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**Maximal determinants of Schrödinger operators on bounded intervals**

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## MAXIMAL DETERMINANTS OF SCHRÖDINGER OPERATORS ON BOUNDED INTERVALS

BY CLARA L. ALDANA, JEAN-BAPTISTE CAILLAU & PEDRO FREITAS

**ABSTRACT.** — We consider the problem of finding extremal potentials for the functional determinant of a one-dimensional Schrödinger operator defined on a bounded interval with Dirichlet boundary conditions under an  $L^q$ -norm restriction ( $q \geq 1$ ). This is done by first extending the definition of the functional determinant to the case of  $L^q$  potentials and showing the resulting problem to be equivalent to a problem in optimal control, which we believe to be of independent interest. We prove existence, uniqueness and describe some basic properties of solutions to this problem for all  $q \geq 1$ , providing a complete characterisation of extremal potentials in the case where  $q$  is one (a pulse) and two (Weierstraß's  $\wp$  function).

**RÉSUMÉ** (Maximisation du déterminant d'opérateurs de Schrödinger sur un intervalle borné)

On cherche les potentiels qui maximisent le déterminant fonctionnel d'un opérateur de Schrödinger sur un intervalle borné, avec conditions aux limites de Dirichlet et sous contrainte de norme  $L^q$  ( $q \geq 1$ ). On commence par étendre la définition du déterminant fonctionnel au cas de potentiels  $L^q$ , en montrant que le problème de maximisation associé est équivalent à un problème de contrôle optimal. On prouve l'existence et l'unicité de solution de ce problème pour tout  $q \geq 1$ , et les principales propriétés de ces solutions sont étudiées. On donne une caractérisation complète des potentiels optimaux dans les cas  $q = 1$  (fonction créneau) et  $q = 2$  (fonction  $\wp$  de Weierstraß).

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## INTRODUCTION

An important quantity arising in connection with self-adjoint elliptic operators is the functional (or spectral) determinant. This has been applied in a variety of settings in mathematics and in physics, and is based on the regularisation of the spectral zeta function associated to an operator  $T$  with discrete spectrum. This zeta function is defined by

$$(1) \quad \zeta_T(s) = \sum_{n=1}^{\infty} \lambda_n^{-s},$$

where the numbers  $\lambda_n$ ,  $n = 1, 2, \dots$  denote the eigenvalues of  $T$  and, for simplicity, and without loss of generality from the perspective of this work as we will see below, we shall assume that these eigenvalues are all positive and with finite multiplicities. Under these conditions, and for many operators such as the Laplace or Schrödinger operators, the above series will be convergent on a right half-plane, and may typically be extended meromorphically to the whole of  $\mathbb{C}$ . Furthermore, zero is not a singularity and since, formally,

$$\zeta'_T(0) = - \sum_{n=1}^{\infty} \log(\lambda_n),$$

the regularised functional determinant is then defined by

$$(2) \quad \det T = e^{-\zeta'_T(0)},$$

where  $\zeta'_T(0)$  should now be understood as referring to the meromorphic extension mentioned above. This quantity appears in the mathematics and physics literature in connection to path integrals, going back at least to the early 1960's. Examples of calculations of determinants for operators with a potential in one dimension may be found in [5, 12, 18] and, more recently, for one-dimensional polyharmonic operators of arbitrary order [11] and the harmonic oscillator in arbitrary dimension [10]. Some of the regularising techniques for zeta functions which are needed in order to define the above determinant were studied in [19], while the actual definition (2) was given in [22]. Within such a context, it is then natural to study extremal properties of these global spectral objects and this question has indeed been addressed by several authors, mostly when the underlying setting is of a geometric nature [3, 21, 20, 2].

In this paper, we shall consider the problem of optimising the functional determinant for a Schrödinger operator defined on a bounded interval together with Dirichlet boundary conditions. More precisely, let  $T_V$  be the operator associated with the eigenvalue problem defined by

$$(3) \quad \begin{cases} -\phi'' + V\phi = \lambda\phi \\ \phi(0) = \phi(1) = 0, \end{cases}$$

where  $V$  is a potential in  $L^q[0, 1]$  ( $q \geq 1$ ). For a given  $q$  and a positive constant  $A$ , we are interested in the problem of optimising the determinant given by

$$(4) \quad \det T_V \longrightarrow \max, \quad \|V\|_q \leq A$$

where  $\|\cdot\|_q$  denotes the norm on  $L^q[0, 1]$ . For smooth bounded potentials the determinant of such operators is known in closed form and actually requires no computation of the eigenvalues themselves. In the physics literature such a formula is sometimes referred to as the Gelfand-Yaglom formula and a derivation may be found in [18], for instance—see also [5]. More precisely, for the operator  $T_V$  defined by (3) we have  $\det T_V = 2y(1)$ , where  $y$  is the solution of the initial value problem

$$(5) \quad \begin{cases} -y'' + Vy = 0 \\ y(0) = 0, \quad y'(0) = 1. \end{cases}$$

We shall show that this expression for the determinant still holds for  $L^q$  potentials and study the problem defined by (4). We then prove that (4) is well-posed and has a unique solution for all  $q \geq 1$  and positive  $A$ . In our first main result we consider the  $L^1$  case where the solution is given by a piecewise constant function.

**THEOREM A** (Maximal  $L^1$  potential). — *Let  $q = 1$ . Then for any positive number  $A$  the unique solution to problem (4) is the symmetric potential given by*

$$V_A(x) = \frac{A}{\ell(A)} \chi_{\ell(A)},$$

where  $\chi_{\ell(A)}$  denotes the characteristic function of the interval of length

$$\ell(A) = \frac{A}{(1 + \sqrt{1 + A})^2}$$

centred at  $1/2$ . The associated maximum value of the determinant is

$$\max_{\|V\|_1=A} \det T_V = \frac{4}{1 + \sqrt{1 + A}} \exp\left(\frac{A}{1 + \sqrt{1 + A}}\right).$$

In the case of general  $q$  we are able to provide a similar result concerning existence and uniqueness, but the corresponding extremal potential is now given as the solution of a second order (nonlinear) ordinary differential equation.

**THEOREM B** (Maximal  $L^q$  potential,  $q > 1$ ). — *For any  $q > 1$  and any positive number  $A$ , there exists a unique solution to problem (4). This maximal potential is given by*

$$V_A = \frac{q}{4q - 2} {}^{q-1}\sqrt{\Psi},$$

where  $\Psi$  is the solution to

$$\Psi'' - |\Psi|^\alpha + 2H = 0, \quad \alpha := q/(q - 1),$$

$$\Psi(0) = 0, \quad \Psi'(0) = H - c(A, q).$$

Here  $c(A, q) := (1/2)(A(4q - 2)/q)^q$ , and  $H$  is a (uniquely defined) constant satisfying  $H > c(A, q)$ . The function  $\Psi$  is non-negative on  $[0, 1]$ , and the maximal potential is symmetric with respect to  $t = 1/2$ , smooth on  $(0, 1)$ , strictly increasing on  $[0, 1/2]$ , with zero derivatives at  $t = 0$  and  $t = 1$  if  $1 < q < 2$ , positive derivative at  $t = 0$  (resp. negative derivative at  $t = 1$ ) if  $q = 2$ , and vertical tangents at both endpoints if  $q > 2$ .

The properties given in the above theorem provide a precise qualitative description of the evolution of maximal potentials as  $q$  increases from 1 to  $+\infty$ . Starting from a rectangular pulse ( $q = 1$ ), solutions become regular for  $q$  on  $(1, 2)$ , having zero derivatives at the endpoints. In the special case of  $L^2$ , the maximising potential can be written in terms of the Weierstraß elliptic function and has finite nonzero derivatives at the endpoints. This marks the transition to potentials with singular derivatives at the boundary for  $q$  larger than two, converging towards an optimal constant potential in the limiting  $L^\infty$  case.

**THEOREM C** (Maximal  $L^2$  potential). — *Let  $q = 2$ . Then for any positive number  $A$  the unique solution to problem (4) is given by*

$$V_A(t) = \frac{1}{3}\wp\left(\frac{2t-1}{2\sqrt{6}} + \omega'\right), \quad t \in [0, 1],$$

where  $\wp$  is the Weierstraß elliptic function associated to invariants

$$g_2 = 24H, \quad g_3 = -6(H - 9A^2/2)^2,$$

and where  $\omega'$  is the corresponding imaginary half-period of the rectangular lattice of periods. The corresponding (unique) value of  $H$  such that

$$\wp\left(\frac{1}{2\sqrt{6}} + \omega'\right) = 0$$

is in  $(9A^2/2, h^*(A))$ , where  $h^*(A)$  is the unique root of the polynomial

$$128H^3 - 9(H - 9A^2/2)^4$$

in  $(9A^2/2, \infty)$ .

Concerning possible extensions of these results to higher dimensions, the underlying space geometry mentioned above may in fact impose certain restrictions that will have to be taken into consideration when studying extremal problems for the determinant. In dimensions higher than one, different issues from those in the more standard situations analysed so far may also come into play. In particular, it is not even guaranteed that, without further restrictions, such extrema do exist – compare the results in the references above with the extremal problems related to the Laplace and Schrödinger operators considered in [6, 13, 14], for instance. This would thus be a first question to address when considering the problem of finding extremal potentials in domains in higher dimensions, where furthermore no formula is known for the determinant of a Schrödinger operator in general.

The paper is structured as follows. In the next section we show that the functional determinant of Schrödinger operators with Dirichlet boundary conditions on bounded intervals and with potentials in  $L^q$  is well-defined and we extend the formula from [18] to this general case. The main properties of the determinant, namely boundedness and monotonicity over  $L^q$ , are studied in Section 2. Having established these, we then consider the optimal control problem (4) of maximising  $y(1)$  in (5) in Sections 3 and 4, where the proofs of our main results Theorems A and B-C are given, respectively.

1. THE DETERMINANT OF ONE-DIMENSIONAL SCHRÖDINGER OPERATORS

We consider the eigenvalue problem defined by (3) associated to the operator  $T_V$  on the interval  $[0, 1]$  with potential  $V \in L^q[0, 1]$  for  $q \geq 1$ . Although no further restrictions need to be imposed on  $V$  at this point, for our purposes it will be sufficient to consider  $V$  to be non-negative, as we will show in Proposition 9 below. This simplifies slightly the definition of the associated zeta function given by (1) and thus also that of the determinant. Hence, in the rest of this section we assume that  $V$  is a non-negative potential.

