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## Periodic functional determinants

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**Abstract.** We examine and evaluate the functional determinants associated with a class of periodic operators which arise in the quantum theory of solitons. The functional determinants are expressed in terms of a finite subset of the spectrum of the operator, a subset which corresponds to the edges of the valency or conduction bands of the Schrödinger equation.

### 1. Introduction

In this paper we shall examine functional determinants associated with a class of periodic operators. Although it is a standard method in field theory to proceed by first considering a system in a large but finite spatial volume and then extracting the infinite volume limit, it is a much harder calculation to keep the finite volume at all stages. While the 'thermodynamic' limit is often the object of an inquiry, situations do arise when we wish to keep some finite dimension present. For instance, the Casimir effect (Toms 1980) and field theory at finite temperature (Dolan and Jackiw 1974, Braden 1982) are two examples. Further examples concern the periodic string (Gervais and Neveu 1982, Mansfield 1983) and solitons; the latter will be amplified shortly.

The class of operators we shall deal with are usually referred to as Hill's operators, which are second-order differential equations of the form  $-d^2/dx^2 + q(x)$  where the potential  $q(x)$  has period  $L$  (Magnus and Winkler 1966, Eastham 1973). These arise naturally when considering quantum mechanics on a lattice (Sutherland 1973). They also arise in the second variation of the action for fields with finite periodicities, and hence our interest in their functional determinants. These operators also arise in the study of quantum mechanical, completely integrable systems (Olshanetsky and Perelomov 1983).

To be more specific consider the following illustrative problem. Let  $\mathcal{L} = \frac{1}{2}(\partial_t \phi)^2 - \frac{1}{2}(\partial_x \phi)^2 - 2m^2 \sin^2 \frac{1}{2} \phi$  be the Lagrangian density for fields on a spacetime with topology  $\mathbb{R} \times S'$  ( $S'$  here is taken to be spatial with period  $L$ ). The time-independent classical equations of motion can be solved. When the combination  $mL$  is large enough, non-trivial, classical solutions exist. This is of course just saying that we can solve the equations of motion for a pendulum: the non-trivial solutions are those that actually go over the top of the circle, there being an energy requirement necessary for this to occur. The lowest-energy non-trivial solution becomes the usual SG soliton in the limit  $L \rightarrow \infty$ . The small oscillations about this classical solution lead to the study of Lamé's

equation (Whittaker and Watson 1978)

$$\left(-\frac{d^2}{dx^2} + p(p+1)k^2 \operatorname{sn}^2(x, k) - a_p\right)y = \lambda y. \tag{1}$$

Here  $p = 1$  for the SG case given above and  $a_p$  is a constant;  $\operatorname{sn}(x, k)$  is an elliptic function. Similarly we get the  $p = 2$  case if we study the analogous  $\phi^4$  case (Avis and Isham 1978). The  $L \rightarrow \infty$  ( $k \rightarrow 1$ ) limit of this equation gives us the usual reflectionless potential Sturm–Liouville equation normally associated with solitons. The  $K \rightarrow 0$ ,  $L \rightarrow \pi$ , limit reduces to simple harmonic motion.

The purpose then of this paper is to examine the functional determinants which are associated with operators of Hill’s type. A useful means of doing this is via the zeta function formed from the operator. This is reviewed in § 2. In constructing the zeta function we use a suitable resolvent of the operator—that is, a function that singles out the eigenvalues. The real difficulty lies in choosing appropriate forms for the resolvent. In § 3 this is studied and the resolvent is constructed from a subset of the eigenvalues. Using the language of solid-state physics, the resolvent is constructed from the knowledge of the edges of the valency and conduction bands. For a generic potential this, of course, may involve all of the eigenvalues, but for the cases that frequently arise it involves far fewer. For instance, the resolvent of equation (1) is given in terms of  $2p + 1$  eigenvalues each of which is known. One of the principal purposes of this paper is to emphasise the utility of this representation. This is illustrated in § 4 by examining the  $p = 1$  form of equation (1). Here we also take the  $L \rightarrow \infty$  limit and in so doing rederive several known results. Section 5 consists of a discussion and conclusions. The appendixes contain some calculations involving elliptic functions.

**2. The zeta function**

One of the advantages of working on a compact space (with appropriate boundary conditions) is that the spectrum becomes discrete. We associate with an operator  $A$  the zeta function  $\zeta_A(s)$  (Dikii 1961) constructed from the eigenvalues  $\lambda_n$  of  $A$

$$\zeta_A(s) = \sum_n \lambda_n^{-s} \equiv \operatorname{Tr}[A^{-s}] \tag{2}$$

considered as a function analytic in  $s$ . The determinant of the operator is then constructed (Hawking 1977) from  $-\operatorname{d}\zeta_A/\operatorname{d}s|_{s=0}$ . If  $A$  has a zero mode we must, as is well known, exclude it from the above and treat it separately.

It is convenient in what follows to explicitly include the vacuum energy subtraction in our treatment. Thus if  $A_0$  is the operator coming from the small oscillations about the vacuum we consider the combination

$$g(s) = \operatorname{Tr}[A^{-s} - A_0^{-s}]. \tag{3}$$

Here equation (3) is a trace over all the (non-zero) eigenvalues of  $A, A_0$ . Then

$$\ln \left[ \det \left( \frac{A}{A_0} \right) \right] = - \left. \frac{\operatorname{d}g(s)}{\operatorname{d}s} \right|_{s=0}. \tag{4}$$

Equation (4), although free from vacuum divergences, may nevertheless be divergent at  $s = 0$  corresponding to needed counterterms. Thus, for a two-dimensional field theory, adding an appropriate mass counterterm makes this finite.

