\zeta} - e^{-it\zeta})dt \quad (4.3)$$

Set

$$F(z, \zeta) = \int_0^\infty \varphi(z+t)(e^{iz\zeta} - e^{-it\zeta})dt \quad (4.4)$$

Then  $F(z, \zeta)$  is holomorphic in  $\zeta \in \mathbb{C}$  with values in continuous functions of  $z \geq 0$  with support in  $[0, 1]$ , and one has

$$K(1_+ e^{iz\zeta})(z) = \hat{\varphi}(\zeta)e^{iz\zeta} + F(z, \zeta) \quad (4.5)$$

One has  $K(1) = 1$ ,  $K(f) \geq 0$  for  $f \geq 0$ , and since  $\varphi(z) = \varphi(-z)$ , for any non negative functions  $f, g \in L^1([0, \infty[)$

$$\int_0^\infty K(f)gdz = \int_0^\infty fK(g)dz \quad (4.6)$$

Therefore, one gets

$$\begin{aligned} \|K(f)\|_{L^\infty} &\leq \|f\|_{L^\infty} \quad \forall f \in L^\infty([0, \infty[) \\ \|K(f)\|_{L^1} &\leq \|f\|_{L^1} \quad \forall f \in L^1([0, \infty[) \end{aligned} \quad (4.7)$$

Thus  $K$  is self-adjoint on  $L^2([0, \infty[)$ , with norm  $\|K\|_{L^2} \leq 1$ .

Observe that by formula 4.5, for any  $\lambda \in \mathbb{C} \setminus 0$  and any  $c \in \mathbb{R}$ ,  $K - \lambda$  maps the closed subspace  $W_\lambda^c$  of  $L_c^2$  (defined in 3.37) continuously into  $L^2([0, 1]) = \{f \in L^2([0, \infty[), \text{support}(f) \subset [0, 1]\}$ . This is obvious by 3.74 since for  $c' > 0$ ,  $c' \geq c$ , one has  $L_{c'}^2 \subset L^2([0, \infty[)$  and the vector space  $W_{\lambda, A}$  in 3.74 has finite dimension by lemma 3.1.

We shall denote by  $S_\lambda^c$  the continuous map

$$\begin{aligned} W_\lambda^c &\longrightarrow L^2([0, 1]) \\ f &\longrightarrow S_\lambda^c(f) = (K - \lambda)f \end{aligned} \quad (4.8)$$

**Theorem 4.1** *For any  $\lambda \in \mathbb{C} \setminus [0, 1/2]$  and any  $c \in \mathbb{R}$ ,  $S_\lambda^c$  is Fredholm, i.e its kernel is finite dimensional and its range is closed, and has finite codimension.*

*Proof.* We start by proving a coercivity estimate.

**Lemma 4.2** *Let  $\lambda_0 \in \mathbb{C} \setminus [0, 1/2]$ . There exists  $r_0 > 0, c_0 \geq 1$  such that for all  $\lambda \in \mathbb{C}, |\lambda - \lambda_0| \leq r_0$  and all  $c \geq c_0$ , there exists  $C$  such that the following inequality holds true*

$$\|f\|_{L^2_\varepsilon} \leq CM_{\lambda, c_0, c} \|(K - \lambda)f\|_{L^2([0,1])}, \quad \forall f \in W_\lambda^c \quad (4.9)$$

*Proof.* We first prove that there exists  $c_0 \geq 1, C_0 > 0$  such that

$$\|f\|_{L^2_1} \leq C_0 \|(K - \lambda_0)f\|_{L^2([0,1])}, \quad \forall f \in W_{\lambda_0}^{c_0} \quad (4.10)$$

In fact, if 4.10 is untrue, there exists a sequence  $c_n \geq 1, c_n \rightarrow +\infty$ , and a sequence  $f_n \in W_{\lambda_0}^{c_n}, \|f_n\|_{L^2_1} = 1$ , such that

$$\lim_{n \rightarrow \infty} \|(K - \lambda_0)f_n\|_{L^2([0,1])} = 0 \quad (4.11)$$

Then, there exists a subsequence of  $f_n$ , that we still denote by  $f_n$ , which converges weakly to  $f$  in  $W_{\lambda_0}^1$ , and since  $W_{\lambda_0}^{c_n}$  is closed in  $W_{\lambda_0}^1$  by lemma 3.7, one has by 3.39  $f \in \bigcap_n W_{\lambda_0}^{c_n} = \{0\}$ , thus  $f = 0$ . One has  $(K - \lambda_0)f_n = (m - \lambda_0)f_n + (\varphi * 1_+ f_n)|_{]0, \infty[}$ . Using lemma 3.8 with  $c = 1$ , we get  $\|(\varphi * 1_+ f_n)|_{]0, \infty[}\|_{L^2_1} \rightarrow 0$  and since the function  $(K - \lambda_0)f_n$  has support in  $[0, 1]$ , we conclude using 4.11 that  $\|(m - \lambda_0)f_n\|_{L^2_1} \rightarrow 0$ , which is impossible since  $\lambda_0 \in \mathbb{C} \setminus [0, 1/2]$  and  $\|f_n\|_{L^2_1} = 1$ . Using 3.82, we get from 4.10

$$\|f\|_{L^2_{c_0}} \leq C_0 M_{\lambda_0, 1, c_0} \|(K - \lambda_0)f\|_{L^2([0,1])}, \quad \forall f \in W_{\lambda_0}^{c_0} \quad (4.12)$$

By proposition 3.3, there exists  $r > 0$  such that  $\lambda \rightarrow W_\lambda^{c_0} \subset L_{c_0}^2$  is analytic for  $|\lambda - \lambda_0| < r$ . Thus there exists a holomorphic map  $A_\lambda$  from the disc  $|\lambda - \lambda_0| < r$  into the space of bounded linear operators from  $W_{\lambda_0}^{c_0}$  into its orthogonal complement  $W_{\lambda_0}^{c_0, \perp}$  in  $L_{c_0}^2$  such that  $g \rightarrow g + A_\lambda g$  is an isomorphism from  $W_{\lambda_0}^{c_0}$  onto  $W_\lambda^{c_0}$ . In particular, for  $r_1 < r$  there exists  $C > 0$  such that for all  $f = g + A_\lambda g$ , one has for all  $|\lambda - \lambda_0| \leq r_1$ , since  $A_{\lambda_0} = 0$

$$\|g\|_{L^2_{c_0}} \leq \|f\|_{L^2_{c_0}} \leq (1 + C|\lambda - \lambda_0|)\|g\|_{L^2_{c_0}} \quad (4.13)$$

One has also, since  $K - \lambda$  is bounded on  $L_{c_0}^2$ , for all  $|\lambda - \lambda_0| \leq r_1$

$$\begin{aligned} (K - \lambda_0)g &= (K - \lambda)f + (\lambda - \lambda_0)g - (K - \lambda)A_\lambda g \\ \|(K - \lambda_0)g\|_{L^2([0,1])} &\leq \|(K - \lambda)f\|_{L^2([0,1])} + C|\lambda - \lambda_0|\|g\|_{L^2_{c_0}} \end{aligned} \quad (4.14)$$

