

# Quantum mechanics versus spectral differential geometry

Peter Collas

*Department of Physics and Astronomy, California State University, Northridge, Northridge, CA 91330, USA*

Received 29 April 1990; revised manuscript received 11 July 1990; accepted for publication 11 July 1990

Communicated by D.D. Holm

We relate the Schrödinger equation for any two-dimensional natural mechanical system to the eigenvalue equation for the Laplace–Beltrami operator associated with the Jacobi metric of the given system, thereby connecting quantum mechanics and spectral geometry. The harmonic oscillator and the Pullen–Edmonds potential are discussed in this context.

By a *natural system* (NMS) [1] we shall mean a conservative system with Hamiltonian of the form

$$H = \frac{1}{2} \sigma^{ij} p_i p_j + V = E. \quad (1)$$

We geometrize such a system by imposing the *scaled Jacobi metric* [1,2]

$$g = (1 - v)\sigma, \quad v = V/E, \quad (2)$$

on the configuration manifold. (We consider  $E > 0$  for notational simplicity.) We shall refer to the resulting Riemannian manifold as the *Jacobi manifold*  $M$  of the NMS. The geodesic flow on  $M$  corresponds to the trajectories of the NMS after a suitable reparametrization. The Jacobi metric (2) is a well-defined Riemannian metric in the region of the configuration space where  $v < 1$  ( $V < E$ ). However, as is the case for example for systems with only bound states, at the physical boundary  $V = E$  and the metric  $g$  becomes degenerate. *In such cases the Jacobi manifold  $M$  is compact with boundary*; moreover its boundary has length equal to zero. In spite of these features, one can, with some care, work with such manifolds.

A Hamiltonian system – but not a NMS – that was recently thoroughly investigated by Balazs and Voros [3] in a study of classical and quantum chaos, is the motion on the compactified pseudosphere. This *compact* two-dimensional system has constant *negative* curvature; these features guarantee its strong chaoticity. Balazs and Voros quantized their system making use of the fact that the quantum Hamilto-

nian associated with the free motion on the pseudosphere is given by the Laplace–Beltrami operator on the pseudosphere. They were thus able to draw on a number of results from spectral Riemannian geometry [4,5], which deals with questions related to the eigenvalue spectrum of the Laplace–Beltrami operator on manifolds. However all NMSs have Jacobi manifolds with variable curvature; furthermore, several widely studied chaotic systems, e.g., the Hénon–Heiles [6], and the Pullen–Edmonds [7], have Gaussian curvature  $K > 0$ . It is therefore desirable to be able to carry out similar investigations on these more general systems.

In this Letter we show that the eigenvalue equation for the Laplace–Beltrami operator associated with the Jacobi metric of any two-dimensional NMS is the Schrödinger equation for the system; thus we connect spectral Riemannian geometry to quantum mechanics. In most cases the manifold  $M$  of a NMS when compact has a boundary, and so the question of boundary conditions of the eigenvalue problem is crucial. We clarify it using the harmonic oscillator potential as an example. We then discuss the use of Weyl’s asymptotic eigenvalue estimate as a rough quantization rule for the harmonic oscillator and the Pullen–Edmonds potential.

The Laplace–Beltrami operator acting on functions on a Riemannian manifold with metric  $g$  is given by

$$\Delta_g \psi = \frac{1}{\sqrt{\det g}} \partial_i (\sqrt{\det g} g^{ij} \partial_j \psi). \quad (3)$$

For the metric (2), in two dimensions, we have  $\det g = (1-v)^2 \det \sigma$ , thus

$$\Delta_g \psi = \frac{1}{(1-v)\sqrt{\det \sigma}} \partial_i (\sqrt{\det \sigma} \sigma^{ij} \partial_j \psi) = \frac{\Delta \psi}{1-v}, \tag{4}$$

where  $\Delta$  is the Laplace–Beltrami operator for the metric  $\sigma$ . The eigenvalue equation for  $\Delta_g$  on  $M$  is