For smooth potentials, and as was already mentioned in the Introduction, it is known that the regularised functional determinant of  $T_V$  is well-defined [5, 18], and this has been extended to potentials with specific singularities [16, 17]. We shall now show that this is also the case for general potentials in  $L^q[0, 1]$ , for  $q \geq 1$ . We first show that the zeta function associated with the operator  $T_V$  as defined by (1) is analytic at the origin and has as its only singularity in the half-plane  $\text{Re}(s) > -1/2$  a simple pole at  $1/2$ . This is done adapting one of the approaches originally used by Riemann (see [23] and also [26, p. 21ff]). We then show that the method from [18] can be used to prove that the determinant is still given by  $2y(1)$ , where  $y$  is the solution of the initial value problem (5).

In order to show these properties of the determinant, it is useful to consider the heat trace associated with  $T_V$ , defined by

$$\text{Tr}(e^{-tT_V}) = \sum_{n=1}^{\infty} e^{-t\lambda_n}.$$

Our first step is to show that the behaviour of the heat trace as  $t$  approaches zero for any non-negative potential in  $L^q(0, 1)$  is the same as in the case of smooth potentials.

**PROPOSITION 1.** — *Let  $T_V$  be the Schrödinger operator defined by problem (3) with  $V \in L^q[0, 1]$ , then*

$$\text{Tr}(e^{-tT_V}) = \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + O(\sqrt{t}), \quad \text{as } t \rightarrow 0.$$

*Proof.* — For potentials which are the derivative of a function of bounded variation it was proved in [25, §3] (see also [24, Th. 1]) that the eigenvalues behave asymptotically as

$$(6) \quad \lambda_n = n^2\pi^2 + O(1), \quad n = 1, 2, \dots$$

when  $n$  goes to  $\infty$ . For a potential in  $L^q$  we may thus assume the above asymptotics which imply the existence of a positive constant  $c$  such that

$$\pi^2 n^2 - c \leq \lambda_n \leq \pi^2 n^2 + c$$

uniformly in  $n$ . For the zero potential the spectrum is given by  $\pi^2 n^2$  and the heat trace associated with it becomes the Jacobi theta function defined by

$$\psi(t) = \sum_{n=1}^{\infty} e^{-n^2\pi^2 t}.$$

We are interested in the behaviour of the heat trace for potentials  $V$  for small positive  $t$ , and we will determine this behaviour by comparing it with that of  $\psi$ . For simplicity, in what follows we write

$$\varphi(t) = \text{Tr}(e^{-tT_V}).$$

We then have

$$(e^{-ct} - 1)\psi(t) \leq \varphi(t) - \psi(t) \leq (e^{ct} - 1)\psi(t),$$

and, since  $\psi$  satisfies the functional equation [26, p. 22]

$$\psi(t) = \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + \frac{1}{\sqrt{\pi t}} \psi(1/\pi^2 t),$$

it follows that

$$\frac{1}{\sqrt{\pi t}} \psi(1/\pi^2 t) + (e^{-ct} - 1)\psi(t) \leq \varphi(t) - \frac{1}{2\sqrt{\pi t}} + \frac{1}{2} \leq \frac{1}{\sqrt{\pi t}} \psi(1/\pi^2 t) + (e^{ct} - 1)\psi(t).$$

Since  $\frac{1}{\sqrt{\pi t}} \psi(1/\pi^2 t) = O(e^{-C/t})$  for some  $C > 0$  and

$$(e^{ct} - 1)\psi(t) = O(\sqrt{t})$$

as  $t \rightarrow 0$ , it follows that

$$\varphi(t) = \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + O(\sqrt{t}) \text{ as } t \rightarrow 0. \quad \square$$

REMARK 2. — Note that although the heat trace for the zero potential  $\psi$  satisfies

$$\psi(t) = \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + O(t^\alpha) \text{ as } t \rightarrow 0^+$$

for any positive real number  $\alpha$ , this will not be the case for general potentials, where we can only ensure that the next term in the expansion will be of order  $\sqrt{t}$ .

We may now consider the extension of  $\zeta_{T_V}$  to a right half-plane containing the origin.

PROPOSITION 3. — *The spectral zeta function associated with the operator  $T_V = -\Delta + V$  with Dirichlet boundary conditions and potential  $V \in L^q[0, 1]$ ,  $q \geq 1$ , defined by (1) may be extended to the half-plane  $\text{Re}(s) > -1/2$  as a meromorphic function with a simple pole at  $s = 1/2$ , whose residue is given by  $1/(2\pi)$ .*

Proof. — We start from

$$\int_0^{+\infty} t^{s-1} e^{-\lambda_n t} dt = \Gamma(s) \lambda_n^{-s},$$

which is valid for  $\text{Re}(s) > 0$ . Summing both sides in  $n$  from one to infinity yields

$$\zeta_{T_V}(s) = \frac{1}{\Gamma(s)} \int_0^{+\infty} t^{s-1} \varphi(t) dt,$$

where  $\varphi$  denotes the heat trace as above and the exchange between the sum and the integral is valid for  $\text{Re}(s) > 1/2$ . By Proposition 1 we may write

$$\varphi(t) = \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + f(t),$$

where  $f(t) = O(\sqrt{t})$  as  $t$  approaches zero. Since, in addition,  $\varphi(t) = O(e^{-ct})$  as  $t$  approaches infinity, for some  $c > 0$ , we have

$$\begin{aligned} \zeta_{T_V}(s) &= \frac{1}{\Gamma(s)} \left[ \int_0^1 \left( \frac{1}{2\sqrt{\pi t}} - \frac{1}{2} + f(t) \right) t^{s-1} dt + \int_1^{+\infty} \varphi(t) t^{s-1} dt \right] \\ &= \frac{1}{\Gamma(s)} \left( \frac{\pi^{-1/2}}{2s-1} - \frac{1}{2s} \right) + F(s), \end{aligned}$$

which is valid for  $\text{Re}(s) > 1$  and where  $F$  is an analytic function in the half-plane  $\text{Re}(s) > -1/2$ . Due to the simple zero of  $1/\Gamma(s)$  at zero we see that the expression in the right-hand side is well-defined and meromorphic in the half-plane  $\text{Re}(s) > -1/2$ , except for the simple pole at  $s = 1/2$ , showing that we may extend  $\zeta_{T_V}(s)$  to this half-plane. The value of the residue is obtained by a standard computation.  $\square$

REMARK 4. — It is clear from the proof that the behaviour on  $\text{Re}(s) \leq 1/2$  will depend on the potential  $V$ . This may be seen from the simple example of a constant potential  $V(x) \equiv a$ , for which the heat trace now satisfies

$$\varphi(t) = e^{-at}\psi(t).$$

From this we see that when  $a$  is nonzero  $\varphi(t)$  has an expansion for small  $t$  with terms of the form  $t^{-(n-1)/2}$ , for all non-negative integers  $n$ . These terms produce simple poles at  $s = -(2n + 1)/2$ ,  $n \geq 0$  an integer, with residues depending on  $a$ . When  $a$  vanishes we recover  $\zeta_{T_V}(s) = \zeta(2s)$  and there are no poles other than the simple pole at  $s = 1/2$ .

We are now ready to extend the result in [18] to the case of  $L^q$  potentials with  $q$  greater than or equal to one.

THEOREM 5. — *The determinant of the operator  $T_V = -\Delta + V$  with Dirichlet boundary conditions and potential  $V \in L^q[0, 1]$ ,  $q \in [1, +\infty]$ , is given by*

$$(7) \quad \det T_V = 2y(1),$$

where  $y$  is the solution of the initial value problem (5).

*Proof.* — We shall follow along the lines of the proof in [18, Th. 1] for smooth potentials, which consists in building a one-parameter family of potentials,  $\alpha V$ , connecting the zero potential, for which the expression for the determinant may be computed explicitly, with the potential  $V$ , and comparing the way these two quantities change. More precisely, the main steps in this approach are as follows. For  $\alpha \in [0, 1]$ , we define



the family of operators  $T_\alpha$  in  $L^2[0, 1]$  by  $T_\alpha u(\alpha, t) := -u''(\alpha, t) + \alpha V(t)u(\alpha, t)$  and consider the eigenvalue problem

$$(8) \quad \begin{cases} T_\alpha u(\alpha, t) = \lambda(\alpha)u(\alpha, t) \\ u(\alpha, 0) = 0, \quad u(\alpha, 1) = 0 \end{cases}$$

with solutions  $\lambda_k(\alpha)$ ,  $u_k(\alpha)$ . We have that  $\{T_\alpha\}_{\alpha \in [0,1]}$  is an analytic family in  $\alpha$  of type  $B$  in the sense of Kato. This follows from [15, Ex. VII.4.24], which covers a more general case. Then, by [15, Rem. VII.4.22 & Th. VII.3.9], we obtain that the eigenvalues  $\lambda_k(\alpha)$  and its associated (suitably normalised) eigenfunction  $u_k(\alpha)$ , for any  $k \geq 1$ , are analytic functions of  $\alpha$ . The corresponding  $\zeta$ -function is given by

$$(9) \quad \zeta_{T_\alpha}(s) = \sum_{j=1}^{\infty} \lambda_j^{-s}(\alpha).$$

Although this series is only defined for  $\text{Re}(s) > 1/2$ , we know from Proposition 3 that the spectral zeta function defined by it can be extended uniquely to a meromorphic function on the half-plane  $\text{Re}(s) > -1/2$  which is analytic at zero. We shall also define  $y(\alpha, t)$  to be the family of solutions of the initial value problem

$$\begin{cases} T_\alpha y(\alpha, t) = 0 \\ y(\alpha, 0) = 0, \quad \frac{\partial y}{\partial t}(\alpha, 0) = 1. \end{cases}$$

By Proposition 7 in the next section the quantity  $2y(\alpha, 1)$  is well-defined for  $V \in L^q[0, 1]$ . The idea of the proof is to show that

$$(10) \quad \frac{d}{d\alpha} \log(\det T_\alpha) = \frac{d}{d\alpha} \log(y(\alpha, 1))$$

for  $\alpha \in [0, 1]$ . Since at  $\alpha = 0$ ,  $\det T_0 = 2y(0, 1)$ , it follows that equality of the two functions will still hold for  $\alpha$  equal to one. The connection between the two derivatives is made through the Green's function of the operator. We shall first deal with the left-hand side of identity (10), for which we need to differentiate the series defining the spectral zeta function with respect to both  $\alpha$  and  $s$ , and then take  $s = 0$ . We begin by differentiating the series in equation (9) term by term with respect to  $\alpha$  to obtain

$$(11) \quad \frac{\partial}{\partial \alpha} \zeta_{T_\alpha}(s) = -s \sum_{j=1}^{\infty} \frac{\lambda'_j(\alpha)}{\lambda_j^{s+1}(\alpha)},$$

where the expression for the derivative of  $\lambda_j$  with respect to  $\alpha$  is given by

$$\lambda'_j(\alpha) = \left( \int_0^1 V(x)u_j^2(\alpha, x) dx \right) \left( \int_0^1 u_j^2(\alpha, x) dx \right)^{-1}.$$