By 4.12, 4.13, and 4.14, we get for all  $|\lambda - \lambda_0| \leq r_1$  and all  $f \in W_\lambda^{c_0}$ , with  $C_1 = C_0 M_{\lambda_0, 1, c_0}$

$$\begin{aligned} \|f\|_{L^2_{c_0}} &\leq (1 + C|\lambda - \lambda_0|)\|g\|_{L^2_{c_0}} \\ &\leq (1 + C|\lambda - \lambda_0|)C_1 \|(K - \lambda_0)g\|_{L^2([0,1])} \\ &\leq (1 + C|\lambda - \lambda_0|)C_1 (\|(K - \lambda)f\|_{L^2([0,1])} + C|\lambda - \lambda_0|\|f\|_{L^2_{c_0}}) \end{aligned} \quad (4.15)$$

Thus for  $r_0 > 0$  small enough, we get that there exists  $C$  such that for all  $|\lambda - \lambda_0| \leq r_0$  and all  $f \in W_\lambda^{c_0}$

$$\|f\|_{L^2_{c_0}} \leq C \|(K - \lambda)f\|_{L^2([0,1])} \quad (4.16)$$

Thus using lemma 3.7, 3.83, we get for  $c \geq c_0, |\lambda - \lambda_0| \leq r_0$  and all  $f \in W_\lambda^c$

$$\|f\|_{L^2_\varepsilon} \leq M_{\lambda, c_0, c} \|f\|_{L^2_{c_0}} \leq CM_{\lambda, c_0, c} \|(K - \lambda)f\|_{L^2([0,1])} \quad (4.17)$$

and thus 4.9 holds true . The proof of lemma 4.2 is complete.  $\square$

The proof of theorem 4.1 now follows easily . Let  $\lambda_0 \in \mathbb{C} \setminus [0, 1/2]$ . Take a continuous path  $s \in [0, 1] \rightarrow \gamma(s)$  in  $\mathbb{C} \setminus [0, 1/2]$  with  $\gamma(0) = \lambda_0, \gamma(1) = 2$ . Since  $\gamma([0, 1])$  is compact, it is covered by a finite union of discs  $D(\lambda_j, r_j)$ ,  $1 \leq j \leq N$ , such that lemma 4.2 holds true with  $c_0 = c_j$  and  $\lambda \rightarrow W_\lambda^{c_j}$  is analytic with values in  $L_{c_j}^2$  for  $|\lambda - \lambda_j| \leq 2r_j$ . Moreover, we can choose the  $r_j$  and the  $c_j$  such that  $Im(\zeta_l) \neq c_j$  for all  $|\lambda - \lambda_j| \leq 2r_j$ .

Then by 4.9,  $S_\lambda^c$  is injective and its range  $S_\lambda^c(W_\lambda^c)$  is closed in  $L^2([0, 1])$  for all  $|\lambda - \lambda_j| \leq r_j$  and all  $c \geq c_j$ .

Let  $d(\lambda, c) \in [0, \infty]$  be the codimension of  $V(\lambda, c) = S_\lambda^c(W_\lambda^c)$  in  $L^2([0, 1])$ . Let  $B(\lambda, c)$  be the inverse map of  $S_\lambda^c$ . Then  $B(\lambda, c)$  is a bounded and one to one operator from  $V(\lambda, c)$  onto  $W_\lambda^c$ , and by 4.14 one has for all  $\lambda, \underline{\lambda}$  such that  $|\lambda - \lambda_j| \leq r_j, |\underline{\lambda} - \lambda_j| \leq r_j$

$$\begin{aligned} V(\lambda, c_j) &= \{u \in L^2([0, 1]), \exists v \in V(\underline{\lambda}, c_j), u = v + R_\lambda v\} \\ R_\lambda &= (K - \lambda)A_\lambda B(\underline{\lambda}, c_j) - (\lambda - \underline{\lambda})B(\underline{\lambda}, c_j) \end{aligned} \quad (4.18)$$

Since  $\lambda \rightarrow R_\lambda$  is analytic with values in bounded operators from  $V(\underline{\lambda}, c_j)$  into  $L^2([0, 1])$  and  $R_{\underline{\lambda}} = 0$ , we get from 4.18 that there exists  $r_{1, \underline{\lambda}}$  such that

$$d(\lambda, c_j) = d(\underline{\lambda}, c_j) \quad \forall \lambda, |\lambda - \underline{\lambda}| \leq r_{1, \underline{\lambda}} \quad (4.19)$$

Thus,

$$d(\lambda, c_j) = d(\lambda', c_j) \quad \forall \lambda, \lambda' \in D(\lambda_j, c_j) \quad (4.20)$$

Take  $c \in \mathbb{R}$ . By 3.74,  $S_\lambda^c$  is Fredholm iff  $S_{\lambda_j}^{c_j}$  is Fredholm. Thus, since  $S_{\lambda_j}^{c_j}$  is injective, it remains to prove

$$d(\lambda_j, c_j) < \infty \quad (4.21)$$

By 4.20, and since  $d(\lambda, c_j) - d(\lambda, c)$  is finite, it remains to prove

$$d(2, c_0) < \infty \quad (4.22)$$

or equivalently, since we know by lemma 4.2 that  $S_2^{c_0}$  is injective, that  $S_2^{c_0}$  is Fredholm, which is equivalent by 3.74 to show that for some  $c$ ,  $S_2^c$  is Fredholm. We shall take  $c = 0$ . Since  $\|K\| \leq 1$ ,  $K - 2$  is one to one from  $L^2([0, \infty])$  into itself. Let  $g \in L^2([0, \infty])$  with support in  $[0, 1]$  and  $f \in L^2([0, \infty])$  such that  $(K - 2)f = g$ . Then one has by 4.2

$$\begin{aligned} (\varphi * 1_+ f - 21_+ f)(z) &= h(z) \quad \forall z \in \mathbb{R} \\ h(z) &= 1_+ g(z) - m(z)1_+ f(z) + (1 - 1_+)(\varphi * 1_+ f)(z) \end{aligned} \quad (4.23)$$

The function  $h \in L^2(\mathbb{R})$  has support in  $[-1, 1]$ . Thus by proposition 3.3, 3.40, one gets  $f \in W_2^0$ . This shows that  $S_2^0$  is bijective, thus is Fredholm. The proof of theorem 4.1 is complete.  $\square$

Let  $c_1 > 0$  be such that one has  $Im(\zeta) \geq 2c_1$  for any  $\zeta \in Z_1^0$ . Let  $U_\delta = \{\lambda, |\lambda - 1| < \delta\}$ . One has  $\hat{\varphi}(\zeta) = 1 - \alpha\zeta^2/2 + \dots$ ,  $\alpha = \int_{-1}^1 z^2 \varphi(z) dz > 0$ . Therefore, for  $\delta > 0$  small,

and  $\lambda \in U_\delta$  the equation  $\hat{\varphi}(\zeta) = \lambda$  has exactly two solutions  $\zeta = \pm\eta(\lambda)$  such that  $|Im(\eta(\lambda))| \leq c_1$ ,  $\lambda \rightarrow \eta(\lambda)^2$  is holomorphic in  $U_\delta$  and  $\eta(1) = 0$ . Moreover, one has

$$\begin{aligned} W_\lambda^{-c_1} &= W_\lambda^{c_1} \oplus V_\lambda^0 \\ V_\lambda^0 &= \text{span}(\cos(\eta(\lambda)z), \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)}) \end{aligned} \quad (4.24)$$