We are interested in the case when—by separation of variables, for instance—the operators  $A, A_0$  contain a part that is a Hill’s operator. To concentrate on this situation we take the remaining coordinates as for free  $d$ -dimensional motion and then we have, with  $K$  representing the Hills operator

$$\begin{aligned} \text{Tr} \left[ -\frac{d^2}{dx_1^2} - \dots - \frac{d^2}{dx_d^2} + K \right]^{-s} \\ = \frac{2\pi^{d/2}}{\Gamma(\frac{1}{2}d)} \text{Tr} \left[ \int_0^\infty \frac{d\omega \omega^{d-1}}{(2\pi)^d} (\omega^2 + K)^{-s} \right] \\ = \frac{1}{\Gamma(\frac{1}{2}d)} \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(\frac{1}{2}d)}{\Gamma(s)} \Gamma(s - \frac{1}{2}d) \text{Tr}[(K)^{d/2-s}]. \end{aligned} \tag{5}$$

For the special case where  $K$  corresponds to free motion with period  $L$ , equation (5) gives a term that is well known—the Casimir term (Hawking 1977, Toms 1980, Braden 1982)

$$-\frac{d}{ds} \zeta_A(s)|_{s=0} = -\frac{2\pi^{d/2}}{L^d} \Gamma(-\frac{1}{2}d) \zeta_R(-d) \tag{6}$$

where  $\zeta_R(-d)$  is the Riemann zeta function which vanishes for  $d$  even, and has a simple form for  $d$  odd. When  $d = 1$  the expression (6) becomes  $-\pi/3L$  and when  $d = 3$  it is  $-\pi^2/45L^3$ .

We are led then to consider the following function of  $s$ :

$$G(s) = \text{Tr}[K^s - K_0^s] \tag{7}$$

where  $K$  and  $K_0$  are the Hill’s operators coming from  $A$  and  $A_0$ . (Of course  $d$  could be zero in what we have said and then  $A$  and  $A_0$  coincide with  $K$  and  $K_0$  respectively.) Equation (5) is, for  $d = 1$ , just the usual combination appearing in soliton mass corrections:  $G(\frac{1}{2})$  typically needs a mass counterterm to make it finite.

In what follows we are going to concentrate on  $G(s)$  with  $s = 0$ . In particular we shall give expressions for  $\text{Tr}[\ln K/K_0]$ . The reason for working with the quantum mechanical case ( $d = 0$ ) is simply to isolate the key features of our approach avoiding the additional complications of counterterms. The results are applied elsewhere to field theories.

The study of  $G(s)$  proceeds via a resolvent  $R(\lambda)$ , a function with only simple poles of residue 1 at the eigenvalues  $\lambda_n$  of  $K$  and residue  $-1$  at the eigenvalues of  $K_0$ . Then

$$G(s) = \frac{1}{2i\pi} \int_{\Gamma'} d\lambda \lambda^s R(\lambda) \tag{8}$$

where the contour  $\Gamma'$  encircles the real  $\lambda$  axis in a positive (anticlockwise) sense about the minimum eigenvalue of  $K$  or  $K_0$ . For a Hill’s operator such an eigenvalue exists (Eastham 1973). Our earlier remark about separating off zero modes means the resolvent is such that it has no pole at zero. Lastly it is possible to remove the (finite) negative eigenvalues from  $K$  and  $K_0$  and treat these separately. Thus we can consider the contour  $\Gamma'$  to encircle the positive  $\lambda$  axis crossing at the origin.

There is a further integral representation of (8) which is frequently useful. This is obtained by completing the contour on a large circle around the  $\lambda$  plane and is valid as long as the contribution from this contour vanishes as the circle becomes increasingly large. (This behaviour is shown to hold in the following section.) Such a contour is

then readily deformed to pick up the discontinuity of  $G$  across the negative  $\lambda$  axis. On the assumption that  $R(\lambda)$  is continuous across this axis, a point justified in the next section, the result is then

$$G(s) = -\frac{\sin \pi s}{\pi} \int_0^\infty d\lambda \lambda^s R(-\lambda). \tag{9}$$

In what follows we shall show  $R(\lambda)$  to have the form  $(d/d\lambda)f(\lambda)$ . When this is the case the functional determinant  $\det K/K_0$  has a particularly simple form

$$\ln \left[ \det \left( \frac{K}{K_0} \right) \right] = - \int_0^\infty d\lambda R(-\lambda) \tag{10a}$$

$$= f(0). \tag{10b}$$

We shall utilise this last representation for  $G(s)$  to make contact with Levinson's theorem later on.

Our next task is to find suitable expressions for the resolvent  $R(\lambda)$ . This is done in the next section. Before proceeding to this, however, it is useful to consider a sample calculation which illustrates the ideas of this section and which is later generalised.

As an example we take the case of a constant potential  $a$ , that is, we have the following two Hill's operators:

$$K = -\frac{d^2}{dx^2} - a \quad K_0 = -\frac{d^2}{dx^2}. \tag{11}$$

To specify the spectrum we need to specify the boundary conditions of the problem. Taking the periodic boundary condition (with period  $L$ ) a suitable resolvent is

$$R(\lambda) = \frac{d}{d\lambda} \ln \left( \frac{\sin^2 \frac{1}{2}(\lambda - a)^{1/2} L}{\sin^2 \frac{1}{2} \sqrt{\lambda} L} \right) \frac{\lambda}{\lambda - a} \tag{12a}$$

$$= +2 \sum_{k=1}^\infty \left( \frac{1}{\lambda - a - (2k\pi/L)^2} - \frac{1}{\lambda - (2k\pi/L)^2} \right). \tag{12b}$$

The choice of this resolvent is motivated in the next section. The factor  $\lambda$  has been included to remove the zero mode. We have included the factor  $(\lambda - a)^{-1}$  for convenience for it allows us to take the limit  $a \rightarrow 0$  without complication. The overall factor of 2 gives us the multiplicity of the eigenvalues.