For potentials in  $L^1[0, 1]$  we have, as we saw above, that the corresponding eigenvalues of problem (8) satisfy the asymptotics given by (6), while the corresponding eigenfunctions satisfy

$$u_j(x) = \sin(j\pi x) + r_j(x),$$

where  $r_j(x) = O(1/j)$  uniformly in  $x$  — see [25, Rem. 2]. We thus have

$$\begin{aligned} \int_0^1 u_j^2(x) \, dx &= \int_0^1 \sin^2(j\pi x) \, dx + 2 \int_0^1 r_j(x) \sin(j\pi x) \, dx + \int_0^1 r_j^2(x) \, dx \\ &= \frac{1}{2} + 2 \int_0^1 r_j(x) \sin(j\pi x) \, dx + \int_0^1 r_j^2(x) \, dx = \frac{1}{2} + O(1/j). \end{aligned}$$

In a similar way, the numerator in the expression for  $\lambda'_j(\alpha)$  satisfies

$$\begin{aligned} \int_0^1 V(x)u_j^2(x) \, dx &= \int_0^1 V(x) \sin^2(j\pi x) \, dx + 2 \int_0^1 V(x)r_j(x) \sin(j\pi x) \, dx + \int_0^1 V(x)r_j^2(x) \, dx \\ &= \frac{1}{2} \int_0^1 V(x) [1 - \cos(2j\pi x)] \, dx + O(1/j) \\ &= \frac{1}{2} \int_0^1 V(x) \, dx - \frac{1}{2} \int_0^1 V(x) \cos(2j\pi x) \, dx + O(1/j) \\ &= \frac{1}{2} \int_0^1 V(x) \, dx + o(1), \end{aligned}$$

where the last step follows from the Riemann-Lebesgue Lemma. Combining the two asymptotics we thus have

$$\lambda'_j(\alpha) = \int_0^1 V(x) \, dx + o(1)$$

and so the term in the series (11) is of order  $O(j^{-2s-2})$ . This series is thus absolutely convergent (and uniformly convergent in  $\alpha$ ) for  $\text{Re}(s) > -1/2$ . This justifies the differentiation term by term, and also makes it possible to now differentiate it with respect to  $s$  to obtain

$$\frac{\partial^2}{\partial s \partial \alpha} \zeta_{T_\alpha}(s) = \sum_{j=1}^\infty [-1 + s \log(\lambda_j(\alpha))] \frac{\lambda'_j(\alpha)}{\lambda_j^{s+1}(\alpha)},$$

which is uniformly convergent for  $s$  in a neighbourhood of zero and  $\alpha$  in  $[0, 1]$ . We thus obtain

$$\left. \frac{\partial}{\partial \alpha} \frac{\partial}{\partial s} \zeta_{T_\alpha}(s) \right|_{s=0} = - \sum_{j=1}^\infty \frac{\lambda'_j(\alpha)}{\lambda_j(\alpha)}$$

and

$$\begin{aligned} \frac{d}{d\alpha} \log [\det T_\alpha] &= \sum_{j=1}^\infty \frac{\lambda'_j(\alpha)}{\lambda_j(\alpha)} = \sum_{j=1}^\infty \lambda_j(\alpha)^{-1} \int_0^1 \frac{u_j(\alpha, x)^2}{\|u_j(\alpha)\|^2} V(t) \, dt \\ &= \int_0^1 \sum_{k=1}^\infty \lambda_k(\alpha)^{-1} \frac{u_k(\alpha, t)}{\|u_k(\alpha)\|} \frac{u_k(\alpha, t)}{\|u_k(\alpha)\|} V(t) \, dt \\ &= \int_0^1 G_\alpha(\lambda = 0, t, t) V(t) \, dt = \text{Tr}(T_\alpha^{-1}V). \end{aligned}$$

Here,  $G_\alpha(\lambda = 0, t, t)$  is the restriction to the diagonal of the Green's function of the boundary value problem (8) at  $\lambda = 0$ . The exchange between the integral and the summation may be justified as above. We will now consider the right-hand side in (10). Here we follow exactly the same computation as in [18]. For that we consider

$$z(\alpha, t) = \frac{\partial y}{\partial \alpha}(\alpha, t).$$

Then  $z(\alpha, t)$  is a solution to the initial value problem:

$$\begin{cases} T_\alpha z(\alpha, t) = -V(t)y(\alpha, t) \\ z(\alpha, 0) = 0, \quad \frac{\partial z}{\partial t}(\alpha, 0) = 0. \end{cases}$$

Using the variation of parameters formula, the solution of this problem is given by

$$z(\alpha, t) = \frac{1}{W} \left[ y(\alpha, t) \int_0^t y(\alpha, r) \tilde{y}(\alpha, r) V(r) dr - \tilde{y}(\alpha, t) \int_0^t y(\alpha, r) y(\alpha, r) V(r) dr \right],$$

where the Wronskian  $W = y(\alpha, t)(\partial \tilde{y} / \partial t)(\alpha, t) - \tilde{y}(\alpha, t)(\partial y / \partial t)(\alpha, t)$  is constant, and  $\tilde{y}(\alpha, t)$  is the solution to the adjoint problem

$$\begin{cases} T_\alpha \tilde{y}(\alpha, t) = 0 \\ \tilde{y}(\alpha, 1) = 0, \quad \frac{\partial \tilde{y}}{\partial t}(\alpha, 1) = 1. \end{cases}$$

Therefore we obtain

$$z(\alpha, 1) = y(\alpha, 1) \frac{1}{W} \int_0^1 y(\alpha, r) \tilde{y}(\alpha, r) V(r) dr = y(\alpha, 1) \int_0^1 G_\alpha(\lambda = 0, r, r) V(r) dr,$$

from which the identity (10) follows. Integrating this with respect to  $\alpha$  yields

$$\det T_\alpha = cy(\alpha, 1),$$

where  $c$  is a constant independent of  $\alpha$ . Since  $\det T_0 = 2y(0, 1)$ , the result follows.  $\square$

We shall finish this section with the example of the pulse potential, of which the optimal potential in the  $L^1$  case is a particular case.

**EXAMPLE 6.** — Let  $S = [x_1, x_2] \subseteq [0, 1]$  and  $m > 0$ . A long but straightforward computation shows that the solution of

$$-y'' + m\chi_S y = 0, \quad y(0) = 0, \quad y'(0) = 1$$

is given by

$$y(t) = \begin{cases} t & t \in [0, x_1] \\ ae^{\sqrt{m}t} + be^{-\sqrt{m}t} & t \in [x_1, x_2], \\ ct + d & t \in [x_2, 1], \end{cases}$$

with

$$\begin{aligned} a &= \frac{1}{2} \left( x_1 + \frac{1}{\sqrt{m}} \right) e^{-\sqrt{m}x_1}, & b &= \frac{1}{2} \left( x_1 - \frac{1}{\sqrt{m}} \right) e^{\sqrt{m}x_1}, \\ c &= \sqrt{m} (ae^{\sqrt{m}x_2} - be^{-\sqrt{m}x_2}), & d &= ae^{\sqrt{m}x_2} (1 - \sqrt{m}x_2) + be^{-\sqrt{m}x_2} (1 + \sqrt{m}x_2). \end{aligned}$$

Therefore the functional determinant of the operator  $T = -d^2/dx^2 + m\chi_S$  with Dirichlet boundary conditions is given by

$$\det(\Delta + m\chi_R) = 2y(1) = e^{-\sqrt{m}x_1} e^{\sqrt{m}x_2} (x_1 + 1/\sqrt{m})(1 + \sqrt{m} - \sqrt{m}x_2) + e^{\sqrt{m}x_1} e^{-\sqrt{m}x_2} (x_1 - 1/\sqrt{m})(1 - \sqrt{m} + \sqrt{m}x_2).$$

2. SOME PROPERTIES OF THE DETERMINANT

Let us denote  $D$  the operator mapping a potential  $V$  in  $L^q[0, 1]$  to  $D_V := y(1)$ , where  $y$  is the solution of

$$-y'' + Vy = 0, \quad y(0) = 0, \quad y'(0) = 1.$$

PROPOSITION 7. — *The operator  $D$  is well-defined, Lipschitz on bounded sets of  $L^q$  (hence continuous), and non-negative for non-negative potentials.*

Proof. — For  $V \in L^q[0, 1]$ , local existence and uniqueness holds by Carathéodory for  $x' = C(V)x$  with

$$(12) \quad C(V) := \begin{bmatrix} 0 & 1 \\ V & 0 \end{bmatrix}, \quad x := (y, y'), \quad x(0) = (0, 1).$$

Gronwall's lemma implies that the solution is defined up to  $t = 1$  and that

$$(13) \quad |x(1)| \leq \exp(1 + \|V\|_1).$$

Let  $V_1$  and  $V_2$  in  $L^q[0, 1]$  be both of norm less or equal to  $A$ . Denote  $x_1$  and  $x_2$  the corresponding solutions defined as in (12). One has

$$x'_1 - x'_2 = (C(V_1) - C(V_2))x_1 + C(V_2)(x_1 - x_2),$$

integrating one obtains

$$|x_1(t) - x_2(t)| \leq \|x_1\|_\infty \|V_1 - V_2\|_1 + \int_0^t |C(V_2(s))| \cdot |x_1(s) - x_2(s)| ds.$$

By the integral version of Gronwall's inequality we obtain

$$\begin{aligned} |x_1(1) - x_2(1)| &\leq \|x_1\|_\infty \|V_1 - V_2\|_1 \exp(1 + \|V_2\|_1) \\ &\leq e^{2(1+A)} \|V_1 - V_2\|_1, \end{aligned}$$

implying that  $D$  is Lipschitz on bounded sets. Let finally  $V$  be non-negative, and assume by contradiction that the associated  $y$  first vanishes at  $\bar{t} > 0$ . As  $y(0) = y(\bar{t}) = 0$  and  $y'(0) > 0$ , the function must have a positive maximum at some  $\tau \in (0, \bar{t})$ . The function  $y$  being continuously differentiable,  $y'(\tau) = 0$ . Now,

$$y'(\tau) = y'(0) + \int_0^\tau y''(t) dt,$$

while  $y'' = Vy \geq 0$  since  $V \geq 0$  and  $y \geq 0$  on  $[0, \tau] \subset [0, \bar{t}]$ . Then  $y'(\tau) \geq 1$ , contradicting the definition of  $\tau$ . □

Being Lipschitz on bounded sets, the operator  $D$  sends Cauchy sequences in  $L^q[0, 1]$  to Cauchy sequences in  $\mathbb{R}$  (Cauchy-continuity). So its restriction to the dense subset of smooth functions has a unique continuous extension to the whole space. As this restriction is equal to the halved determinant whose definition for smooth potentials is recalled in Section 1 for the operator  $-\Delta + V$  with Dirichlet boundary conditions,  $D_V$  is indeed the unique continuous extension of this determinant to  $L^q[0, 1]$  and, in agreement with Theorem 5,

$$D_V = \frac{1}{2} \det T_V.$$

We begin by proving a uniform upper bound on the maximum value of  $y(1)$  for the control problem (5), and thus for the determinant of the original Schrödinger operator given by (3).