**Theorem 4.3** *There exists  $\delta > 0$  such that for any  $\lambda \in U_\delta$ , the map  $S_\lambda^{-c_1}$  is surjective onto  $L^2([0, 1])$ , and its kernel  $Ker(S_\lambda^{-c_1}) \subset W_\lambda^{c_1} \oplus V_\lambda^0$  is one dimensional, and spanned by the function*

$$e_\lambda(z) = \cos(\eta(\lambda)z) + b(\lambda) \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} + g_\lambda(z) \quad (4.25)$$

where  $b(\lambda)$  is holomorphic in  $U_\delta$ ,  $b(\lambda) \in \mathbb{R}$  for  $\lambda \in \mathbb{R}$ ,  $b(1) = 0$ , and  $g_\lambda$  is holomorphic in  $U_\delta$  with values in  $W_\lambda^{c_1}$  and  $g_1 = 0$ . Moreover, there exists  $C > 0$  such that

$$|g_\lambda(z)| \leq C|\lambda - 1|e^{-c_1 z} \quad \forall z \geq 0, \forall \lambda \in U_\delta \quad (4.26)$$

*Proof.* By the end of proof of theorem 4.1, we know that  $S_\lambda^0$  is bijective for any  $\lambda > 1$ . For  $\lambda \in U_\delta$  with  $\delta > 0$  small, and  $\lambda > 1$ , the two roots  $\pm\eta(\lambda)$  are purely imaginary and non zero ; thus  $W_\lambda^0$  has codimension 1 in  $W_\lambda^{-c_1}$ , and therefore,  $S_\lambda^{-c_1}$  is Fredholm of index 1. For  $\lambda \in U_\delta$ , let  $A_\lambda$  be the holomorphic map from  $W_1^{-c_1}$  into its orthogonal complement in  $L_{-c_1}^2$  such that any  $f \in W_\lambda^{-c_1}$  is of the form  $f = g + A_\lambda g$  with  $g \in W_1^{-c_1}$ . Then  $1 + A_\lambda$  is an isomorphism from  $W_1^{-c_1}$  onto  $W_\lambda^{-c_1}$  and one has

$$S_\lambda^{-c_1}(1 + A_\lambda)g = (K - 1)g + (1 - \lambda)g + (K - \lambda)A_\lambda g \quad (4.27)$$

Thus  $S_\lambda^{-c_1}(1 + A_\lambda)$  is an analytic family of Fredholm operators from  $W_1^{-c_1}$  into  $L^2([0, 1])$ , therefore its index is independent of  $\lambda \in U_\delta$ , and since  $1 + A_\lambda$  is an isomorphism, this index is equal to 1. Thus, for  $\delta > 0$  small, one gets

$$\dim Ker(S_\lambda^{-c_1}) - \text{codim} Im(S_\lambda^{-c_1}) = 1 \quad \forall \lambda \in U_\delta \quad (4.28)$$

One has , since  $z = -i\partial_\zeta e^{iz\zeta}|_{\zeta=0}$  and using 4.3

$$\begin{aligned} W_1^{-c_1} &= W_1^{c_1} \oplus \text{span}(1, z) \\ K(1) &= 1 \\ K(z) &= z + \int_0^1 \varphi(z+t)(z+t)dt \end{aligned} \quad (4.29)$$

Since  $W_\lambda^{c_1}$  has codimension 2 in  $W_\lambda^{-c_1}$ , by 4.28,  $S_\lambda^{c_1}$  is Fredholm of index  $-1$  for  $\lambda \in U_\delta$ . Observe that  $S_1^{c_1}$  is injective ; in fact, if  $g \in W_1^{c_1} \subset L^1([0, \infty[)$  is such that  $(K - 1)g = 0$ , one has  $\|Kg\|_{L^1} = \|g\|_{L^1}$ , thus by 4.7,  $K(|g|) = |g|$ , and thus we may assume  $g \geq 0$ . From

$$g = Kg = mg + (\varphi * 1_+g)|_{z>0} \quad (4.30)$$

and  $0 \leq m \leq 1/2$ , we get that  $g$  is continuous. Since  $g \in W_1^{c_1}$ , one has  $\lim_{z \rightarrow \infty} g(z) = 0$  (see 3.57). Thus  $g$  reaches its maximum on  $[0, \infty[$ , and we get easily  $g = 0$  from 4.30 .

Thus for  $\delta$  small and  $\lambda \in U_\delta$ ,  $S_\lambda^{c_1}$  is injective, and since its index is  $-1$ , we get for all  $\lambda \in U_\delta$

$$\begin{aligned} \text{Ker}(S_\lambda^{c_1}) &= \{0\} \\ \text{codimIm}(S_\lambda^{c_1}) &= 1 \end{aligned} \quad (4.31)$$

For  $f = g + a + bz \in W_1^{-c_1}$ ,  $g \in W_1^{c_1}$ , one has

$$(K - 1)f = (K - 1)g + b \int_0^1 \varphi(z + t)(z + t)dt \quad (4.32)$$

Let us show that the function  $(K - 1)(z) = \int_0^1 \varphi(z + t)(z + t)dt \in L^2([0, 1])$  is not in the range of  $S_1^{c_1}$ . In fact, since  $K(1) = 1$  and  $K$  is self adjoint on  $L^2$ , one has for any  $g \in W_1^{c_1} \subset L^1[0, \infty[$ , since  $(K - 1)g$  has support in  $[0, 1]$

$$\int_0^1 (K - 1)(g)(z)dz = \lim_{M \rightarrow \infty} \int_0^\infty g(z)(K - 1)(1_{[0, M]})(z)dz = \int_0^\infty g(z)(K - 1)(1)(z)dz = 0 \quad (4.33)$$

Since  $\varphi$  is non negative, one has obviously  $\int_0^1 \int_0^1 \varphi(z + t)(z + t)dt dz > 0$ . Therefore,  $\text{Ker}(S_1^{-c_1})$  has dimension 1 and is spanned by the constant function 1. Thus for  $\delta$  small and  $\lambda \in U_\delta$ ,  $\dim \text{Ker}(S_\lambda^{-c_1}) \leq 1$ , and from 4.28, this implies  $\dim \text{Ker}(S_\lambda^{-c_1}) = 1$ , and  $\text{codimIm}(S_\lambda^{-c_1}) = 0$ . For  $\lambda \in U_\delta$ , there exists a holomorphic family  $h_\lambda(z) \in L^2([0, 1])$  such that

$$u \in \text{Im}(S_\lambda^{c_1}) \quad \text{iff} \quad \int_0^1 u(z)h_\lambda(z)dz = 0 \quad (4.34)$$

Therefore, for  $f = g + a \cos(\eta(\lambda)z) + b \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} \in W_\lambda^{-c_1}$ ,  $g \in W_\lambda^{c_1}$ , the equation  $(K - \lambda)f = 0$  is equivalent to

$$a\theta^0(\lambda) + b\theta^1(\lambda) = 0 \quad \text{and} \quad g = -(S_\lambda^{c_1})^{-1}(K - \lambda) \left( a \cos(\eta(\lambda)z) + b \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} \right) \quad (4.35)$$

where the two holomorphic functions  $\theta^0, \theta^1$  are given by

$$\begin{aligned} \theta^0(\lambda) &= \int_0^1 (K - \lambda) \left( \cos(\eta(\lambda)z) \right) h_\lambda(z) dz \\ \theta^1(\lambda) &= \int_0^1 (K - \lambda) \left( \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} \right) h_\lambda(z) dz \end{aligned} \quad (4.36)$$