As  $\lambda \rightarrow \infty$ ,  $R(\lambda)$  goes like  $\lambda^{-3/2}$ . Thus for  $s < \frac{1}{2}$  we may use the representation (9). Note, for  $s = \frac{1}{2}$  which appears in a two-dimensional soliton calculation, we can only use this representation for subtracted (renormalised) quantities. Equation (10b) then gives us

$$\frac{1}{2} \ln \left[ \det \left( \frac{-d^2/dx^2 - a}{-d^2/dx^2} \right) \right] = \ln \left( \frac{\sinh \frac{1}{2} \sqrt{a} L}{\frac{1}{2} \sqrt{a} L} \right). \tag{13}$$

This is the usual result which may be derived in this case by an explicit summation. From (4) we have

$$\begin{aligned} \ln \left[ \det \left( \frac{K}{K_0} \right) \right] &= \sum_{n=-\infty}^\infty \ln \left( \frac{a + (2n\pi/L)^2}{(2n\pi/L)^2} \right) \\ &= \ln \left[ \prod_{n=1}^\infty \left( 1 + \frac{a}{(2n\pi/L)^2} \right)^2 \right]. \end{aligned} \tag{14}$$

The result (13) follows now by using the identity

$$\sin z = z \prod_{k=1}^{\infty} \left( 1 - \frac{z^2}{k^2 \pi^2} \right). \tag{15}$$

### 3. The resolvent for the periodic potential

The purpose of this section is to construct a suitable resolvent for the Hill's operators. To do this we must first recall some standard results from the theory of these operators. In order to provide a self-contained account we shall briefly do this, referring the reader to the standard sources (Magnus and Winkler 1966, Eastham 1973, McKean and van Moerbeke 1975) for further information.

Let  $y_1(x, \lambda)$ ,  $y_2(x, \lambda)$  be the solutions of the Hill's equation

$$Ky = \lambda y \quad K = -\frac{d^2}{dx^2} + q(x) \tag{16}$$

with boundary conditions  $y_1(0, \lambda) = y_2(0, \lambda) = 1$ ,  $y_1'(0, \lambda) = y_2'(0, \lambda) = 0$ . Now any two independent solutions at  $x = L$  are related to those at the  $x = 0$  by a matrix, the monodromy matrix. Here we have

$$\begin{pmatrix} y_1(L) \\ y_2(L) \end{pmatrix} = \begin{pmatrix} y_1(L) & y_1'(L) \\ y_2(L) & y_2'(L) \end{pmatrix} \begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \mathbf{M}_\lambda \begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix}. \tag{17}$$

The determinant of this matrix is just the Wronskian of the two solutions, i.e. 1. Defining the discriminant  $\Delta(\lambda)$  of Hill's equation

$$\Delta(\lambda) = \text{Tr}[\mathbf{M}_\lambda] = y_1(L) + y_2'(L) \tag{18}$$

then the characteristic equation for the eigenvalues of  $\mathbf{M}_\lambda$  is

$$p^2 - \Delta(\lambda)p + 1 = 0 \tag{19a}$$

$$p_{\pm} = \frac{\Delta(\lambda) \pm (\Delta^2(\lambda) - 4)^{1/2}}{2} \quad p_+ p_- = 1. \tag{19b}$$

Setting  $p_{\pm} = \exp(\pm i\alpha L)$ , Floquet's theorem tells us that when these roots are distinct, equation (16) has two linearly independent solutions  $f_1, f_2$  such that

$$f_1(x) = \exp(i\alpha x)p_1(x) \quad f_2(x) = \exp(-i\alpha x)p_2(x) \tag{20}$$

where  $p_1, p_2$  are periodic functions of period  $L$ .

From (19) and (20) we see the Hill's equation has stable solutions provided  $|\Delta(\lambda)| < 2$ . The solutions of  $|\Delta(\lambda)| = 2$  give the intervals of stability and instability. Let  $\lambda_i$  be the solutions of this equation (see figure 1).

Then for  $(\lambda_{2i-1}, \lambda_{2i})$  ( $i = 1, 2, \dots$ ) we have an interval of instability: no solution here is bounded. The complementary intervals  $(\lambda_{2i}, \lambda_{2i+1})$  ( $i = 0, 1, 2, \dots$ ) are the intervals of stability: here every solution is bounded, but none is of period  $L$  or  $2L$ . These intervals of stability are just the conduction and valence bands for the Schrödinger equation (16). The  $\lambda_i$  represent the periodic spectrum; the solutions have period  $L$  for  $\lambda_0, \lambda_{4i-1}, \lambda_{4i}$  ( $i = 1, 2, \dots$ ) and period  $2L$  for  $\lambda_{4i+1}, \lambda_{4i+2}$  ( $i = 0, 1, 2, \dots$ ). In general the solutions at the end points are unstable. This is always true for  $\lambda_0$ . Solutions are stable if an interval of instability collapses, i.e., if we have a double root  $\lambda_{2i-1} = \lambda_{2i}$ .

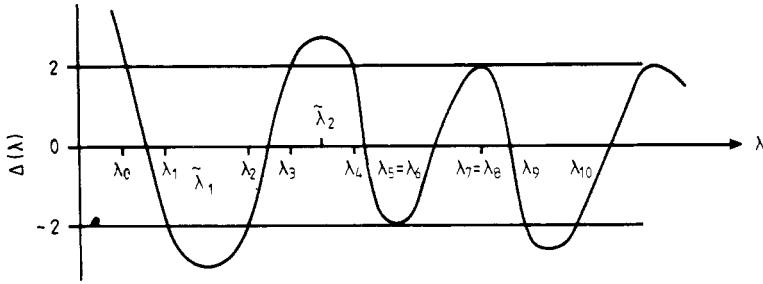


Figure 1. The discriminant  $\Delta(\lambda)$ .

We call the simple roots the simple periodic spectrum. Obviously these come in pairs apart from  $\lambda_0$ .

We now construct resolvents—depending on the boundary conditions—from the monodromy matrix  $\mathbf{M}_\lambda$ . Obviously  $\Delta(\lambda) \pm 2 (= \text{Tr}[\mathbf{M}_\lambda \pm 1]) = 0$  has the antiperiodic and periodic spectrum as roots. Dirichlet boundary conditions are given by the roots of  $(M_\mu)_{21} = y_2(L, \mu) = 0$ . The roots  $\mu_i$  of this latter equation form the auxiliary spectrum. These interlace the periodic spectrum,  $\mu_i \in [\lambda_{2i-1}, \lambda_{2i}]$  ( $i = 1, 2, \dots$ ). In what follows we shall concentrate on the former boundary conditions even though similar results are available for the auxiliary spectrum.