**PROPOSITION 8.** — *Assume the potential  $V$  is in  $L^q[0, 1]$ ,  $q \in [1, \infty]$ . Then*

$$|D_V - 1| \leq \sum_{m=1}^{\infty} \frac{\|V\|_1^m}{(m+1)^{m+1}}.$$

*Proof.* — To prove the proposition it is enough to treat the case  $q = 1$ . The initial value problem given by equation (5) is equivalent to the integral equation

$$y(t) = t + \int_0^t (t-s)V(s)y(s) \, ds.$$

We now build a standard iteration scheme defined by

$$(14) \quad \begin{cases} y_{m+1}(t) = t + \int_0^t (t-s)V(s)y_m(s) \, ds, \\ y_0(t) = t, \end{cases}$$

which converges to the solution of equation (5) — this is a classical result from the theory of ordinary differential equations which may be found, for instance, in [8], and which also follows from the computations below.

We shall now prove by induction that

$$(15) \quad |y_m(t) - y_{m-1}(t)| \leq \frac{t^{m+1}}{(m+1)^{m+1}} \left[ \int_0^t |V(s)| \, ds \right]^m.$$

From (14) it follows that

$$y_1(t) - y_0(t) = \int_0^t (t-s)V(s)y_0(s) \, ds,$$

and thus

$$|y_1(t) - y_0(t)| \leq \int_0^t s(t-s)|V(s)| \, ds.$$

If we define the sequence of functions  $f_m$  by

$$f_m(s) = (t-s) \frac{s^{m+1}}{(m+1)^{m+1}},$$

the above may be written as

$$|y_1(t) - y_0(t)| \leq \int_0^t f_0(s)|V(s)| \, ds.$$

Since  $f_0(s) = s(t - s) \leq t^2/4$ , we have that

$$|y_1(t) - y_0(t)| \leq \frac{t^2}{4} \int_0^t |V(s)| \, ds,$$

and thus the induction hypothesis (15) holds for  $m = 1$ . Assume now that (15) holds.

It follows from (14) that

$$\begin{aligned} |y_{m+1}(t) - y_m(t)| &= \left| \int_0^t (t - s)V(s) [y_m(s) - y_{m-1}(s)] \, ds \right| \\ &\leq \int_0^t (t - s) \cdot |V(s)| \cdot |y_m(s) - y_{m-1}(s)| \, ds, \end{aligned}$$

and, using (15), we obtain

$$\begin{aligned} |y_{m+1}(t) - y_m(t)| &\leq \int_0^t (t - s)|V(s)| \frac{s^{m+1}}{(m + 1)^{m+1}} \left[ \int_0^s |V(r)| \, dr \right]^m \, ds \\ &= \int_0^t f_m(s)|V(s)| \left[ \int_0^s |V(r)| \, dr \right]^m \, ds. \end{aligned}$$

Differentiating  $f_m(s)$  with respect to  $s$  and equating to zero, we obtain that this is maximal for  $s = (m + 1)t/(m + 2)$ , yielding

$$f_m(s) \leq \frac{t^{m+2}}{(m + 2)^{m+2}},$$

and so

$$|y_{m+1}(t) - y_m(t)| \leq \frac{t^{m+2}}{(m + 2)^{m+2}} \left[ \int_0^t |V(s)| \, ds \right]^{m+1}$$

as desired. Hence

$$\sum_{m=0}^{\infty} |y_{m+1}(t) - y_m(t)| \leq \sum_{m=0}^{\infty} \frac{t^{m+2}}{(m + 2)^{m+2}} \left[ \int_0^t |V(s)| \, ds \right]^{m+1}.$$

On the other hand,

$$\sum_{m=0}^{\infty} [y_{m+1}(t) - y_m(t)] = -y_0 + \lim_{m \rightarrow \infty} y_m(t) = y(t) - t,$$

yielding

$$|y(t) - t| \leq \sum_{m=0}^{\infty} \frac{t^{m+2}}{(m + 2)^{m+2}} \left[ \int_0^t |V(s)| \, ds \right]^{m+1}.$$

Taking  $t$  to be one finishes the proof. □

We shall finally present a proof of the fact that in order to maximise the determinant it is sufficient to consider non-negative potentials. This is based on a comparison result for linear second order ordinary differential equations which we believe to be interesting in its own right, but which we could not find in the literature.

**PROPOSITION 9.** — Assume  $V$  is in  $L^q[0, T]$ , and let  $u$  and  $v$  be the solutions of the initial value problems defined by

$$\begin{cases} -u''(t) + |V(t)|u(t) = 0 \\ u(0) = 0, \quad u'(0) = 1 \end{cases} \quad \text{and} \quad \begin{cases} -v''(t) + V(t)v(t) = 0 \\ v(0) = 0, \quad v'(0) = 1. \end{cases}$$

Then  $u(t) \geq v(t)$  for all  $0 \leq t \leq T$ .

*Proof.* — The proof is divided into two parts. We first show that if the potential  $V$  does not remain essentially non-negative, then  $u$  must become larger than  $v$  at some point, while never being smaller for smaller times. We then prove that once  $u$  is strictly larger than  $v$  for some time  $t_1$ , then it must remain larger for all  $t$  greater than  $t_1$ .

We first note that solutions of the above problems are at least in  $AC^2[0, T]$ , and thus continuously differentiable on  $[0, T]$ . Furthermore,  $u$  is always positive, since  $u(0) = 0$ ,  $u'(0) = 1$  and  $u''(0) \geq 0$ . Let now  $w = u - v$ . While  $V$  remains essentially non-negative,  $v$  also remains positive and  $w$  vanishes identically. Assume now that there exists a time  $t_0$  such that for  $t$  in  $(0, t_0)$  the potential  $V$  is essentially non-negative and on arbitrarily small positive neighbourhoods of  $t_0$   $V$  takes on negative values on sets of positive measure. Then  $w''(t) = |V(t)|w(t) + [|V(t)| - V(t)]v$  close to  $t_0$  (and zero elsewhere on these small neighbourhoods of  $t_0$ ). Since  $w(t_0) = w'(t_0) = 0$  and  $w''$  is non-negative and strictly positive on sets of positive measure contained in these neighbourhoods,  $w$  will take on positive values on arbitrarily small positive neighbourhoods of  $t_0$ . Define now  $z(t) = (u^2(t) - v^2(t))/2$ . Then

$$z'(t) = u(t)u'(t) - v(t)v'(t),$$

$$\begin{aligned} \text{and} \quad z''(t) &= [u'(t)]^2 + u(t)u''(t) - [v'(t)]^2 - v(t)v''(t) \\ &= [u'(t)]^2 - [v'(t)]^2 + |V(t)|z(t) + [|V(t)| - V(t)]v^2. \end{aligned}$$

From the previous discussion above, we may assume the existence of a positive value  $t_1$  such that both  $z$  and  $z'$  are positive at  $t_1$  (and thus in a small positive neighbourhood  $(t_1, t_1 + \delta)$ ), while  $z$  is non-negative for all  $t$  in  $(0, t_1)$ . Letting

$$a(t) = \frac{[u'(t)]^2 - [v'(t)]^2}{u(t)u'(t) - v(t)v'(t)},$$

which is well-defined and bounded on  $[t_1, t_1 + \delta)$ , we may thus write

$$z''(t) = a(t)z'(t) + |V(t)|z(t) + [|V(t)| - V(t)]v^2 \geq a(t)z'(t),$$

for  $t$  in  $[t_1, t_1 + \delta)$ . Then  $z''(t) - a(t)z'(t) \geq 0$  and upon multiplication by

$$e^{-\int_{t_1}^t a(s)ds}$$

and integration between  $t_1$  and  $t$  we obtain

$$z'(t) \geq e^{\int_{t_1}^t a(s)ds} z'(t_1).$$

This yields the positivity of  $z'(t)$  (and thus of  $z(t)$ ) for  $t$  greater than  $t_1$ . Combining this with the first part of the proof shows that  $z$  is never negative for positive  $t$ .  $\square$

Henceforth, we restrict the search for maximising potentials to non-negative functions. Besides, it is clear from the proof that the result may be generalised to the comparison of two potentials  $V_1$  and  $V_2$  where  $V_1 \geq V_2$ , provided  $V_1$  is non-negative.

### 3. MAXIMIZATION OF THE DETERMINANT OVER $L^1$ POTENTIALS

By virtue of the analysis of the previous sections, problem (4) for  $q = 1$  can be recast as the following optimal control problem:

$$(16) \quad y(1) \longrightarrow \max,$$

$$(17) \quad -y'' + Vy = 0, \quad y(0) = 0, \quad y'(0) = 1,$$

over all non-negative potentials  $V \geq 0$  in  $L^1[0, 1]$  such that

$$(18) \quad \int_0^1 V(t) dt \leq A$$

for fixed positive  $A$ . In order to prove Theorem A, a family of auxiliary problems is introduced: in addition to (17), the potentials are assumed essentially bounded and such that

$$(19) \quad 0 \leq V(t) \leq B, \quad \text{a.a. } t \in [0, 1],$$

for a fixed positive  $B$ . To avoid the trivial solution  $V \equiv B$ , we suppose  $B > A$  and henceforth study the properties of problem (16)–(19).

Setting  $x := (y, y', x_3)$ , the auxiliary problem can be rewritten  $-x_1(1) \rightarrow \min$  under the dynamical constraints

$$(20) \quad x'_1 = x_2,$$

$$(21) \quad x'_2 = Vx_1,$$

$$(22) \quad x'_3 = V,$$

$V$  measurable valued in  $[0, B]$ , and the boundary conditions  $x(0) = (0, 1, 0)$ , free  $x_1(1)$  and  $x_2(1), x_3(1) \leq A$ .