One has  $\theta^0(1) = 0$  and  $\theta^1(1) = \int_0^1 (K - 1)(z)h_\lambda(z)dz \neq 0$ . Therefore with

$$\begin{aligned} b(\lambda) &= -\frac{\theta^0(\lambda)}{\theta^1(\lambda)} \\ g_\lambda &= -(S_\lambda^{c_1})^{-1}(K - \lambda) \left( \cos(\eta(\lambda)z) + b(\lambda) \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} \right) \end{aligned} \quad (4.37)$$

we get that the function  $e_\lambda$  defined in 4.25 spans the kernel of  $S_\lambda^{-c_1}$ . One has  $b(1) = 0$  and by 4.37  $g_1 = 0$ . For  $\lambda \in \mathbb{R}$ , and  $u \in \text{Im}(S_\lambda^{c_1})$ , one has  $\bar{u} \in \text{Im}(S_\lambda^{c_1})$  and thus we may

assume  $h_\lambda(z) \in \mathbb{R}$  for  $\lambda \in \mathbb{R}$ , and by 4.36 we get  $b(\lambda) \in \mathbb{R}$  for  $\lambda \in \mathbb{R}$ . One has by 4.37, 4.5, 4.4 and  $b(1) = 0$

$$\begin{aligned} (K - \lambda)g_\lambda &= -(K - \lambda) \left( \cos(\eta(\lambda)z) + b(\lambda) \frac{\sin(\eta(\lambda)z)}{\eta(\lambda)} \right) \\ &= -\frac{1}{2}(F(z, \eta(\lambda)) + F(z, -\eta(\lambda))) - \frac{b(\lambda)}{2i\eta(\lambda)}(F(z, \eta(\lambda)) - F(z, -\eta(\lambda))) \\ &\in (\lambda - 1)L_z^\infty([0, 1]) \end{aligned} \quad (4.38)$$

and therefore, since  $\varphi^*$  is bounded from  $L_{c_1}^2$  into  $e^{-c_1 z}L^\infty$ , and  $\lambda \notin [0, 1/2]$ , we get 4.26 from 4.38 and  $g_1 = 0$ . The proof of theorem 4.3 is complete.  $\square$

The main theorem of this section can now be stated. It says that if  $f$  is approximately an eigenfunction of  $K$ , with eigenvalue  $\lambda$ , then  $f$  is proportional to  $e_\lambda$  of theorem 4.3 up to an exponentially small correction.

**Theorem 4.4** *Let  $\alpha \in ]0, 1[$ . There exists  $\delta > 0, C_1 > 0$  such that for any  $M > 1$  large, any  $\lambda \in U_\delta$  and any  $f \in L^2([0, \infty[)$  with support in  $[0, M + 1]$  such that  $(K - \lambda)f = g$  satisfies  $g(z) = 0 \forall z \in [0, M[$ , one has*

$$\begin{aligned} f(z) &= ae_\lambda(z) + r(z) \\ \|r\|_{L^2([0, \alpha M])} &\leq e^{-C_1 M} \|f\|_{L^2([0, M+1])} \end{aligned} \quad (4.39)$$

*Proof.* The function  $g$  has support in  $[M, M + 2]$  and one has

$$\begin{aligned} (\varphi - \lambda) * 1_+ f &= g + \theta \\ \theta &= -mf + 1_{z \leq 0}(\varphi * 1_+ f) \end{aligned} \quad (4.40)$$

Let  $\delta > 0$  small and  $c_1(\delta) < c_1$  be such that one has  $|Im(\eta(\lambda))| \leq c_1(\delta)$  for  $|\lambda - 1| \leq \delta$ . Then  $c_1(\delta) \rightarrow 0$  when  $\delta \rightarrow 0$ . One has  $\theta \in L^2([-1, 1])$ , and  $\hat{f}(\zeta)$  is holomorphic in  $Im(\zeta) < 0$ . From 4.40 we get  $(\hat{\varphi}(\zeta) - \lambda)\hat{f}(\zeta) = \hat{g}(\zeta) + \hat{\theta}(\zeta)$ , and thus by the Fourier inversion formula, one has the equality in  $L_{-c_1}^2$

$$\begin{aligned} f &= f_1 + f_2 \\ f_1(z) &= \frac{1}{2\pi} \int_{Im(\zeta)=-c_1} e^{iz\zeta} \frac{\hat{\theta}(\zeta)}{(\hat{\varphi}(\zeta) - \lambda)} d\zeta \\ f_2(z) &= \frac{1}{2\pi} \int_{Im(\zeta)=-c_1} e^{iz\zeta} \frac{\hat{g}(\zeta)}{(\hat{\varphi}(\zeta) - \lambda)} d\zeta \end{aligned} \quad (4.41)$$

By the same proof as the one of 3.40 in proposition 3.3, one has for  $\lambda \in U_\delta$

$$f_1|_{]0, \infty[} \in W_\lambda^{-c_1(\delta)} \quad (4.42)$$

Let us estimate  $f_2$ . One has for  $z \leq \alpha M$ ,  $\int_{Im(\zeta)=-c_1} e^{iz\zeta} \hat{g}(\zeta) d\zeta = 0$ , and thus, using the new integration variable  $\zeta = -ic_1 + s$ , we get for all  $z \in [0, \alpha M]$

$$f_2(z) = \frac{e^{(z-M)c_1}}{2\pi} \int_{-\infty}^{\infty} \left( \frac{1}{(\hat{\varphi}(-ic_1 + s) - \lambda)} - \frac{1}{\lambda} \right) e^{i(z-M)s} \left( \int_0^2 e^{-its} e^{-c_1 t} g(M+t) dt \right) ds \quad (4.43)$$

From 4.43, and since  $\frac{1}{(\hat{\varphi}(\zeta)-\lambda)} - \frac{1}{\lambda} \in L^2(\text{Im}(\zeta) = -c_1)$  we get for some  $C$

$$\|f_2\|_{L^2([0, \alpha M])} \leq C e^{-c_1 M(1-\alpha)} \|g\|_{L^2([M, M+2])} \leq C e^{-c_1 M(1-\alpha)} \|f\|_{L^2([0, M+1])} \quad (4.44)$$

One has

$$(K - \lambda)f_1 = G = g - (K - \lambda)f_2 \quad (4.45)$$

From 4.42, the function  $G$  is supported in  $[0, 1]$ , and since we may assume  $1 \leq \alpha M - 1$ , we get from 4.44  $\|G\|_{L^2} \leq C e^{-c_1 M(1-\alpha)} \|f\|_{L^2([0, M+1])}$ . By theorem 4.3 we thus get from 4.45

$$\begin{aligned} f_1(z) &= a e_\lambda(z) + R(z) \\ \|R\|_{L^2_{-c_1(\delta)}} &\leq C e^{-c_1 M(1-\alpha)} \|f\|_{L^2([0, M+1])} \end{aligned} \quad (4.46)$$

Thus we get  $\|R\|_{L^2([0, \alpha M])} \leq C e^{-(c_1(1-\alpha) - \alpha c_1(\delta))M} \|f\|_{L^2([0, M+1])}$ . For  $\delta$  small, one has  $c_1(1-\alpha) - \alpha c_1(\delta) \geq C_1 > 0$ , and thus by 4.41, 4.44 and 4.46, we get that 4.39 holds true for  $M$  large enough. The proof of theorem 4.4 is complete.  $\square$