To construct the resolvent  $R(\lambda)$  we use the fact that  $\Delta(\lambda)$  and  $\Delta(\lambda) \pm 2$  are integral functions of order  $\frac{1}{2}$ . This means that they possess product expansions of the form  $c_i \prod_n (1 - \lambda/\lambda_n)$  where  $\lambda_n$  are the zeros of the appropriate function, and  $c_i$  is a constant readily obtained by asymptotic analysis. An appropriate resolvent is

$$R(\lambda) = \frac{d}{d\lambda} \ln(\Delta(\lambda) \pm 2) = \sum_n \frac{1}{\lambda - \lambda_n} \tag{21}$$

which has simple poles of residue 1 at the zeros of the function being considered.

To illustrate, consider  $K_0 = -d^2/dx^2$ . The appropriate monodromy matrix is then

$$\mathbf{M}_\lambda = \begin{pmatrix} \cos \sqrt{\lambda} L & -\sqrt{\lambda} \sin \sqrt{\lambda} L \\ (\sin \sqrt{\lambda} L)/\sqrt{\lambda} & \cos \sqrt{\lambda} L \end{pmatrix} \tag{22}$$

$$\text{Tr}[\mathbf{M}_\lambda - 1] = \Delta(\lambda) - 2 = 2 \cos \sqrt{\lambda} L - 2 = -4 \sin^2 \frac{1}{2} \sqrt{\lambda} L \tag{23}$$

$$R(\lambda) = \frac{d}{d\lambda} \ln(\Delta(\lambda) - 2) = \frac{L}{2\sqrt{\lambda}} \cot \frac{1}{2} \sqrt{\lambda} L = \sum_{k=-\infty}^{\infty} \frac{1}{\lambda - (2k\pi/L)^2}. \tag{24}$$

Here we have the resolvent for periodic boundary conditions we used in (12a), though the zero mode has yet to be subtracted. A similar result holds for the antiperiodic boundary conditions.

To utilise the resolvent (21) we are required to find expressions for  $\Delta(\lambda) \pm 2$ . Of course we can solve the Hill's equation and construct solutions  $y_1(x, \lambda)$ ,  $y_2(x, \lambda)$  with the required boundary conditions. A simpler method is, however, often available. It uses a remarkable result of Hochstadt: the simple periodic spectrum determines both the double periodic spectrum and the non-trivial roots of  $\Delta'(\lambda) = 0$  (Hochstadt 1965). Physically this is saying that given the edges of the various conduction bands for the potential, we can construct the periodic spectrum. Furthermore, we have a simple representation for this. Suppose there are  $n + 1$  bands with edges  $\lambda_0^0, \dots, \lambda_{2n}^0$ . The

non-trivial roots  $\tilde{\lambda}_j$  of  $\Delta'(\lambda) = 0$  are determined by the condition

$$0 = \int_{\lambda_{2j-1}^0}^{\lambda_{2j}^0} \prod_{j=1}^n (\mu - \tilde{\lambda}_j) \frac{d\mu}{l(\mu)} \tag{25}$$

where  $l(\mu)$  in (25) is determined by the simple periodic spectrum:

$$l(\mu) = \left( -\prod_{i=0}^{2n} (\lambda - \lambda_i^0) \right)^{1/2}. \tag{26}$$

Having determined the non-trivial roots  $\tilde{\lambda}_j$  the discriminant may be expressed (McKean and van Moerbeke 1975) in the following form

$$\Delta(\lambda) = 2 \cos \psi(\lambda) L \tag{27}$$

with

$$\psi(\lambda) = \frac{i}{2} \int_{\lambda_0}^{\lambda} \prod_{j=1}^n (\mu - \tilde{\lambda}_j) \frac{d\mu}{l(\mu)} \quad \psi(\lambda_0) = 0. \tag{28}$$

Hochstadt's result then says  $\psi(\lambda) = \pm m\pi/L$  iff  $\lambda = \lambda_{2m-1}$  or  $\lambda = \lambda_{2m}$ . That is (25) and (27) show the simple periodic spectrum determines both the non-trivial roots of  $\Delta'(\lambda) = 0$  as well as the double periodic spectrum.

For our simple example  $K_0$  we find  $l(\lambda) = \sqrt{-\lambda}$ ,  $\psi(\lambda) = \sqrt{\lambda}$  and  $\Delta(\lambda) = 2 \cos \sqrt{\lambda} L$  which is the result of (22). Hochstadt's formula (27) is particularly useful as we may readily generalise the results already obtained for the simple harmonic motion  $K_0$ . In particular (23) becomes

$$\Delta(\lambda) - 2 = -4 \sin^2 \frac{1}{2} \psi(\lambda) L. \tag{29}$$

Using this expression, suitable resolvents for both periodic boundary conditions ( $R_+$ ) and for antiperiodic boundary conditions ( $R_-$ ) are easily constructed. For the subtracted combination  $K - K_0$  these are

$$R_+(\lambda) = 2 \frac{d}{d\lambda} \ln \left( \frac{\sin \frac{1}{2} \psi(\lambda) L}{\sin \frac{1}{2} \sqrt{\lambda} L} \right) \frac{\sqrt{\lambda}}{(\lambda - \lambda_a)^{1/2}} \tag{30}$$

$$R_-(\lambda) = 2 \frac{d}{d\lambda} \ln \left( \frac{\cos \frac{1}{2} \psi(\lambda) L}{\cos \frac{1}{2} \sqrt{\lambda} L} \right). \tag{31}$$

In constructing  $R_+$  we have included the possibility  $K$  that has a zero mode  $\lambda_a$  and introduced factors which serve to remove it. We observe  $R_{\pm}(\lambda)$  are continuous across the negative  $\lambda$  axis, the assumption we made in the previous section.