**PROPOSITION 10.** — *Every auxiliary problem has a solution.*

*Proof.* — The set of admissible controls is obviously nonempty, the control is valued in a fixed compact set, and the field of velocities

$$\{(x_2, Vx_1, V), V \in [0, B]\} \subset \mathbb{R}^3$$

is convex for any  $x \in \mathbb{R}^3$ ; according to Filippov Theorem [1], existence holds. □

Let  $V$  be a maximising potential for (16)–(19), and let  $x = (y, y', x_3)$  be the associated trajectory. According to Pontryagin maximum principle [1], there exists a nontrivial pair  $(p^0, p) \neq (0, 0)$ ,  $p^0 \leq 0$  a constant and  $p : [0, 1] \rightarrow (\mathbb{R}^3)^*$  a Lipschitz covector function such that, a.e. on  $[0, 1]$ ,

$$(23) \quad x' = \frac{\partial H}{\partial p}(x, V, p), \quad p' = -\frac{\partial H}{\partial x}(x, V, p),$$



and

$$(24) \quad H(x(t), V(t), p(t)) = \max_{v \in [0, B]} H(x(t), v, p(t)),$$

where  $H$  is the Hamiltonian function

$$H(x, V, p) := pf(x, V) = p_1x_2 + (p_2x_1 + p_3)V.$$

(There  $f(x, V)$  denotes the dynamics (20)–(22) in compact form.) Moreover, in addition to the boundary conditions on  $x$ , the following transversality conditions hold:  $p_1(1) = -p^0$ ,  $p_2(1) = 0$ , and  $p_3(1) \leq 0$  with complementarity

$$(x_3(1) - A)p_3(1) = 0.$$

As is clear from (23),  $p_3$  is constant,  $p'_1 = -p_2$  and

$$(25) \quad -p''_2 + Vp_2 = 0.$$

The dynamical system (20)–(22) is bilinear in  $x$  and  $V$ ,

$$x' = F_0(x) + VF_1(x), \quad F_0(x) = \begin{bmatrix} x_2 \\ 0 \\ 0 \end{bmatrix}, \quad F_1(x) = \begin{bmatrix} 0 \\ x_1 \\ 1 \end{bmatrix},$$

so

$$H = H_0 + VH_1 \quad \text{with} \quad H_0(x, p) = pF_0(x), \quad H_1(x, p) = pF_1(x).$$

Let  $\Phi(t) := H_1(x(t), p(t))$  be the evaluation of  $H_1$  along the extremal  $(x, V, p)$ ; it is a Lipschitz function, and the maximisation condition (24) implies that  $V(t) = 0$  when  $\Phi(t) < 0$ ,  $V(t) = B$  when  $\Phi(t) > 0$ . If  $\Phi$  vanishes identically on some interval of nonempty interior, the control is not directly determined by (24) and is termed *singular*. Subarcs of the trajectory corresponding to  $V = 0$ ,  $V = B$  and singular control, are labelled  $\gamma_0$ ,  $\gamma_+$  and  $\gamma_s$ , respectively. Differentiating once, one obtains  $\Phi'(t) = H_{01}(x(t), p(t))$ , where  $H_{01} = \{H_0, H_1\}$  is the Poisson bracket of  $H_0$  and  $H_1$ ;  $\Phi$  is so  $W^{2, \infty}$  and, differentiating again,

$$(26) \quad \Phi'' = H_{001} + VH_{101}$$

with length-three brackets  $H_{001} = \{H_0, H_{01}\}$ ,  $H_{101} = \{H_1, H_{01}\}$ . Computing,

$$H_{01} = -p_1x_1 + p_2x_2, \quad H_{001} = -2p_1x_2, \quad H_{101} = 2p_2x_1.$$

In particular, using the definition of  $H$ ,

$$(27) \quad \Phi'' - 4V\Phi = -2(H + p_3V), \quad \text{a.a. } t \in [0, 1],$$

where  $H$  and  $p_3$  are constant along any extremal.

There are two possibilities for extremals depending on whether  $p'_2(1) = p^0$  is zero or not (so-called abnormal or normal cases).

LEMMA 11. — *The cost multiplier  $p^0$  is negative and one can set  $p'_2(1) = -1$ .*

*Proof.* — Suppose by contradiction that  $p^0 = 0$ . Then  $p_2(1) = p'_2(1) = 0$ , so (25) implies that  $p_2$  (and  $p_1$ ) are identically zero. Since  $(p^0, p) \neq (0, 0)$ ,  $p_3$  must be negative so  $\Phi = p_2x_1 + p_3 = p_3 < 0$  and  $V$  is identically zero on  $[0, 1]$ , which is impossible (the zero control is admissible but readily not optimal). Hence  $p^0$  is negative, and one can choose  $p^0 = -1$  by homogeneity in  $(p^0, p)$ .  $\square$

LEMMA 12. — *The constraint  $\int_0^1 V dt \leq A$  is strongly active ( $p_3 < 0$ ).*

*Proof.* — Assume by contradiction that  $p_3 = 0$ . Since  $-x''_1 + Vx_1 = 0$  with  $x_1(0) = 0$ ,  $x'_1(0) = 1$  and  $V \geq 0$ ,  $x_1$  is non-negative on  $[0, 1]$  (see Proposition 7). Integrating, one has  $x_1(t) \geq t$  on  $[0, 1]$ . Symmetrically,  $-p''_2 + Vp_2 = 0$  with  $p_2(1) = 0$ ,  $p'_2(1) = -1$ , so one gets that  $p_2(t) \geq 1 - t$  on  $[0, 1]$ . Now,  $p_3 = 0$  implies  $\Phi = p_2x_1 \geq t(1 - t)$ , so  $\Phi > 0$  on  $(0, 1)$ :  $V = B$  a.e., which is impossible since  $B > A$ .  $\square$

As a result, since  $\Phi(0) = \Phi(1) = p_3$ ,  $\Phi$  is negative in the neighbourhood of  $t = 0+$  and  $t = 1-$ , so an optimal trajectory starts and terminates with  $\gamma_0$  arcs.

LEMMA 13. — *There is no interior  $\gamma_0$  arc.*

*Proof.* — If such an interior arc existed, there would exist  $\bar{t} \in (0, 1)$  such that  $\Phi(\bar{t}) = 0$  and  $\Phi'(\bar{t}) \leq 0$  ( $\Phi'(\bar{t}) > 0$  would imply  $\Phi > 0$  in the neighbourhood of  $\bar{t}+$ , contradicting  $V = 0$ ); but then  $\Phi'' = -2H < 0$  for  $t \geq \bar{t}$  would result in  $\Phi < 0$  for  $t > \bar{t}$ , preventing  $\Phi$  for vanishing again before  $t = 1$ .  $\square$

LEMMA 14. — *If  $H + p_3B < 0$ , there is no interior  $\gamma_+$  arc.*

*Proof.* — By contradiction again: there would exist  $\bar{t} \in (0, 1)$  such that  $\Phi(\bar{t}) = 0$  and  $\Phi'(\bar{t}) \geq 0$  ( $\Phi'(\bar{t}) < 0$  would imply  $\Phi < 0$  in the neighbourhood of  $\bar{t}+$ , contradicting  $V = B$ ); along  $\gamma_+$ ,

$$\Phi'' - 4B\Phi = -2(H + p_3B) > 0,$$

so

$$(28) \quad \Phi = \frac{H + p_3B}{2B} (1 - \text{ch}(2\sqrt{B}(t - \bar{t}))) + \frac{\Phi'(\bar{t})}{2\sqrt{B}} \text{sh}(2\sqrt{B}(t - \bar{t})),$$

and  $\Phi > 0$  if  $t > \bar{t}$ , preventing  $\Phi$  for vanishing again before  $t = 1$ .  $\square$

Along a singular arc,  $\Phi \equiv 0$  so (26) allows to determine the singular control provided  $H_{101} \neq 0$  (“order one” singular). A necessary condition for optimality (the Legendre-Clebsch condition) is that  $H_{101} \geq 0$  along such an arc; order one singular arcs such that  $H_{101} > 0$  are called *hyperbolic* [4].

LEMMA 15. — *Singulars are of order one and hyperbolic; the singular control is constant and equal to  $-H/p_3$ .*

*Proof.* —  $\Phi = p_2x_1 + p_3 \equiv 0$  implies  $H_{101} = 2p_2x_1 = -2p_3 > 0$ , so any singular is of order one and hyperbolic; (27) then tells  $H + p_3V = 0$ , hence the expression of the singular control.  $\square$

PROPOSITION 16. — *A maximising potential is piecewise constant.*

*Proof.* — According to the maximum principle, the trajectory associated with an optimal potential is the concatenation of (possibly infinitely many)  $\gamma_0$ ,  $\gamma_+$  and  $\gamma_s$  subarcs. By Lemma 13, there are exactly two  $\gamma_0$  arcs; if  $V$  has an infinite number of discontinuities, it is necessarily due to the presence of infinitely many switchings between  $\gamma_+$  and  $\gamma_s$  subarcs with  $H + p_3B < 0$  (this quantity must be nonpositive to ensure admissibility of the singular potential,  $V = -H/p_3 \leq B$ , and even negative since otherwise  $\gamma_+$  and  $\gamma_s$  would be identical, generating no discontinuity at all). By Lemma 14, there is no  $\gamma_+$  subarc if  $H + p_3B < 0$ . There are thus only finitely many switchings of the potential between the constant values 0,  $B$  and  $-H/p_3$ .  $\square$

**COROLLARY 17.** — *An optimal trajectory is either of the form  $\gamma_0\gamma_+\gamma_0$ , or  $\gamma_0\gamma_s\gamma_0$ .*

*Proof.* — There is necessarily some minimum  $\bar{t} \in (0, 1)$  such that  $\Phi(\bar{t}) = 0$  (otherwise  $V \equiv 0$  which would contradict the existence of solution). There are two cases, depending on the order of the contact of the extremal with  $H_1 = 0$ .

(i)  $\Phi'(\bar{t}) \neq 0$  (“regular switch” case). Having started with  $\Phi(0) = p_3 < 0$ , necessarily  $\Phi'(\bar{t}) > 0$  and there is a switch from  $V = 0$  to  $V = B$  at  $\bar{t}$ . According to Lemma 14, this is only possible if  $H + p_3B \geq 0$ . Along  $\gamma_+$ ,  $\Phi$  is given by (28) and vanishes again at some  $\tilde{t} \in (\bar{t}, 1)$  as the trajectory terminates with a  $\gamma_0$  subarc. Since  $H + p_3B \geq 0$  and  $\Phi'(\tilde{t}) < 0$ ,  $\Phi'(\tilde{t})$  is necessarily negative, so  $\Phi < 0$  for  $t > \tilde{t}$  and the structure is  $\gamma_0\gamma_+\gamma_0$ .