## 5 The Metropolis Kernel $K_h$ on the interval $[-1, 1]$

Let  $h \in ]0, 1[$  be a small parameter. Let  $\varphi$  be as in section 3 and set

$$\varphi_h(x) = \frac{1}{h} \varphi\left(\frac{x}{h}\right) \quad (5.1)$$

Let  $m_h(x)$  be the non negative, continuous function on  $[-1, 1]$  equal to

$$m_h(x) = 1 - \int_{-1}^1 \varphi_h(x-y) dy \quad (5.2)$$

Then  $m_h(-x) = m_h(x)$ ,  $m_h(x) = 0$  for all  $x \in [-1+h, 1-h]$ ,  $m_h(\pm 1) = 1/2$  and for any  $x = -1 + hz \in [-1, 1-h]$  one has

$$m_h(-1 + hz) = m(z) \quad (5.3)$$

where  $m$  is defined by 4.1. For  $f \in L^1([-1, 1])$  and  $x \in [-1, 1]$  set

$$K_h(f)(x) = m_h(x)f(x) + (\varphi_h * f)(x) = m_h(x)f(x) + \int_{-1}^1 \varphi_h(x-y)f(y)dy \quad (5.4)$$

Then  $K_h$  maps  $L^1([-1, 1])$  into itself, one has  $K_h(1) = 1$ ,  $K_h(f) \geq 0$  for  $f \geq 0$ , and for any non negative functions  $f, g \in L^1([-1, 1])$

$$\int_{-1}^1 K_h(f)g dx = \int_{-1}^1 f K_h(g) dx \quad (5.5)$$

Therefore, one has  $\|K_h(f)\|_{L^\infty} \leq \|f\|_{L^\infty}$  for all  $f \in L^\infty([-1, 1])$ ,  $\|K_h(f)\|_{L^1} \leq \|f\|_{L^1}$  for all  $f \in L^1([-1, 1])$ . Let  $L^2 = L^2([-1, 1], dx/2)$ . Then  $K_h$  is self-adjoint on  $L^2$ , with norm  $\|K_h\|_{L^2} = 1$ , and since the operator  $f \mapsto \varphi_h * f$  is compact on  $L^2$ , and  $m_h$  takes values

in  $[0, 1/2]$ , the essential spectrum of  $K_h$  is equal to  $[0, 1/2]$ . We shall denote by  $\text{Spec}(K_h)$  the spectrum of the self-adjoint operator  $K_h$  acting on  $L^2$ . Recall that the holomorphic function  $b$  is defined in theorem 4.3. For  $\eta \in \mathbb{C}$  close to 0, set

$$2i\Gamma(\eta) = \log \left( \frac{1 + \frac{b(\hat{\varphi}(\eta))}{i\eta}}{1 - \frac{b(\hat{\varphi}(\eta))}{i\eta}} \right) \quad (5.6)$$

Observe that since  $b(1) = 0$ ,  $\frac{b(\hat{\varphi}(\eta))}{i\eta}$  is a well defined holomorphic function of  $\eta$  near  $\eta = 0$ , which vanishes at  $\eta = 0$ . Thus  $\Gamma$  is holomorphic near 0,  $\Gamma(-\eta) = -\Gamma(\eta)$ , and  $\Gamma(\eta) \in \mathbb{R}$  for  $\eta \in \mathbb{R}$ . We denote by  $B(\mu, h)$  the holomorphic function defined near  $(0, 0)$  such that

$$\eta = B(\mu, h) \quad \text{iff} \quad \eta + h\Gamma(\eta) = \mu \quad (5.7)$$

**Theorem 5.1** *For all  $h$ , with  $\nu_0 \in ]0, 1[$  from 3.5, one has  $\text{Spec}(K_h) \subset [-\nu_0, 1]$  and  $\text{Spec}(K_h)$  is discrete on  $[-\nu_0, 0[$  and  $]1/2, 1]$ . There exists  $\delta_1 \in ]0, 1/2[$  independent of  $h$ , such that all the eigenvalues of  $K_h$  in the interval  $[1 - \delta_1, 1]$  are simple. For  $0 < \delta \leq \delta_1$ , let  $k_h(\delta)$  be the number of eigenvalues of  $K_h$  in the interval  $[1 - \delta, 1]$ , and for  $0 \leq k \leq k_h(\delta_1)$ , let  $\{\lambda_k(h)\}$  be the eigenvalues of  $K_h$  in the interval  $[1 - \delta_1, 1]$*

$$\text{Spec}(K_h) \cap [1 - \delta, 1] = \{\lambda_{k_h(\delta)}(h) < \dots < \lambda_{k+1}(h) < \lambda_k(h) < \dots < \lambda_1(h) < \lambda_0(h) = 1\} \quad (5.8)$$

Then for  $\delta_1 > 0$  small,  $k_h(\delta)$  satisfies the Weyl law

$$k_h(\delta) \simeq \frac{1}{2\pi} \text{vol}([-1, 1]) \int_{\hat{\varphi}(h\xi) \geq 1 - \delta} d\xi = \frac{1}{\pi h} \int_{\hat{\varphi}(\zeta) \geq 1 - \delta} d\zeta \quad (5.9)$$

There exists  $c_1 > 0, c_2 > 0$  independent of  $h$  such that for all  $0 \leq k \leq k_h(\delta_1)$ , one has

$$|\lambda_k(h) - \hat{\varphi}(B(hk\pi/2, h))| \leq c_1 \exp(-c_2/h) \quad (5.10)$$

In particular, since  $\hat{\varphi}(\zeta) = 1 - \alpha\zeta^2/2 + \dots$  with  $\alpha = \int_{-1}^1 z^2 \varphi(z) dz > 0$ , and since by 5.7 one has  $B(h\pi/2, h) = \frac{h\pi}{2} + \mathcal{O}(h^2)$  the spectral gap  $1 - \lambda_1(h)$  satisfies

$$1 - \lambda_1(h) = \frac{\alpha h^2 \pi^2}{8} + \mathcal{O}(h^3) \quad (5.11)$$

Moreover, the eigenfunction  $\varepsilon_{k,h}$  of  $K_h$  associated to the eigenvalue  $\lambda_k(h)$  satisfies with  $\eta_{k,h} = B(hk\pi/2, h)$ , and for all  $x \in [-1, 1]$

$$\begin{aligned} \varepsilon_{k,h}(x) &= \cos\left(\eta_{k,h} \frac{x+1}{h}\right) + \frac{b(\hat{\varphi}(\eta_{k,h}))}{\eta_{k,h}} \sin\left(\eta_{k,h} \frac{x+1}{h}\right) + r_{k,h}(x) \\ |r_{k,h}(x)| &\leq c_1 |\lambda_k(h) - 1| \exp\left(-\frac{c_2}{h} \text{dist}(x, \{[-1, -1+h] \cup [1-h, 1]\})\right) \end{aligned} \quad (5.12)$$

Theorem 5.1 matches numerical approximations surprisingly closely. We have illustrated this for the spectral gap in 2.13. Consider the Weyl law 5.9 when  $\varphi$  is the uniform probability on  $[-1, 1]$ . Then the Weyl law predicts  $\pi h k_h(\delta) \simeq 2a(\delta)$ ,  $\sin(a(\delta)) = (1 - \delta)a(\delta)$ , while the numerical computations of J. Neuberger are given in the following table with  $h = 0.05$ . The integer  $i$  on the left is the number of eigenvalues in the interval

$]1 - \delta, 1]$ , for  $\delta$  such that  $1 - \delta$  is an eigenvalue, the second number is the numerical value of the eigenvalue  $\lambda_i$  equal to  $1 - \delta$ , and the last number is the value of  $1 - \delta = \sin(a(\delta))/a(\delta)$  predicted by the Weyl law, with  $a(\delta) = \pi hi/2$ .