To make connection with the different representations of § 2 we must now look at the asymptotics of  $R(\lambda)$ . Using standard methods we have

$$\frac{\Delta(\lambda) - 2}{\Delta^0(\lambda) - 2} = 1 + \cot \frac{1}{2} \sqrt{\lambda} L \frac{1}{\sqrt{\lambda}} \int_0^L q(z) dz + O(\lambda^{-1}). \tag{32}$$

Thus as  $\lambda \rightarrow \infty$ ,  $R(\lambda) \sim \lambda^{-3/2}$ , as stated earlier. Further, the second term in (32) is precisely the mass counterterm needed in connection with  $G(\frac{1}{2})$  and soliton calculations. Utilising equations (10) we find

$$\frac{1}{2} \ln \left[ \det \left( \frac{K}{K_0} \right) \right] = \ln \left( \frac{\sin \frac{1}{2} \psi(0) L}{\frac{1}{2} \sqrt{-\lambda_a} L} \right). \tag{33}$$

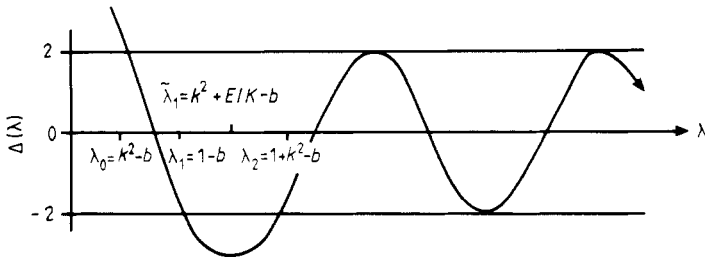


This straightforwardly gives (13) for the case  $K = -d^2/dx^2 - a_0$ . To illustrate these results we turn to the first non-trivial example,  $n = 1$ , in the next section.

**4. An example: the two-band potential**

In the previous section we used Hochstadt's formula to give expressions for the resolvent  $R(\lambda)$  in terms of the simple periodic spectrum of the Hill's operator  $K = -d^2/dx^2 + q(x)$ . Thinking of  $K$  as a Schrödinger equation,  $R(\lambda)$  is constructed from the edges of the conduction and valence bands. For  $n + 1$  bands it is constructed from  $2n + 1$  simple eigenvalues. A theorem of Borg tells us that  $n = 0$  if and only if  $q$  is a constant then this gives the simple harmonic oscillatory example so far considered. Similarly a result of Hochstadt tells us  $n = 1$  if and only if  $q(x) = 2k^2 \text{sn}^2(x, k) - b$ , i.e. the  $p = 1$  form of Lamé's equation (equation (1)). Indeed the  $n = p$  form of Lamé's equation always gives us  $n + 1$  bands. In this section we shall consider in some detail the  $n = 1$ , two band situation. This is relevant to the example discussed in the introduction.

Suppose we have a potential with bands  $(\alpha, \beta), (\gamma, \infty)$ ; the former would be viewed as a valence band, the latter a conduction band. By rescaling  $\alpha \leq \beta \leq \gamma$  can be brought to the form  $\eta(k^2 - b), \eta(1 - b), \eta(1 + k^2 - b)$  with  $\eta = \gamma - \alpha, k^2 = (\gamma - \beta)/(\gamma - \alpha), b = (\gamma - \alpha)^2 - \beta/(\gamma - \alpha)$ . A further rescaling of  $x$  means we may set  $\eta = 1$ . In this form the band edges  $k^2 - b, 1 - b$  and  $1 + k^2 - b$  are just those that come from the  $n = 1$  form of Lamé's equation written above. In figure 2 we draw the discriminant  $\Delta(\lambda)$  for this equation.



**Figure 2.** The discriminant  $\Delta(\lambda)$  for the potential  $q(x) = 2k^2 \text{sn}^2(x, k) - b$ .

If we calculate  $\Delta(\lambda)$  from the monodromy matrix we need the solutions  $y_1(x, \lambda), y_2(x, \lambda)$  to the Schrödinger equation (16) with our chosen potential. These are in fact

$$y_1(x, \lambda) = y_+(x, \lambda) - y_-(x, \lambda) \tag{34a}$$

$$y_2(x, \lambda) = \frac{\text{sn } \alpha}{\text{cn } \alpha \text{ dn } \alpha} (y_+(x, \lambda) + y_-(x, \lambda)) \tag{34b}$$

$$y_{\pm}(x, \lambda) = \frac{\Theta(0)}{2H(\alpha)} \frac{H(x \pm \alpha)}{\Theta(x)} \exp(\mp xZ(\alpha)) \tag{35}$$

$$y_{\pm}(-x, \lambda) = -y_{\mp}(x, \lambda)$$

$$\lambda = 1 - b + k^2 \text{cn}^2(\alpha, k). \tag{36}$$

Here  $\text{sn}$ ,  $\text{cn}$ ,  $\text{dn}$  are Jacobi elliptic functions,  $H$ ,  $\Theta$  are theta functions and  $Z$  is the Jacobi zeta function.

The solutions  $y_{\pm}$  may be straightforwardly generalised to the  $n = p$  form of Lamé's equation following Hermite (1912). It becomes more difficult, however, to find the appropriate combinations giving  $y_1, y_2$ . We show in appendix 1 these solutions possess the appropriate  $k \rightarrow 0$  limit:

$$\lim_{k \rightarrow 0} y_1(x, \lambda) = \cos x(\lambda + b)^{1/2} \quad \lim_{k \rightarrow 0} y_2(x, \lambda) = \frac{\sin x(\lambda + b)^{1/2}}{(\lambda + b)^{1/2}}. \quad (37)$$

The solutions  $y_{1,2}(x, \lambda)$  we have constructed are linearly independent within the intervals of stability. At the end points, however, these solutions coalesce. Here there is a non-periodic eigenfunction and a periodic eigenfunction. This behaviour is general to all Lamé's equations: the periodic eigenfunctions are in fact polynomials (the Lamé polynomials) in the Jacobi elliptic functions. Table 1 gives these solutions for the  $n = 1$  case. We note that the  $k \rightarrow 1$  limit of Lamé's equation gives us the usual reflectionless potential—this limit of the Lamé polynomials gives the Legendre polynomials.