(ii)  $\Phi'(\bar{t}) = 0$ . The potential being piecewise continuous,  $\Phi''$  has left and right limits at  $\bar{t}$  (see (26)). Having started with  $V = 0$ ,  $\Phi''(\bar{t}-) = -2H$  is negative; assume the contact is of order two, that is  $\Phi''(\bar{t}+) \neq 0$  (“fold” case, [4]). Clearly,  $\Phi''(\bar{t}+) < 0$  is impossible as it would imply  $\Phi < 0$  for  $t > \bar{t}$  (and hence  $V \equiv 0$  on  $[0, 1]$ ). So  $\Phi''(\bar{t}+) > 0$  (“hyperbolic fold”, *ibid.*), and there is a switching from  $V = 0$  to  $V = B$ . Along  $\gamma_+$ ,

$$\Phi = \frac{H + p_3B}{2B} (1 - \text{ch}(2\sqrt{B}(t - \bar{t})))$$

by (28) again, and  $H + p_3B$  must be negative for  $\Phi''(\bar{t}+) > 0$  to hold. Then  $\Phi > 0$  for  $t > \bar{t}$ , which contradicts the termination by a  $\gamma_0$  subarc. So  $\Phi''(\bar{t}+) = 0$ , that is  $V$  jumps from 0 to singular,  $V = -H/p_3$ , at  $\bar{t}$ . As it must be admissible,  $H + p_3B \leq 0$ . If  $H + p_3B = 0$ , the singular control is saturating,  $V = B$ , and  $\gamma_+$  and  $\gamma_s$  arcs are identical; there cannot be interior  $\gamma_0$  (Lemma 13), so the structure is  $\gamma_0\gamma_s\gamma_0$  ( $= \gamma_0\gamma_+\gamma_0$ , in this case). Otherwise,  $H + p_3B < 0$  and Lemma 14 asserts that  $\gamma_s\gamma_+$  connections are not possible: The structure is also  $\gamma_0\gamma_s\gamma_0$ .  $\square$

*Proof of Theorem A.* — The proof is done in three steps: first, existence and uniqueness are obtained for each auxiliary problem (17)–(19) with bound  $V \leq B$  on the potential,  $B$  large enough; then existence for the original problem (16)–(19) with unbounded control is proved. Finally, uniqueness is obtained.

(i) As a result of Corollary 17, each auxiliary problem can be reduced to the following finite dimensional question: given  $B > A > 0$ , maximise  $y(1) = y(s, \ell)$  with respect to  $s \in [0, 1]$ ,  $\ell \leq 2 \min\{s, 1 - s\}$  and  $\ell \geq A/B$ , where  $y(s, \ell)$  is the value at

$t = 1$  of the solution of (17) generated by the potential equal to the characteristic function of the interval  $[s - \ell/2, s + \ell/2]$  times  $A/\ell$  (the constraint (18) is active by virtue of Lemma 12). Computing,

$$y(s, \ell) = (1 - \ell) \operatorname{ch} \sqrt{A\ell} + A[(s - s^2) + (1/A - 1/2)\ell + \ell^2/4] \operatorname{shc} \sqrt{A\ell},$$

where  $\operatorname{shc}(z) := (1/z) \operatorname{sh} z$ . The function to be maximised is continuous on the compact triangle defining the constraints on  $(s, \ell)$ , so one retrieves existence. As we know that an optimal arc must start and end with  $\gamma_0$  arcs, the solution cannot belong to the part of the boundary corresponding to  $\ell = 2 \min\{s, 1 - s\}$ , extremities included; as a result,  $\partial y/\partial s$  must be zero at a solution, so  $s = 1/2$  (potential symmetric with respect to  $t = 1/2$ ). Since one has  $y(s = 1/2, \ell) = (1 + A/4) + A^2\ell/24 + o(\ell)$ , too small a  $\ell$  cannot maximise the function; so, for  $B$  large enough, the point on the boundary  $\ell = A/B$  cannot be solution, and one also has that

$$\frac{\partial y}{\partial \ell}(s, \ell)|_{s=1/2} = \frac{(A(\ell - 1)^2 - 4\ell)(\operatorname{ch} \sqrt{A\ell} - \operatorname{shc} \sqrt{A\ell})}{8\ell}$$

must vanish. As  $\ell < 1$ , one gets  $\ell = \ell(A) := A/(1 + \sqrt{1 + A})^2$ , hence the expected value for the maximum determinant.

(ii) The mapping  $V \mapsto -y(1)$  is continuous on  $L^1[0, 1]$  by Proposition 7. Let  $C := \{V \in L^1[0, 1] \mid \|V\|_1 \leq A, V \geq 0 \text{ a.e.}\}$ ; it is closed and nonempty. For  $k \in \mathbb{N}$ ,  $k > A$  ( $A > 0$  fixed), consider the sequence of auxiliary problems with essential bounds  $V \leq k$ . For  $k$  large enough, the solution does not depend on  $k$  according to point (i), hence the stationarity of the sequence of solutions to the auxiliary problems. The sequence of subsets  $C \cap \{V \in L^\infty[0, 1] \mid \|V\|_\infty \leq B_k\}$  is increasing and dense in  $C$ , so the lemma below ensures existence for the original problem.

LEMMA 18. — *Let  $f : E \rightarrow \mathbb{R}$  be continuous on a normed space  $E$ , and consider*

$$f(x) \longrightarrow \min, \quad x \in C \text{ nonempty closed subset of } E.$$

*Assume that there exists an increasing sequence  $(C_k)_k$  of subsets of  $C$  such that*

- (i)  $\bigcup_k C_k$  is dense in  $C$ ,
- (ii) for each  $k \in \mathbb{N}$ , there is a minimiser  $x_k$  of  $f$  in  $C_k$ .

*Then, if  $(x_k)_k$  is stationary,  $\lim_{k \rightarrow \infty} x_k$  is a minimiser of  $f$  on  $E$ .*

*Proof.* — Let  $\bar{x}$  be the limit of the stationary sequence  $(x_k)_k$ ; assume, by contradiction, that  $\bar{f} := f(\bar{x}) > \inf_C f$  (including the case  $\inf_C f = -\infty$ ). Then there is  $y \in C$  such that  $f(y) < \bar{f}$ . By density, there is  $k \in \mathbb{N}$  and  $y_k \in C_k$  such that  $\|y - y_k\| \leq \varepsilon$  where, by continuity of  $f$  at  $y$ ,  $\varepsilon > 0$  is chosen such that

$$\|x - y\| \leq \varepsilon \implies |f(x) - f(y)| \leq d/2 \quad (d := \bar{f} - f(y) > 0);$$

then  $f(y_k) \leq f(y) + d/2 < \bar{f}$ , which is contradictory as  $k$  can be taken large enough in order that  $x_k = \bar{x}$ . So  $f(\bar{x}) = \inf_C f$ , whence existence. □

*End of proof of Theorem A*

(iii) The Pontryagin maximum principle can be applied to (16)–(18) with an optimal potential  $V$  in  $L^1[0, 1]$  since the function  $f(x, V)$  defining the dynamics (20)–(22) has a partial derivative uniformly (with respect to  $x$ ) dominated by an integrable function (see [7, §4.2.C, Rem. 5]):

$$\left| \frac{\partial f}{\partial x}(x, V(t)) \right| \leq 1 + |V(t)|, \quad \text{a.a. } t \in [0, 1].$$

The Hamiltonian is unchanged, but the constraint on the potential is now just  $V \geq 0$ ; as a consequence,  $\Phi = p_2x_1 + p_3$  must be nonpositive because of the maximisation condition. Normality is proved as in Lemma 11 and  $p_2(1)$  can be set to  $-1$ . Regarding strong activation of the  $L^1$  constraint ( $p_3 < 0$ ) the argument at the beginning of the proof of Lemma 12 immediately implies that  $p_3$  must be negative as  $\Phi$  cannot be positive, now. So  $\Phi(0) = \Phi(1) = p_3 < 0$  and  $V$  is equal to 0 in the neighbourhood of  $t = 0+$  and  $t = 1-$ . Because existence holds,  $\Phi$  must first vanish at some  $\bar{t} \in (0, 1)$  (otherwise  $V \equiv 0$  which is obviously not optimal); necessarily,  $\Phi'(\bar{t}) = 0$ . One verifies as before that there cannot be interior  $\gamma_0$  subarcs, which prevents accumulation of  $\gamma_0\gamma_s$  or  $\gamma_s\gamma_0$  switchings. In particular,  $V$  must be piecewise constant and the right limit  $\Phi''(\bar{t}+)$  exists. The same kind of reasoning as in the proof of Corollary 17 rules out the fold case  $\Phi''(\bar{t}+)$  nonzero; so  $\Phi''(\bar{t}+) = 0$  and  $V$  switches from 0 to singular at  $\bar{t}$ . The impossibility of interior  $\gamma_0$  subarcs implies a  $\gamma_0\gamma_s\gamma_0$  structure, which is the solution obtained before.  $\square$

**REMARK 19.** — This proves in particular that the generalised “impulsive” potential equal to  $A$  times the Dirac mass at  $t = 1/2$  is not optimal, whatever  $A > 0$ , the combination  $\gamma_0\gamma_s\gamma_0$  giving a better cost. More precisely, the optimal value of the determinant is  $1 + A/4 + A^3/192 + o(A^3)$ , so it is asymptotic when  $A$  tends to zero to the value obtained for the Dirac mass (equal to  $1 + A/4$ , as is clear from (i) in the proof above).