$$\Delta_g \psi = -\lambda \psi, \tag{5}$$

which may be rewritten using (4) as

$$\Delta \psi + \lambda(1-v)\psi = 0; \tag{6}$$

if we now let  $\lambda = 2E$ , eq. (6) is the Schrödinger equation (with  $m = \hbar = 1$ ). In spectral geometry one seeks connections between the spectrum of (5) and the geometry of  $M$ . If, as is the case for bound state problems,  $M$  is compact with boundary, then mathematicians study (5) with Dirichlet ( $\psi = 0$  on  $\partial M$ ), or Neumann ( $\nu \psi = 0$  on  $\partial M$ , with  $\nu$  a normal vector field on  $\partial M$ ) boundary conditions. In contrast, the boundary conditions for the corresponding problem in quantum mechanics require that  $\psi = 0$  (exponentially) [8] at spatial infinity.

Let  $x_1, x_2$ , be the coordinates of the metric (2), then the element of area on  $M$  is given by

$$dA = \sqrt{\det g} dx_1 dx_2. \tag{7}$$

We let  $L^2(M)$  be the space of measurable functions  $\psi$  on  $M$  for which  $\int_M |\psi|^2 dA < +\infty$ . On  $L^2(M)$  we have the usual Hermitian inner product

$$(\psi_i | \psi_j) = \int_M \bar{\psi}_i \psi_j dA. \tag{8}$$

With the inner product (8),  $L^2(M)$  is a Hilbert space.

The Jacobi metric for the two-dimensional harmonic oscillator is

$$g = [1 - (\omega^2/2E)r^2] (dr^2 + r^2 d\phi^2), \tag{9}$$

its Gaussian curvature  $K > 0$ .  $M$  is homeomorphic to a disk and so its Euler characteristic  $\chi(M) = 1$ <sup>#1</sup>. We

<sup>#1</sup> It is interesting that one can obtain this obvious result also by making use of the Gauss–Bonnet formula. Special care is required since  $K \rightarrow +\infty$  at  $\partial M$ , and a limit must be taken as one approaches  $\partial M$ . However, the divergence from  $K$  is cancelled by a corresponding divergence in the geodesic curvature of  $\partial M$ .

write  $\psi = F(\phi)R(r)$ , for the solutions of eqs. (5) or (6) with Dirichlet boundary conditions. For  $F(\phi)$  we obtain

$$F_l(\phi) = \frac{\exp(il\phi)}{\sqrt{2\pi}}, \tag{10}$$

where  $l = 0, \pm 1, \pm 2, \dots$  in order to guarantee the single-valuedness of  $F_l$  on  $M$ . The radial part of the differential equation can as usual be transformed into Whittaker’s equation, whose normalizable solution gives us

$$R(r) = C e^{-z/2} z^{|l|/2} \times {}_1F_1(\frac{1}{2}(1+|l|) - \kappa; 1+|l|; z), \tag{11}$$

where  $C$  is a normalization constant,  ${}_1F_1$  the confluent hypergeometric function, and

$$\kappa = (E\lambda/8\omega^2)^{1/2}, \quad z = (\omega^2\lambda/2E)^{1/2}r^2. \tag{12}$$

The  $\partial M$  is given by the condition  $v = 1$ , or  $r^2 = 2E/\omega^2$ ; thus we have

$$z_{\max} = (2E\lambda/\omega^2)^{1/2} = 4\kappa, \tag{13}$$

so the Dirichlet boundary conditions on (11) require that

$${}_1F_1(\frac{1}{2}(1+|l|) - \kappa; 1+|l|; 4\kappa) = 0. \tag{14}$$

Eq. (14) then yields the spectrum of  $M$ ,  $\text{Spec}(M)$ . Information about the zeros of  ${}_1F_1$  along with useful asymptotic expansions can be found in ref. [9]. For example, the number of positive (real) zeros  $N_+$  of (11) in  $z$  is