Table 1. Solutions  $y_{1,2}(x, \lambda)$  for  $n = 1$ .

Eigenvalue	Periodic eigenfunction	Period	Non-periodic eigenfunction
$\lambda_0 = k^2 - b$	$\text{dn } x$	$2K$	$\text{dn } x \left( \frac{\Theta_1'(x)}{\Theta_1(x)} \right)$
$\lambda_1 = 1 - b$	$\text{cn } x$	$4K$	$\text{cn } x \left( \frac{H_1'(x)}{H_1(x)} - xk'^2 \right)$
$\lambda_2 = 1 + k^2 - b$	$\text{sn } x$	$4K$	$\text{sn } x \left( \frac{H'(x)}{H(x)} - x \right)$

To calculate  $\Delta(\lambda)$  we now use equation (18) with period  $L = 2K$ . Using the periodicity properties of elliptic functions this reduces to

$$\Delta(\lambda) = -2 \cos 2iKZ(\alpha). \quad (38)$$

Hochstadt's formula is also easy to calculate. We find from (26)  $\tilde{\lambda}_1 = k^2 + E/K - b$ . Thus using  $\lambda_0 = k^2 - b$  equation (28) yields

$$\psi(\lambda) = \frac{i}{2} \int_{k^2-b}^{\lambda} \frac{(\mu - \tilde{\lambda}_1) d\mu}{[-(\mu - k^2 + b)(\mu - 1 + b)(\mu - 1 - k^2 + b)]^{1/2}} \quad (39)$$

$$= -i \left( Z(\alpha) + \frac{i\pi}{2K} \right). \quad (40)$$

Again we have the relation between  $\lambda$  and  $\alpha$  given by (36). Further the range of  $\alpha$  comes from (39). We find

$$\alpha = iu + K + iK' \quad u \in (0, K') \quad \text{for } k^2 - b \leq \lambda \leq 1 - b \quad (41a)$$

$$\alpha = iu \quad u \in (0, K') \quad \text{for } 1 + k^2 - b \leq \lambda. \quad (41b)$$

These correspond to the solutions  $y_{\pm}$  (35) being bounded.

By now using the general formulae (30) or (31) for the resolvent we can construct the regularised determinants for finite period. We make contact with other known results by taking the  $k \rightarrow 0,1$  limit of these expressions. The  $k \rightarrow 1$  limit yields the scattering result for solitons on the line, and the  $k \rightarrow 0$  limit gives the simple harmonic oscillator. We shall now study these limits.

Consider initially  $k \rightarrow 1$ . In this limit  $L = 2K \rightarrow \infty$ . Several observations are in order. As  $K \rightarrow 1$  the first stability interval shrinks to a point:  $\lambda_0 = \lambda_1 = 1 - b$ . This corresponds to the bound state of the reflectionless potential  $1/\cosh^2 x$ . Secondly the second stability interval gives us a continuum of eigenvalues greater than  $\lambda_2 = 2 - b$ . For a finite interval  $L$  we can regularise our operators by a term by term subtraction. This allows  $b$  to take any finite value as there will only be a finite number of eigenvalues in the range  $(\lambda_2, 0)$ . Here 0 appears as the lowest eigenvalue of  $K_0$ , the operator whose eigenvalues we are subtracting. As  $L \rightarrow \infty$ , however, this number diverges unless  $\lambda_2 = 0$ , i.e. we need  $b = 2$  for the  $k \rightarrow 1$  limit. (Physically we need to subtract the right vacuum energy.) This limit gives of course the usual reflectionless potential

$$\left(-\frac{d^2}{dx^2} + \frac{2}{\cosh^2 x}\right)y = \lambda y. \tag{42}$$

Also, we observe that denominator terms like  $\cos \sqrt{\lambda}L$  in (31), which are irrelevant for  $\lambda = 0$  with  $L$  finite, become necessary when taking the  $L \rightarrow \infty$  limit.

Our general discussion has shown that the functional determinant is given via (10b), where  $f(\lambda)$  is the function:

$$f^{1/2}(\lambda) = \frac{1}{2} \ln \left( \frac{\Delta(\lambda) - 2}{\Delta^0(\lambda) - 2} \right) = \ln \left( \frac{\sin \frac{1}{2}\psi(\lambda)L}{\sin \frac{1}{2}\sqrt{\lambda}L} \right) \tag{43}$$

$$= \ln[\sin \frac{1}{2}(\psi(\lambda) - \sqrt{\lambda})L \cot \frac{1}{2}\sqrt{\lambda}L + \cos \frac{1}{2}(\psi(\lambda) - \sqrt{\lambda})L]. \tag{44}$$

To calculate the  $L \rightarrow \infty$  limit we wish to know the  $k \rightarrow 0$  limit of this expression. The relevant piece in this limit is the phaseshift

$$\frac{1}{2}\delta(\lambda) = \lim_{k \rightarrow 1} \frac{1}{2}(\psi(\lambda) - \sqrt{\lambda})L. \tag{45}$$

Because of some errors in the standard texts on elliptic functions pertaining to the  $k \rightarrow 1$  of this combination we evaluate it in appendix 2. There we obtain

$$\delta(\lambda) = \pi - 2 \tan^{-1} \sqrt{\lambda}. \tag{46}$$

This phaseshift is just the usual soliton (Dashen *et al* 1975) result, yet obtained by a rather different route. Again by our formulae (10) we have for the continuum

$$\ln \left[ \det \left( \frac{-d^2/dz^2 - 2/\cosh^2 z}{-d^2/dz^2} \right) \right] = i\delta(0) = i\pi. \tag{47}$$

This agrees with the result

$$\det \left( \frac{-d^2/dz^2 - p(p+1)/\cosh^2 z + \lambda}{-d^2/dz^2 + \lambda} \right) = \frac{\Gamma(\sqrt{\lambda})\Gamma(\sqrt{\lambda} + 1)}{\Gamma(\sqrt{\lambda} - p)\Gamma(\sqrt{\lambda} + p + 1)}. \tag{48}$$

For  $p = 1$ ,  $\lambda = 0$  (48) gives  $-1$ , and hence is in agreement with (47).