1	$9.989722428485196e - 01$	.998972	
2	$9.958930275350699e - 01$	.995892	
3	$9.907745076776656e - 01$	.990772	
4	$9.836368902724804e - 01$	.983631	
5	$9.745083632747128e - 01$	.974495	
6	$9.634249965720746e - 01$	.963397	
7	$9.504306189559230e - 01$	.950379	
8	$9.355766748412645e - 01$	.935489	
9	$9.189220660414982e - 01$	.918781	
10	$9.005329861140520e - 01$	.900316	
11	$8.804827580693300e - 01$	.880162	
12	$8.588516912824048e - 01$	.858393	
13	$8.357269815204014e - 01$	.835088	(5.13)
14	$8.112026914185695e - 01$	.810332	
15	$7.853798719863048e - 01$	.784213	
16	$7.583669278963340e - 01$	.756826	
17	$7.302804099850302e - 01$	.728270	
18	$7.012465827712518e - 01$	.698646	
19	$6.714044765792206e - 01$	.668060	
20	$6.409120114034490e - 01$	.636620	
21	$6.099591983143240e - 01$	.604435	
22	$5.788003857189301e - 01$	.571620	
23	$5.478518797340648e - 01$	.538287	
24	$5.181463472827430e - 01$	.504551	

*Proof.*

We may and will assume  $h \in ]0, h_0]$  with  $h_0$  small. (since we know that 1 is a simple eigenvalue of  $K_h$ , there is nothing to prove for  $h \geq h_0$  if one takes  $\delta$  small). Set

$$-\nu_h = \text{infimum}(\text{Spec}(K_h)) \quad (5.14)$$

Then one has  $\nu_h \leq 1$  since  $\|K_h\| = 1$ . The essential spectrum of  $K_h$  is equal to  $[0, 1/2]$ , and therefore,  $\text{Spec}(K_h)$  is discrete on  $[-\nu_h, 0[$  and  $]1/2, 1]$ . For any  $f \in L^2(\mathbb{R})$ , with support in  $[-1, 1]$ , one has

$$\begin{aligned} (K_h f | f)_{L^2(-1,1)} &= (\varphi_h * f | f)_{L^2(\mathbb{R})} + \int_{-1}^1 m_h(x) |f(x)|^2 dx \\ &\geq (\min_{\mathbb{R}} \hat{\varphi}) \|f\|_{L^2}^2 = -\nu_0 \|f\|_{L^2}^2 \end{aligned} \quad (5.15)$$

From 5.15, we get for all  $h$ ,  $\nu_h \leq \nu_0 < 1$ .

In the sequel,  $C > 0$  denotes a constant independent of  $h$ , which may change from line to line. Let  $\delta > 0$  small. Let  $\lambda \in [1 - \delta, 1]$  be an eigenvalue of  $K_h$  and  $f$  an associated eigenfunction such that  $\|f\|_{L^2} = 1$ . Let  $J_- = [0, \frac{2}{h} - 1]$ , and let  $1_{J_-}$  be the characteristic function of  $J_-$ . Set

$$\begin{aligned} F(z) &= f(-1 + hz) \quad \forall z \in [0, 2/h] \\ F_-(z) &= 1_{J_-} f(-1 + hz) \quad \forall z \geq 0 \end{aligned} \quad (5.16)$$

From  $(K_h - \lambda)f = 0$  and 5.3 we get by the change of variable  $x = -1 + hz$

$$(m(z) - \lambda)f(-1 + hz) + \int_0^{2/h} \varphi(z - u)f(-1 + hu)du = 0 \quad \forall z \in J_- \quad (5.17)$$

□

Taking the product of 5.17 with  $1_{J_-}$  we thus get

$$(m(z) - \lambda)F_-(z) + 1_{J_-} \int_0^{2/h} \varphi(z - u)F_-(u)du = 1_{J_-} \int_{2/h-1}^{2/h} \varphi(z - u)(F_- - F)(u)du \quad \forall z \geq 0 \quad (5.18)$$

that we rewrite in the form

$$\begin{aligned} (m(z) - \lambda)F_-(z) + \int_0^\infty \varphi(z - u)F_-(u)du &= G_-(z) \quad \forall z \geq 0 \\ G_-(z) &= (1 - 1_{J_-}) \int_0^\infty \varphi(z - u)F_-(u)du + 1_{J_-} \int_0^{2/h} \varphi(z - u)(F_- - F)(u)du \end{aligned} \quad (5.19)$$

The function  $G_-(z)$  is equal to 0 outside  $[2/h - 2, 2/h]$ , and the support of  $F_-(z)$  is contained in  $[0, 2/h - 1]$ . Let  $\alpha \in ]0, 1[$  be close to 1. By theorem 4.4, with  $M = 2/h - 2$ , we thus get from 5.19

$$\begin{aligned} f(x) &= a_- e_\lambda\left(\frac{x+1}{h}\right) + r_-(x, h) \quad \forall x \in [-1, 1 - h] \\ \|r_-\|_{L^2([-1, -1+2\alpha(1-h)])} &\leq e^{-C/h} \end{aligned} \quad (5.20)$$

The same argument at the other end point ( $x = 1 - hz$ ) gives

$$\begin{aligned} f(x) &= a_+ e_\lambda\left(\frac{1-x}{h}\right) + r_+(x, h) \quad \forall x \in [-1 + h, 1] \\ \|r_+\|_{L^2([1-2\alpha(1-h), 1])} &\leq e^{-C/h} \end{aligned} \quad (5.21)$$

From 5.20, 5.21 and  $\|f\|_{L^2} = 1$ , we get

$$\exists C > 0, \quad \min(|a_-|, |a_+|) \geq C \quad (5.22)$$

For  $h$  small and  $\alpha$  close to 1, the two formulas 5.20, 5.21 are valid on the interval  $[-1/2, 1/2]$ , and thus we get from theorem 4.3, with  $\eta = \eta(\lambda) \geq 0$  the solution closest to 0 of  $\hat{\varphi}(\eta) = \lambda$ ,

$$\begin{aligned} Ae^{i\eta x/h} + Be^{-i\eta x/h} &= r(x, h) \quad \forall x \in [-1/2, 1/2] \\ \|r\|_{L^2([-1/2, 1/2])} &\leq e^{-C/h} \end{aligned} \quad (5.23)$$

with

$$\begin{aligned} A &= a_- e^{i\eta/h} \left(1 + \frac{b(\lambda)}{i\eta}\right) - a_+ e^{-i\eta/h} \left(1 - \frac{b(\lambda)}{i\eta}\right) \\ B &= a_- e^{-i\eta/h} \left(1 - \frac{b(\lambda)}{i\eta}\right) - a_+ e^{i\eta/h} \left(1 + \frac{b(\lambda)}{i\eta}\right) \end{aligned} \quad (5.24)$$

From 5.23 and 5.24, one has, since  $\eta$  is real,  $|A| + |B| \leq e^{-C/h}$ , and thus 5.24 is a  $2 \times 2$  matrix equation

$$M \begin{pmatrix} a_- \\ -a_+ \end{pmatrix} = \mathcal{O}(e^{-C/h}) \quad (5.25)$$

with

$$M = \begin{pmatrix} e^{i\eta/h} \left(1 + \frac{b(\lambda)}{i\eta}\right) & e^{-i\eta/h} \left(1 - \frac{b(\lambda)}{i\eta}\right) \\ e^{-i\eta/h} \left(1 - \frac{b(\lambda)}{i\eta}\right) & e^{i\eta/h} \left(1 + \frac{b(\lambda)}{i\eta}\right) \end{pmatrix} \quad (5.26)$$

From 5.22, we get  $\det(M) \leq e^{-C/h}$  which is exactly the equation

$$e^{4i(\eta/h + \Gamma(\eta))} = 1 + \mathcal{O}(e^{-C/h}) \quad (5.27)$$

Therefore, there must exist an integer  $k$  such that

$$|\eta + h\Gamma(\eta) - hk\pi/2| \leq e^{-C/h} \quad (5.28)$$

Since we have chosen  $\eta = \eta(\lambda) \geq 0$  the solution closest to 0 of  $\hat{\varphi}(\eta) = \lambda$ , we get  $k \geq 0$ , and with  $\eta_{k,h} = B(hk\pi/2, h)$ ,

$$|\eta - \eta_{k,h}| \leq e^{-C/h} \quad (5.29)$$

Let  $I_{k,h,C}$  be the interval

$$I_{k,h,C} = [\hat{\varphi}(\eta_{k,h}) - e^{-C/h}, \hat{\varphi}(\eta_{k,h}) + e^{-C/h}] \quad (5.30)$$

Let  $C > 0$  given. Then for  $h$  small and  $0 \leq kh \leq c$  with  $c > 0$  small, these intervals are disjoint. From the above discussion, the following lemma holds true.