#### 4. MAXIMIZATION OF THE DETERMINANT OVER $L^q$ POTENTIALS, $q > 1$

We begin the section by proving that maximising the determinant over  $L^1$  potentials is estimated by maximising the determinant over  $L^q$ , letting  $q$  tend to one. To this end, we first establish the following existence result. (Note that the proof is completely different from the existence proof in Theorem A.) Let  $A > 0$ , and consider the following family of problems for  $q$  in  $[1, \infty]$ :

$$(29) \quad D_V = \frac{1}{2} \det(-\Delta + V) \longrightarrow \max, \quad \|V\|_q \leq A.$$

**PROPOSITION 20.** — *Existence holds for  $q \in [1, \infty]$ .*

*Proof.* — The case  $q = \infty$  is obvious, while Theorem A deals with  $q = 1$ . Let then  $q$  belong to  $(1, \infty)$ . By using Gronwall lemma as in (13), it is clear that  $D$  is bounded on the closed ball of radius  $A$  of  $L^q[0, 1]$ . So the value of the problem is finite. Let  $(V_k)_k$  be a maximising sequence. As  $\|V_k\|_q \leq A$  for any  $k$ , up to taking a subsequence one

can assume the sequence to be weakly- $*$  converging in  $L^q \simeq (L^r)^*$  ( $1/q + 1/r = 1$ ) towards some  $\bar{V}$ . Clearly,  $\|\bar{V}\|_q \leq A$ . Let  $x_k$  be associated with  $V_k$  according to (12). The sequence  $(x_k)_k$  so defined is bounded and equicontinuous as, for any  $t \leq s$  in  $[0, 1]$ ,

$$\begin{aligned} |x_k(t) - x_k(s)| &\leq \int_t^s |C(V_k(\tau))| \cdot |x_k(\tau)| \, d\tau \\ &\leq \|x_k\|_\infty \|1 + |V_k|\|_q |t - s|^{1/r} \\ &\leq e^{1+A}(1 + A)|t - s|^{1/r} \end{aligned}$$

by Hölder inequality. Using Ascoli's Theorem (and taking a subsequence),  $(x_k)_k$  converges uniformly towards some  $\bar{x}$ . As  $\bar{x}(1) = \lim_k x_k(1)$  is equal to the value of the problem, it suffices to check that  $\bar{x}' = C(\bar{V})\bar{x}$  to conclude. Being a bounded sequence,  $(C(V_k))_k$  is equicontinuous in  $L^q \simeq (L^r)^*$ , and  $(x_k \cdot \chi_{[0,t]})_k$  converges towards  $\bar{x} \cdot \chi_{[0,t]}$  in  $L^r$  for any  $t$  in  $[0, 1]$  ( $\chi_{[0,t]}$  denoting the characteristic function of the interval  $[0, t]$ ). So

$$\begin{aligned} \bar{x}(t) &= \bar{x}(0) + \lim_k \int_0^t C(V_k(\tau))x_k(\tau) \, d\tau \\ &= \bar{x}(0) + \int_0^t C(\bar{V}(\tau))\bar{x}(\tau) \, d\tau, \quad t \in [0, 1], \end{aligned}$$

which concludes the proof. □

**REMARK 21.** — The same proof also gives existence for the minimisation problem in  $L^q[0, 1]$ ,  $q \in (1, \infty)$ .

**PROPOSITION 22.** — *For a fixed  $A > 0$ , the value function*

$$v_q := \sup_{\|V\|_q \leq A} D_V, \quad q \in [1, \infty],$$

*is decreasing and  $v_q$  tends to  $v_1$  when  $q \rightarrow 1+$ .*

*Proof.* — Let  $1 \leq q \leq r \leq \infty$ . For  $V$  in  $L^r[0, 1] \subset L^q[0, 1]$ ,  $\|V\|_q \leq \|V\|_r$  so the radius  $A$  ball of  $L^r$  is included in the radius  $A$  ball of  $L^q$ . As a result of the inclusion of the admissible potentials,  $v_q \geq v_r$ . Because of monotonicity, the limit  $\bar{v} := \lim_{q \rightarrow 1+} v_q$  exists, and  $\bar{v} \leq v_1$ . Moreover, as proved in Theorem A, the unique maximising potential  $V_1$  for  $q = 1$  is actually essentially bounded so

$$D(A \cdot V_1 / \|V_1\|_q) \leq v_q$$

for any  $q \geq 1$ . By continuity of  $D$  on  $L^1$ , the left-hand side of the previous inequality tends to  $D_{V_1} = v_1$  when  $q \rightarrow 1+$ , and one conversely gets that  $v_1 \leq \bar{v}$ . □

Fix  $q > 1$  and  $A > 0$ . As in Section 3, we set  $x := (y, y', x_3)$  to take into account the  $L^q$  constraint. Then problem (29) can be rewritten  $-x_1(1) \rightarrow \min$  under the dynamical constraints

$$(30) \quad x'_1 = x_2,$$

$$(31) \quad x'_2 = Vx_1,$$

$$(32) \quad x'_3 = V^q,$$

and the boundary conditions  $x(0) = (0, 1, 0)$ , free  $x_1(1)$  and  $x_2(1)$ ,  $x_3(1) \leq A^q$ . The potential is measurable and can be assumed non-negative thanks to the comparison result from Proposition 9. For such an  $L^q$  optimal potential  $V$ , the Pontryagin maximum principle holds for the same reason as in the proof of Theorem A (see step (iii)). So there exists a nontrivial pair  $(p^0, p) \neq (0, 0)$ ,  $p^0 \leq 0$  a constant and  $p : [0, 1] \rightarrow (\mathbb{R}^3)^*$  a Lipschitz covector function such that, a.e. on  $[0, 1]$ ,

$$x' = \frac{\partial H}{\partial p}(x, V, p), \quad p' = -\frac{\partial H}{\partial x}(x, V, p),$$

and

$$H(x(t), V(t), p(t)) = \max_{v > 0} H(x(t), v, p(t))$$

where the Hamiltonian  $H$  is now equal to

$$\begin{aligned} H(x, V, p) &:= pf(x, V) \\ &= p_1 x_2 + p_2 x_1 V + p_3 V^q. \end{aligned}$$

(With  $f(x, V)$  denoting the dynamics (30)–(32) in compact form.) In addition to the boundary conditions on  $x$ , the following transversality conditions hold (note that  $p_3$  is again a constant):  $p_1(1) = -p^0$ ,  $p_2(1) = 0$ , and  $p_3 \leq 0$  with complementarity

$$(x_3(1) - A^q) p_3 = 0.$$

Although the system is not bilinear in  $(x, V)$  anymore, the adjoint equation

$$(33) \quad -p_2'' + V p_2 = 0$$

holds unchanged, and one proves normality and strong activation of the  $L^q$  constraint similarly to the case  $q = 1$ .

LEMMA 23. — *The cost multiplier  $p^0$  is negative.*

*Proof.* — By contradiction: if  $p^0 = 0$ , one has  $p_2$  (and  $p_1$ ) identically zero by (33), so  $p_3$  cannot also be zero and must be negative. Then,  $H = p_3 V^q$  and the maximisation condition implies  $V = 0$  a.e. since  $V$  is non-negative. This is contradictory as the zero control is admissible but clearly not optimal.  $\square$

We will not set  $p^0 = -1$  but will use the fact that  $p_3$  is also negative to use a different normalisation instead.

LEMMA 24. — *The constraint  $\int_0^1 V^q dt \leq A^q$  is strongly active ( $p_3 < 0$ ).*

*Proof.* — Observe that, as in Lemma 12,  $p_2 x_1$  is positive on  $(0, 1)$ . Now, assume by contradiction that  $p_3 = 0$ : then  $H = p_1 x_2 + p_2 x_1 V$ , which would prevent maximisation of  $H$  on a nonzero measure subset.  $\square$

Define  $\Psi := p_2 x_1$ . As we have just noticed, it is positive on  $(0, 1)$ , and  $\Psi(0) = \Psi(1) = 0$  because of the boundary and transversality conditions ( $x_1(0) = 0$  and  $p_2(1) = 0$ , respectively).

PROPOSITION 25. — *One has*

$$\begin{aligned} \Psi'' - |\Psi|^\alpha + 2H &= 0, \quad \alpha = q/(q-1), \\ \Psi(0) &= 0, \quad \Psi(1) = 0, \end{aligned}$$

and

$$(34) \quad V = \frac{q}{4q-2} {}^{q-1}\sqrt{\Psi}.$$

*Proof.* — Because  $\Psi$  is non-negative, it is clear from the maximisation condition that

$$V(t) = {}^{q-1}\sqrt{\frac{\Psi(t)}{-qp_3}}$$

for all  $t \in (0, 1)$ . Since  $\Psi$  is an absolutely continuous function, we can differentiate once to get

$$\Psi' = -p_1x_1 + p_2x_2,$$

and iterate to obtain

$$\Psi'' = 2(p_2x_1V - p_1x_2) = 2(V\Psi - p_1x_2).$$

Using the fact that the Hamiltonian  $H$  is constant along an extremal, and substituting  $p_1x_2$  by  $H - V\Psi - p_3V^q$  and  $V$  by its expression, the following second order differential equation is obtained for  $\Psi$ :

$$\Psi'' - \frac{B_q}{{}^{q-1}\sqrt{-p_3}} |\Psi|^{q/(q-1)} + 2H = 0$$

with

$$B_q = \frac{4}{q^{1/(q-1)}} - \frac{2}{q^{q/(q-1)}}.$$

We can normalise  $p_3$  in order that  $-p_3 = B_q^{-1}$ , which gives the desired differential equation for  $\Psi$ , as well as the desired expression for  $V$ . □

COROLLARY 26. — *The function  $\Psi$  (and so  $V$ ) is symmetric with respect to  $t = 1/2$ , and  $\Psi'(0) = H - c(A, q)$  with*

$$c(A, q) = \frac{1}{2} \left( \frac{A(4q-2)}{q} \right)^q.$$

*Proof.* — As a result of the previous proposition, the quantity

$$\frac{1}{2}\Psi'^2 - \frac{1}{\alpha+1} \Psi |\Psi|^\alpha + 2H\Psi$$

is constant. In particular,  $\Psi(0) = \Psi(1) = 0$  implies that  $\Psi'^2(0) = \Psi'^2(1)$ . Now,  $\Psi'(0) = p_2(0) > 0$  and  $\Psi'(1) = -x_1(1) < 0$  (same estimates as in Lemma 12), so  $\Psi'(1) = -\Psi'(0)$ . Setting  $\widehat{\Psi}(t) := \Psi(1-t)$ , one then checks that both  $\Psi$  and  $\widehat{\Psi}$  satisfy the same differential equation, with the same initial conditions:  $\widehat{\Psi} = \Psi$  and symmetry holds. Finally, since the  $L^q$  constraint is active (Lemma 24),

$$A^q = \int_0^1 |V|^q dt = \left( \frac{q}{4q-2} \right)^q \int_0^1 |\Psi|^\alpha dt,$$



and one can replace  $|\Psi|^\alpha$  by  $\Psi'' + 2H$  to integrate and obtain

$$\Psi'(1) - \Psi'(0) + 2H = \left(\frac{A(4q-2)}{q}\right)^q.$$

Hence the conclusion using  $\Psi'(0) - \Psi'(1) = 2\Psi'(0)$ .  $\square$

According to what has just been proved,  $t \mapsto (\Psi(t), \Psi'(t))$  parametrises the curve  $y^2 = f(x)$  where  $f$  (that depends on  $H$ ,  $A$  and  $q$ ) is

$$(35) \quad f(x) = \frac{2}{\alpha+1}x|x|^\alpha - 4Hx + (H - c(A, q))^2 \quad (\alpha = q/(q-1)).$$

Since  $\Psi'(0) = H - c(A, q)$  is positive,  $H > c(A, q) > 0$  and  $f$  has a local minimum (resp. maximum) at  $x = \sqrt[\alpha]{2H}$  (resp.  $-\sqrt[\alpha]{2H}$ ).