The generalisation of (46) and (47) is straightforward: we get Levinson's theorem  $\delta(0) = \pi n$ , where  $n$  is the number of bound states. It is also useful to note that this result is independent of the boundary conditions contained in the resolvent before the

limit was taken. (Equivalently the periodic and antiperiodic spectrum coalesce in the  $L \rightarrow \infty$  limit.) We remark in passing that it is possible to give an expansion of (44) in terms of  $k^2$  (or  $k'^2$ ), i.e.  $L$  using developments similar to those in the appendix.

Lastly we describe the  $k \rightarrow 0$  limit regaining the simple harmonic oscillator. Because the period  $L$  is finite the value of  $b$  can be arbitrary. The only point to note in taking this limit is the possible appearance of zero modes depending on the value of  $b$  and the need to separate off the negative eigenvalues from the resolvent. Figure 3 shows the position of the three lowest eigenvalues in relation to the eigenvalues of the subtraction simple harmonic oscillator.

In calculating the  $k \rightarrow 0$  limit we have from (40) and (36) after some evaluation (appendix 1)

$$\lim_{k \rightarrow 0} \psi(\lambda) = (\lambda + b)^{1/2} \tag{49}$$

which is precisely the simple harmonic value (28). Again we arrive at the usual results (33) and (13) for the determinant after removing the zero eigenvalue.

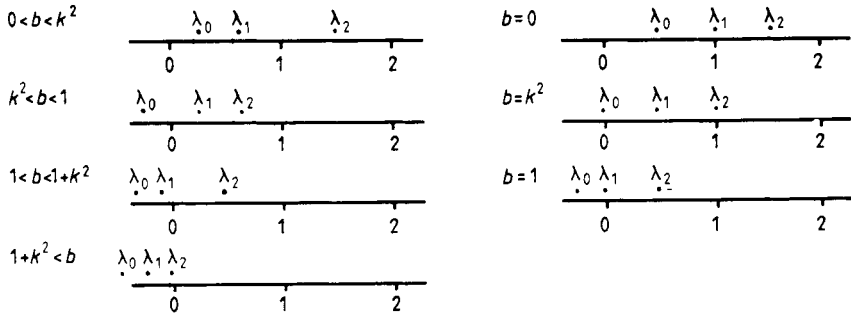


Figure 3. Simple periodic spectrum of  $K$  depending on the value of the constant  $b$  compared with the harmonic oscillator eigenvalues.

### 5. Conclusions

This paper has considered the evaluation of functional determinants associated with periodic operators and specifically with one-dimensional Hill's operators. We have shown how to construct these determinants in terms of a special subset of eigenvalues of the operator: those corresponding to the edges of the valency or conduction bands of the associated Schrödinger equation. For many potentials of interest, including those related to solitons, this subset is finite and known. Thus we can explicitly evaluate the functional determinant. We should note that the remaining eigenvalues are the solutions to a transcendental equation, and so to express the determinant in terms of a finite set of eigenvalues is a significant simplification. As an application of this representation we evaluated the first non-trivial example, that related to the sine-Gordon. There we took the limit of the period tending to infinity, so regaining the usual soliton phaseshift by a very different method. The representation we have used here is readily applied to field theories and gives the usual soliton masses in the appropriate limit. One particular advantage of this approach is that finite length contributions are accounted for and a perturbative expansion is allowed. This is to be discussed elsewhere.

**Appendix 1. The  $k \rightarrow 0$  limit**

Here we evaluate the  $k \rightarrow 0$  limit of  $\psi(\lambda)$  (49) and the eigenfunctions (37). Firstly we recall  $K(0) = \frac{1}{2}\pi$ ,  $K'(0) = \infty$ , thus the limit of the nome  $q = \exp(-\pi K'/K)$  is 0 as  $k \rightarrow 0$ . Further for

$$\text{cn}^2(\alpha, k) = (\lambda + b - 1)/k^2 \tag{A1.1}$$

we deduce  $\alpha \rightarrow iK'$  as  $k \rightarrow 0$ . To evaluate  $\psi(\lambda)$  we use

$$Z[iu] = i[\text{tn}(u, k') \text{dn}(u, k') - Z[u, k'] - (\pi u/2KK')] \tag{A1.2}$$

$$\begin{aligned} \text{tn}(u, k') \text{dn}(u, k') &= -i\text{tn}(iu, k) \text{dn}(iu, k) \\ &= -i \frac{(1 + k^2 - \lambda - b)^{1/2}(\lambda + b - k^2)^{1/2}}{(\lambda + b - 1)^{1/2}}. \end{aligned} \tag{A1.3}$$

Here we have used (A1.1) and the usual elliptic function relations. Thus

$$\lim_{k \rightarrow 0} Z(\alpha) = i[(\lambda + b)^{1/2} - 1] \tag{A1.4}$$

whence using (40) we establish (49):

$$\lim_{k \rightarrow 0} \psi(\lambda) = (\lambda + b)^{1/2}. \tag{A1.5}$$

To evaluate the limits of the eigenfunctions  $y_1, y_2$  we first establish the limits of  $y_{\pm}$ . From (35)

$$y_{\pm}(x, \lambda) = \frac{\Theta(0)H(x \pm \alpha)}{2H(\alpha)\Theta(x)} \exp(\mp xZ(\alpha)). \tag{A1.6}$$