**Lemma 5.2** *Let  $h_0 > 0$  and  $\delta > 0$  small. There exist  $C > 0, c > 0$  such that for all  $h \in ]0, h_0]$  one has*

$$\text{Spec}(K_h) \cap [1 - \delta, 1] \subset \bigcup_{0 \leq k \leq c/h} I_{k,h,C} \quad (5.31)$$

In order to complete the proof of theorem 5.1, it remains to show that  $\text{Spec}(K_h) \cap I_{k,h,C}$  contains exactly one element, since then, the formula 5.12 will be a consequence of theorem 4.3 and of the formulas 5.20 and 5.21.

The proof of  $\text{Spec}(K_h) \cap I_{k,h,C} \neq \emptyset$  is easy. In fact, set

$$\begin{aligned} f_{k,h}(x) &= a_- e_\lambda \left(\frac{x+1}{h}\right) \quad \forall x \in [-1, 0] \\ f_{k,h}(x) &= a_+ e_\lambda \left(\frac{1-x}{h}\right) \quad \forall x \in ]0, 1] \end{aligned} \quad (5.32)$$

where  $a_-, a_+$  is a non zero solution of  $M_{k,h} \begin{pmatrix} a_- \\ -a_+ \end{pmatrix} = 0$ , with  $M_{k,h}$  the matrix defined by 5.26 with  $\eta = \eta_{k,h}$  and  $\lambda = \hat{\varphi}(\eta_{k,h})$ , so that we have  $\det(M_{k,h}) = 0$ . Then  $|a_-|, |a_+|$  are

of the same magnitude, and we can normalize such that  $\|f_{k,h}\|_{L^2} = 1$ . By the preceding discussion, the jump at  $x = 0$  of  $f_{k,h}$  is  $\mathcal{O}(e^{-C/h})$ , and one has

$$(K_h - \hat{\varphi}(\eta_{k,h}))f_{k,h} \in \mathcal{O}(e^{-C/h}) \quad (5.33)$$

Since  $K_h$  is self adjoint, this implies

$$\text{dist}(\text{Spec}(K_h), \hat{\varphi}(\eta_{k,h})) \leq e^{-C/h} \quad (5.34)$$

and thus, there exist  $C > 0$  such that  $\text{Spec}(K_h) \cap I_{k,h,C} \neq \emptyset$  for all  $h$  small and  $0 \leq kh \leq c$  with  $c > 0$  small.

It remains to show that  $\text{Spec}(K_h) \cap I_{k,h,C}$  contains exactly one element. Let  $\lambda_j \in \text{Spec}(K_h) \cap I_{k,h,C}$  and let  $f_j$  be the associated normalized eigenfunctions. By 5.21, 5.22 and 5.25, one gets that

$$\text{dist}_{L^2}(f_j, f_{k,h}) \leq e^{-C/h} \quad (5.35)$$

and therefore  $\text{Spec}(K_h) \cap I_{k,h,C}$  contains at most one element, since for two orthogonal vectors  $f_1, f_2$  on the unit sphere, one has  $\|f_1 - f_2\| = \sqrt{2}$ .

Finally, since by 5.7, one has  $B(\frac{hk\pi}{2}, h) = \frac{hk\pi}{2}(1 + \mathcal{O}(h))$ , the Weyl law 5.9 is an easy byproduct of 5.10. The proof of theorem 5.1 is complete.  $\square$

## 6 The total variation estimate

**1. Background on total variation.** If  $P$  and  $Q$  are probability measures on  $\mathbb{R}$ , we define

$$\|P - Q\|_{TV} = \sup_A |P(A) - Q(A)| = \frac{1}{2} \sup_{\|g\|_\infty \leq 1} |P(g) - Q(g)| = \frac{1}{2} \int_{-\infty}^{\infty} \left| \frac{dP}{d\lambda} - \frac{dQ}{d\lambda} \right| d\lambda \quad (6.1)$$

In 6.1, the sup in  $A$  is over Borel sets,  $P(f) = \int f dP$ , and  $\lambda$  is any  $\sigma$ -finite measure that dominates both  $P$  and  $Q$  (eg  $P + Q$ ). We thus see that, if  $P$  and  $Q$  are compactly supported as in our case,  $2\|P - Q\|$  is the usual dual norm for the measures as the dual of bounded continuous functions. Probabilists put the  $1/2$  in because of the first identity. There is also a dual version

$$\|P - Q\|_{TV} = \inf_V V(\Delta^c) \quad (6.2)$$

with the inf over probability measures  $V$  in  $\mathbb{R} \times \mathbb{R}$  with  $V(\mathbb{R}, A) = P(A)$ ,  $V(A, \mathbb{R}) = Q(A)$ .

**2. A proof of theorem 2.1 .** We may assume  $h \in ]0, h_0]$  with  $h_0 > 0$  small. We denote by  $e_{k,h} = a_{k,h} \varepsilon_{k,h}$ ,  $\|e_{k,h}\| = 1$  the normalized eigenvectors of  $K_h$  with  $\varepsilon_{k,h}$  given in 5.12. The lower bound 2.14 is a simple consequence of the evaluation 5.10 of the top eigenvalues, since 5.11 implies (we use 6.1 with  $g = \frac{e_{k,h}(x)}{\|e_{k,h}\|_{L^\infty}}$ )

$$\|m_x^n - f\|_{TV} \geq \frac{e_{k,h}(x)}{2\|e_{k,h}\|_{L^\infty}} \lambda_k(h)^n \quad (6.3)$$

Then, we use 6.3 with  $k = 1$  and  $k = 2$  and the fact that by 5.12, for  $h_0$  small, there exists  $C > 0$  such that  $|e_{1,h}(x)| + |e_{2,h}(x)| \geq C$  for all  $x \in [-1, 1]$ . From 6.3, we get also

that the lower bound in 2.15 holds true.