LEMMA 27. — *On  $(c(A, q), \infty)$ , there exists a unique  $H$ , denoted  $h(A, q)$ , such that  $\sqrt[\alpha]{2H}$  is a double root of  $f$ .*

*Proof.* — Evaluating,

$$f(\sqrt[\alpha]{2H}) = (H - c(A, q))^2 - \frac{2\alpha}{\alpha+1}(2H)^{1+1/\alpha} =: g(H).$$

As  $g(c(A, q)) < 0$  and  $g(H) \rightarrow \infty$  when  $H \rightarrow \infty$  (note that  $1 + 1/\alpha < 2$ ),  $g$  has one zero in  $(c(A, q), \infty)$ , and only one in this interval as is clear inspecting  $g''$ .  $\square$

PROPOSITION 28. — *The value  $H$  of the Hamiltonian must belong to the nonempty open interval  $(c(A, q), h(A, q))$ .*

*Proof.* — As a result of the previous lemma, for  $H > c(A, q)$  there are three possibilities for the curve  $y^2 = f(x)$  parametrised by  $(\Psi, \Psi')$  depending on whether (i)  $H$  belongs to  $(c(A, q), h(A, q))$ , (ii)  $H = h(A, q)$ , (iii)  $H > h(A, q)$ . As is clear from Figure 1, given the boundary conditions  $\Psi(0) = \Psi(1) = 0$ ,  $\Psi'(0) > 0$  and  $\Psi'(1) < 0$ , case (iii) is excluded. Now, in case (ii), the point  $(\sqrt[\alpha]{2h(A, q)}, 0)$  is a saddle equilibrium point, which prevents connexions between  $(\Psi, \Psi') = (0, h(A, q) - c(A, q))$  and  $(0, c(A, q) - h(A, q))$ .  $\square$

COROLLARY 29. — *The function  $\psi$  (and so  $V$ ) is strictly increasing on  $[0, 1/2]$ .*

*Proof.* — The derivative of  $\psi$  is strictly positive for  $t$  in  $(0, 1/2)$  as is clear from Figure 1, case (i). As a consequence,  $\psi$  is strictly increasing on  $[0, 1/2]$ , and so is  $V$  by virtue of (34).  $\square$

*Proof of Theorem B.* — Let  $q > 1$  and  $A > 0$  be given. Optimal potentials exist by Proposition 20. Such an optimal potential must be given by  $\Psi$  according to Proposition 25. By virtue of Proposition 28, this function  $\Psi$  is obtained as the solution  $\Psi(\cdot, H)$  of

$$(36) \quad \Psi'' - |\Psi|^\alpha + 2H = 0, \quad \Psi(0) = 0, \quad \Psi'(0) = H - c(A, q),$$

for some  $H$  in  $(c(A, q), h(A, q))$  such that  $\Psi(1, H) = 0$ . For any  $H$  in this interval, let us first notice that  $(\Psi, \Psi')$  define a parametrisation of the bounded component of

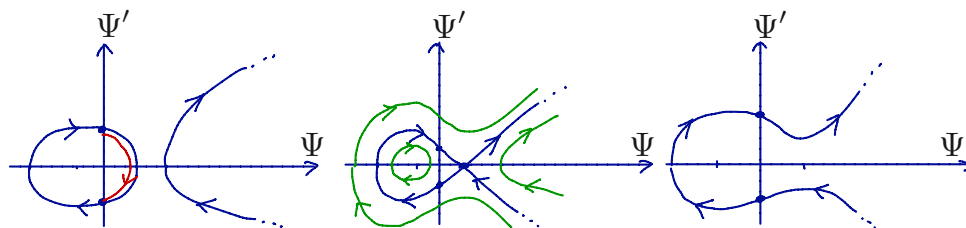


FIGURE 1. Portraits of the curve  $y^2 = f(x)$  parametrised by  $(\Psi, \Psi')$ . From left to right: case (i)  $H \in (c(A, q), h(A, q))$  (the red part corresponds to  $t \in [0, 1]$ ), (ii)  $H = h(A, q)$  (phase portrait in green for other boundary conditions close to the saddle equilibrium), (iii)  $H > h(A, q)$ .

the curve  $y^2 = f(x)$  (see Figure 1). Accordingly, both  $\Psi$  and  $\Psi'$  are bounded, and the solution  $\Psi(\cdot, H)$  of (36) is defined globally, for all  $t \in \mathbb{R}$ . Hence, the function  $H \mapsto \Psi(1, H)$  is well-defined on  $(c(A, q), h(A, q))$ . Proving that this mapping is injective will entail uniqueness of an  $H$  such that  $\Psi(1, H) = 0$ , and thus uniqueness of the optimal potential for the given  $q > 1$  and positive  $L^q$  bound  $A$ . Now, this mapping is differentiable, and  $(\partial\Psi/\partial H)(1, H) = \Phi(1)$  where  $\Phi$  is the solution of the following linearised differential equation (note that  $\alpha = q/(q - 1) > 1$ ):

$$\Phi'' - \alpha\Psi^{\alpha-1}\Phi + 2 = 0, \quad \Phi(0) = 0, \quad \Phi'(0) = 1.$$

The function  $\Phi$  is non-negative in the neighbourhood of  $t = 0+$ . Let us denote  $\tau \in (0, \infty]$  the first possible zero of  $\Phi$ , and  $\tau' := \min\{\tau, 1\}$  (remember that  $\Psi > 0$  on  $(0, 1)$ ). On  $(0, \tau')$ ,

$$\Phi'' = \alpha\Psi^{\alpha-1}\Phi - 2 > -2,$$

so  $\Phi > t(1 - t)$  on  $(0, \tau']$  by integration: necessarily,  $\tau > 1$ . Then  $\Phi(1) > 0$ , so the mapping  $H \mapsto \Psi(1, H)$  is strictly increasing on  $(c(A, q), h(A, q))$  and uniqueness is proved. Regarding the regularity of the optimal potential, it is clear that  $\Psi$  is smooth on  $(0, 1)$ . Besides,  $\Psi'(0)$  is positive and it suffices to write, for small enough  $t > 0$ ,

$$\frac{\Psi^{1/(q-1)}(t) - 0}{t - 0} = t^{(2-q)/(q-1)} \left(\frac{\Psi(t)}{t}\right)^{1/(q-1)}$$

to evaluate the limit when  $t \rightarrow 0+$  and obtain the desired conclusion for the tangencies. (Note the bifurcation at  $q = 2$ .) Same proof when  $t \rightarrow 1-$ . □

*Proof of Theorem C.* — In the particular case  $q = 2$ , one has  $\alpha = 2$  and  $t \mapsto (\psi(t), \psi'(t))$  parametrises the elliptic curve (compare with (35))

$$y^2 = \frac{2}{3}x^3 - 4Hx + (H - c(A, 2))^2.$$

We know that this elliptic curve is not degenerate for  $H$  in  $(c(A, 2), h(A, 2))$ . The value  $c(A, 2) = 9A^2/2$  is explicit (Corollary 26), while  $h^*(A) := h(A, 2)$  is implicitly

defined Lemma 27. Using the birational change of variables  $u = x$ ,  $v = y\sqrt{6}$ , the elliptic curve can be put in Weierstraß form,  $v^2 = 4u^3 - g_2u - g_3$ , with

$$(37) \quad g_2 = 24H, \quad g_3 = -6(H - 9A^2/2)^2.$$

For  $H$  in  $(c(A, 2), h(A, 2))$ , the real curve has two connected components in the plane and is parametrised by  $z \mapsto (\wp(z), \wp'(z))$ , where  $\wp$  is the Weierstraß elliptic function associated to the invariants (37). Since  $g_2$  and  $g_3$  are real, and since the curve has two components, the lattice  $2\omega Z + 2\omega' Z$  of periods of  $\wp$  is rectangular:  $\omega$  is real,  $\omega'$  is purely imaginary, and the bounded component of the curve is obtained for  $z \in \mathbb{R} + \omega'$ . The curve degenerates for  $H = h^*(A)$ , so  $h^*(A)$  can also be retrieved as the unique root in  $(9A^2/2, \infty)$  of the discriminant

$$\Delta = g_2^3 - 27g_3^2 = 3 \cdot 6^2(128H^3 - 9(H - 9A^2/2)^4)$$

of the cubic. We look for a time parametrisation  $z(t)$  such that  $\wp(z(t)) = \psi(t)$  (since  $u = x$ ), and  $\wp'(z(t)) = \psi'(t)\sqrt{6}$  (since  $v = y\sqrt{6}$ ).

LEMMA 30. —  $z(t) = \frac{2t-1}{2\sqrt{6}} + \omega'$ .

*Proof.* — One has  $dz/dt = 1/\sqrt{6}$ . Moreover, there exists a unique  $\xi_0$  in  $(0, \omega)$  such that  $\wp(\xi_0 + \omega') = 0$  (with  $\wp'(\xi_0 + \omega') < 0$ ); by symmetry,  $\wp(-\xi_0 + \omega') = 0$  (with  $\wp'(-\xi_0 + \omega') > 0$ ), so  $\psi(0) = 0$  (with  $\psi'(0) > 0$ ) implies  $z(0) = -\xi_0 + \omega'$ , that is  $z(t) = t/\sqrt{6} - \xi_0 + \omega'$ . As  $\psi(1) = 0$ , necessarily  $z(1) = \xi_0 + \omega'$ , so  $\xi_0 = 1/(2\sqrt{6})$ .  $\square$

Recalling Proposition 25, one eventually gets that the maximal potential for  $q = 2$  is

$$V(t) = \frac{1}{3}\Psi(t) = \frac{1}{3}\wp\left(\frac{2t-1}{2\sqrt{6}} + \omega'\right)$$

for the unique  $H$  in  $(9A^2/2, h^*(A))$  such that  $\Psi(1) = 0$ , that is

$$\wp\left(\frac{1}{2\sqrt{6}} + \omega'\right) = 0.$$

This proves Theorem C.  $\square$

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