From the fact the nome  $q \rightarrow 0$  we find the limit of (A1.6) by expressing this in terms of theta functions. Then we find, using  $a \rightarrow iK'$

$$\lim_{k \rightarrow 0} \frac{\Theta(0)H(x \pm \alpha)}{H(\alpha)\theta(x)} = \lim_{k \rightarrow 0} \frac{\sin(x \pm \alpha)}{\sin \alpha} = \pm \exp(\mp ix). \tag{A1.7}$$

Therefore using (A1.4)

$$\lim_{k \rightarrow 0} y_{\pm}(x, \lambda) = \pm \exp[\mp ix(\lambda + b)^{1/2}]. \tag{A1.8}$$

We have then

$$\lim_{k \rightarrow 0} y_1(x, \lambda) = \cos x(\lambda + b)^{1/2} \tag{A1.9}$$

$$\begin{aligned} \lim_{k \rightarrow 0} y_2(x, \lambda) &= \lim_{k \rightarrow 0} \frac{\text{sn}(\alpha_1)}{\text{cn} \alpha_1 \text{dn} \alpha} \left( \frac{\exp[-ix(\lambda + b)^{1/2}] - \exp[ix(\lambda + b)^{1/2}]}{2} \right) \\ &= -i \sin x(\lambda + b)^{1/2} \lim_{k \rightarrow 0} \frac{(1 + k^2 - \lambda - b)^{1/2}}{(\lambda + b - 1)^{1/2}(\lambda + b - k^2)^{1/2}} \\ &= \frac{\sin x(\lambda + b)^{1/2}}{(\lambda + b)^{1/2}}. \end{aligned} \tag{A1.10}$$

**Appendix 2. The phaseshift**

We calculate the limit of the phaseshift (45)

$$\lim_{k \rightarrow 1} \frac{1}{2} \delta(\lambda) = \frac{1}{2} (\psi(\lambda) - \sqrt{\lambda}) L. \tag{A2.1}$$

Rewriting (36)  $\lambda = 1 - b + k^2 \operatorname{cn}^2 \alpha$  we have

$$\operatorname{sn}^2 \alpha = \frac{1 + k^2 - b - \lambda}{k^2} \quad \operatorname{cn}^2 \alpha = \frac{\lambda + b - 1}{k^2} \quad \operatorname{dn}^2 \alpha = \lambda + b - k^2. \tag{A2.2}$$

Thus

$$\frac{k^2 \operatorname{sn} \alpha \operatorname{cn} \alpha}{\operatorname{dn} \alpha} = \left( \frac{(1 + k - b - \lambda)(\lambda + b - 1)}{\lambda + b - k^2} \right)^{1/2} \tag{A2.3}$$

$$\lim_{k \rightarrow 1} \frac{k^2 \operatorname{sn} \alpha \operatorname{cn} \alpha}{\operatorname{dn} \alpha} = i(\lambda + b - 2)^{1/2}. \tag{A2.4}$$

To evaluate (A2.1), we use the following limit:

$$\lim_{k \rightarrow 1} K \left( Z(\alpha) - \frac{k^2 \operatorname{sn} \alpha \operatorname{cn} \alpha}{\operatorname{dn} \alpha} \right) = -\tanh^{-1}(\sin \beta) \tag{A2.5a}$$

$$\sin \beta = \lim_{k \rightarrow 1} \operatorname{sn} \alpha. \tag{A2.5b}$$

Note this limit is incorrectly given in Byrd and Friedman (1971, p 34). The limit is established using the developments

$$\begin{aligned} Z(\phi, k) &= E(\phi, k) - (E/K)F(\phi, k) & \phi &= \operatorname{am} \alpha \\ E(\phi, k) &= \sum_{m=0}^{\infty} \binom{1/2}{m} k'^{2m} d_{2m}(\phi) & d_0(\phi) &= \sin \phi \\ F(\phi, k) &= \sum_{m=0}^{\infty} \binom{-1/2}{m} k'^{2m} \rho_{2m}(\phi) & \rho_0(\phi) &= \ln \left( \frac{1 + \sin \phi}{\cos \phi} \right) \end{aligned} \tag{A2.6}$$

valid for  $0 < k'^2 \tan^2 \phi < 1, k^2 < 1$ . Then using the limit

$$\lim_{k \rightarrow 1} \left( K - \ln \frac{4}{k'} \right) = 0 \tag{A2.7}$$

only the term  $\rho_0(\phi)$  contributes to (A2.5a). Thus

$$\lim_{k \rightarrow 1} K \left( Z(\alpha) - \frac{k^2 \operatorname{sn} \alpha \operatorname{cn} \alpha}{\operatorname{dn} \alpha} \right) = -\ln \left( \frac{1 + \sin \beta}{\cos \beta} \right)$$

and  $\sin \beta = \lim(\operatorname{sn} \alpha) = \tanh u$ . Hence

$$\lim_{k \rightarrow 1} K \left( Z(\alpha) - \frac{k^2 \operatorname{sn} \alpha \operatorname{cn} \alpha}{\operatorname{dn} \alpha} \right) = -u = -\tanh^{-1}(\sin \beta)$$

which establishes (A2.5a).

Now using

$$\psi(\lambda) = -iZ(\alpha) + \pi/2k \tag{A2.8}$$

we have

$$\begin{aligned} \lim_{k \rightarrow 1} \frac{1}{2} [\psi(\lambda) - (\lambda + b - 2)^{1/2}] L &= \frac{1}{2} \pi - i \lim_{k \rightarrow 1} [Z(\alpha) - i(\lambda + b - 1)^{1/2}] \\ &= \frac{1}{2} \pi - \tan^{-1}(\lambda + b - 2)^{1/2}. \end{aligned} \quad (\text{A2.9})$$

Again we see the necessity for  $b$  to equal 2 to derive the limit (A2.1), for  $L[(\lambda + b - 2)^{1/2} - \sqrt{\lambda}]$  diverges if  $b \neq 2$ . We obtain then with  $b = 2$

$$\frac{1}{2} \delta(\lambda) = \frac{1}{2} \pi - \tan^{-1} \sqrt{\lambda}. \quad (\text{A2.10})$$

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