Let us prove that the upper bound in 2.15 holds true. By theorem 5.1, there exists  $\delta > 0$  such that the spectrum of  $K_h$  is a subset of  $[-1 + \delta, 1]$ , and moreover, the spectrum of  $K_h$  in  $[1 - \delta, 1]$  satisfies all the assertions of theorem 5.1. By the spectral theorem for self-adjoint operators, we can write  $K_h = K_{h,1} + K_{h,2}$ , with  $K_{h,1}K_{h,2} = K_{h,2}K_{h,1} = 0$ , so that  $K_{h,1}$  is the spectral restriction of  $K_h$  on  $[1 - \delta, 1]$ , and  $K_{h,2}$  is the spectral restriction of  $K_h$  on  $[-1 + \delta, 1 - \delta[$ . Obviously, one has with the notations of theorem 5.1

$$\begin{aligned} \|K_{h,2}\| &\leq 1 - \delta \\ K_{h,1}(x, y) &= \sum_{0 \leq k \leq k_h(\delta)} \lambda_k(h) e_{k,h}(x) e_{k,h}(y) \end{aligned} \quad (6.4)$$

Thus, the distribution kernel of  $m_x^n - f$  is equal to

$$(m_x^n - f)(x, y) = \sum_{1 \leq k \leq k_h(\delta)} \lambda_k(h)^n e_{k,h}(x) e_{k,h}(y) + K_{h,2}^n(x, y) \quad (6.5)$$

Let us evaluate separately the total variation of each contribution on the right hand side of 6.5. By 5.12, the eigenvectors  $e_{k,h}$  are uniformly (with respect to  $k, h$ ) bounded by some constant  $C$ , and thus

$$\left\| \sum_{1 \leq k \leq k_h(\delta)} \lambda_k(h)^n e_{k,h}(x) e_{k,h}(y) \right\|_{TV} \leq 2C^2 \sum_{1 \leq k \leq k_h(\delta)} \lambda_k(h)^n \quad (6.6)$$

From 5.10, we thus get what we want, i.e, there exist universal constants  $A, B$  such that

$$\sup_{x \in [-1, 1]} \left\| \sum_{1 \leq k \leq k_h(\delta)} \lambda_k(h)^n e_{k,h}(x) e_{k,h}(y) \right\|_{TV} \leq A(1 - Bh^2)^n \quad (6.7)$$

uniformly in  $n = 1, 2, \dots$  and  $h \in ]0, h_0]$ , and for  $h_0$  small,  $B$  is close to  $\alpha\pi^2/8$  with  $\alpha$  given in 5.11.

It remains to evaluate the contribution of  $K_{h,2}^n(x, y)$  to the total variation. Observe that for this part, we have no good information on the spectrum, so we will use crude estimates. One has  $K_{h,2}^n = K_h K_{h,2}^{n-1}$ , and therefore for  $\text{dist}(x, \{\pm 1\}) \geq h$ , the kernel of  $K_{h,2}^n(x, y)$  is given by

$$K_{h,2}^n(x, y) = \int \varphi_h(x - z) K_{h,2}^{n-1}(z, y) dz \quad (6.8)$$

One has  $\|K_{h,2}\| \leq 1 - \delta$  and  $\|\varphi_h\|_{L^2} \leq Ch^{-1/2}$ , and thus from 6.8, we get for any  $g \in L^2$  and any  $x$  such that  $\text{dist}(x, \{\pm 1\}) \geq h$

$$\left| \int K_{h,2}^n(x, y) g(y) dy \right| \leq Ch^{-1/2} \|g\|_{L^2} (1 - \delta)^{n-1} \quad (6.9)$$

which is far smaller than  $A(1 - Bh^2)^n$  for  $n \geq M/h^2$ .

Thus for some universal constants  $A, B$ , uniformly in  $x \in [-1+h, 1-h]$  and  $l = 1, 2, \dots$  and  $h \in ]0, h_0]$ , the following inequality holds true

$$\|m_x^l - f\|_{TV} \leq A(1 - Bh^2)^l \quad (6.10)$$

and for  $h_0$  small,  $B$  is close to  $\alpha\pi^2/8$  with  $\alpha$  given in 5.11.

To conclude the proof, it remains to understand what happens to the walk if it starts (say) at  $y \in [-1, -1+h]$ . For all we know,  $\varphi_h$  could be extremely concentrated near 0 (even if  $\hat{\varphi}_h \in C^\infty$  and  $\varphi_h(\pm h) > 0$ ). Then the walk would spend a very long time near  $-1$ .

Thus let

$$\begin{aligned} \gamma &= \text{Probability that in two steps we cross } -1+h \text{ starting at } -1 \\ \gamma &= \int_0^h \int_{x>h} \varphi_h(x-y)\varphi_h(y)dydx \in ]0, 1[ \end{aligned} \quad (6.11)$$

Note that this doesn't depend on  $h$ . Consider the Markov chain  $\{X_l\}_{l=0}^\infty$  started at  $X_0 = x$ . Let  $T$  be the first time that the chain enters  $[-1+h, 1-h]$ . Thus  $T = 0$  if  $x \in [-1+h, 1-h]$ . We have for all  $A$

$$P_x(X_l \in A) = \sum_{j=0}^l P_x(X_l \in A \text{ and } T = j) + P_x(X_l \in A \text{ and } T > l) \quad (6.12)$$

Now

$$\begin{aligned} P_x(X_l \in A \text{ and } T = j) &= P_x(X_l \in A \mid T = j)P_x(T = j) \\ &= P_x(T = j) \int_{-1+h \leq y \leq 1-h} P_y(X_{l-j} \in A)Q_{x,j}(dy) \end{aligned} \quad (6.13)$$

Here  $Q_{x,j}(dy) = P_x(X_j = y \mid T = j)$  and we have used the Markov property. From 6.10,  $P_y(X_{l-j} \in A) = \text{mes}(A)/2 + \varepsilon_{l-j}$  with  $\varepsilon_{l-j}$  bounded by the right hand side of 6.10. Thus

$$|P_x(X_l \in A) - \text{mes}(A)/2| \leq \sum_{j=0}^l \varepsilon_{l-j}P_x(T = j) + 2P_x(T > l) \quad (6.14)$$

Now,

$$\begin{aligned} \varepsilon_{l-j} &\leq A(1 - Bh^2)^{l-j}, \quad 0 \leq j \leq l \\ P_x(T = j) &\leq (1 - \gamma)^{\lfloor \frac{j-1}{2} \rfloor}, \quad 0 \leq j \leq l \\ P_x(T > l) &\leq (1 - \gamma)^{\lfloor \frac{l}{2} \rfloor} \end{aligned} \quad (6.15)$$

Here,  $\lfloor z \rfloor$  is the integer part of  $z$ . The last two inequalities in 6.15 follow from the following considerations. Let  $A = \{T = j\}$ . Let  $A_1$  the event that the sum of the two first steps of the  $\lfloor \frac{j-1}{2} \rfloor$  walk are at most  $h$ . Let  $A_2$  the event that the sum of steps three and four are at most  $h$ . Similarly,  $A_i$ ,  $1 \leq i \leq \lfloor \frac{j-1}{2} \rfloor$  are defined. Clearly,  $A \subset \cap A_i$ , since if  $A$  occurs, each  $A_i$  must occur. Next use

$$P(\cap A_i) = P_x(A_1)P_x(A_2|A_1)\dots P_x(A_{\lfloor \frac{j-1}{2} \rfloor}|A_1 \cap \dots \cap A_{\lfloor \frac{j-1}{2} \rfloor - 1})$$

By monotonicity, each conditional probability is at most  $1 - \gamma$ . This proves the second line of 6.15, and the proof of the third inequality in 6.15 is similar.

Since for  $h_0$  small, one has  $1 - \gamma < (1 - Bh^2)^2$ , from 6.15, we get for all  $x \in [-1, 1]$

$$\|m_x^l - f\|_{TV} \leq A_\gamma(1 - Bh^2)^l + 2(1 - \gamma)^{\lfloor \frac{l}{2} \rfloor} \quad (6.16)$$

The proof of theorem 2.1 is complete.

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