$$N_+ = -[\frac{1}{2}(1+|l|) - \kappa]. \tag{15}$$

In (15)  $[\alpha]$  is the largest integer  $\leq \alpha$ . It follows that

$$\kappa > \frac{1}{2}(1+|l|), \tag{16}$$

for (11) to have at least one positive zero. To get some idea of what  $\text{Spec}(M)$  looks like, we use an asymptotic expansion of (14) valid for large  $\kappa$  (see ref. [9], eq. (19) on p. 109, and ref. [10]). Eq. (14) then reduces to

$$\sin\{\pi[\frac{1}{2}(1+|l|) - \kappa + \frac{1}{6}]\} = 0, \tag{17}$$

where we also assume  $\kappa^{4/3} \gg 0.07|l^2 - 0.3|$ . We find that

$$\kappa = n_r + \frac{1}{2}|l| + \frac{2}{3}, \tag{18}$$

where the radial quantum number  $n_r=0, 1, 2, \dots$ ; the  $\kappa$  given by (18) satisfies (16), and gives  $N_+ = n_r + 1$ . We now define the principal quantum number

$$n = 2n_r + |l|, \tag{19}$$

and so the eigenvalues  $\lambda_n$  of  $\text{Spec}(M)$  are given by (12) and (18)

$$\lambda_n = \frac{2\omega^2}{E} \left(n + \frac{4}{3}\right)^2. \tag{20}$$

From (19) and (20) we see that the *multiplicity* of  $\lambda_n$  is  $n+1$ ; i.e., they are  $(n+1)$ -fold *degenerate* (just like the usual two-dimensional harmonic oscillator). The orthogonality of the  $\psi_{n_l}$  with the inner product (18) on  $M$  can be easily verified (see ref. [9], eq. (4) on p. 112). Now using the fact that  $\lambda=2E$  we can also obtain the energy spectrum

$$E_n = \omega \left(n + \frac{4}{3}\right). \tag{21}$$

The spectrum of (21) is, of course, asymptotic to the usual harmonic oscillator spectrum,  $\omega(n+1)$ , for large  $n$ . This could have been anticipated from eqs. (11)–(14) since

$$\lim_{\substack{z \rightarrow \infty \\ \text{large } E}} R(z) \sim \lim_{\kappa \rightarrow \infty} R(4\kappa). \tag{22}$$

We expect this behavior to be typical for any potential with only bound states since in the *semi-classical limit* large  $n$  implies large  $E$ , and for large  $E$  the Dirichlet boundary conditions  $\psi=0$  on  $\partial M$  will approach the usual quantum mechanical  $\psi=0$  at  $\infty$  as the distance of  $\partial M$  from the origin approaches infinity. To put it another way, since in classical mechanics there is not penetration into the forbidden region,  $E < V$ , one anticipates that as quantum mechanics approaches classical mechanics, solutions obtained in the semi-classical approximation will approach solutions obtained with Dirichlet boundary conditions. However, one should not lose sight of the different meaning of eqs. (20) and (21): *The  $\sqrt{\lambda_n}$  can be thought of as the eigenfrequencies of the “membrane”  $M$ , whose geometry is determined by  $g$ , and whose area is fixed by the classical energy  $E$  and the coupling constant.  $E_n$  on the other hand is simply the semi-classical energy spectrum and is asymptotically related to the  $\lambda_n$ .*

Weyl’s asymptotic formula for Dirichlet eigenval-

ues [4,5] gives the number of eigenvalues  $N(\lambda)$ , counted with multiplicity,  $\leq \lambda$ . For two-dimensional compact manifolds with boundary, Weyl’s formula is

$$N(\lambda) \sim \frac{A(M)\lambda}{4\pi}, \text{ as } \lambda \uparrow +\infty, \tag{23}$$

where  $A(M) = \text{Area } M$  (calculated using (7)). The next correction term in an improved estimate known as Weyl’s conjecture [5] involves the length of  $\partial M$  (calculated using (2))  $L(\partial M)$ ; however,  $L(\partial M) = 0$  since  $g$  is degenerate on  $\partial M$ , and so we get no contribution from this term. If we let  $N(\lambda) = m$ ,  $m = \text{integer}$ , we have the estimate (see ref. [4], p. 172)

$$\lambda_m \sim \frac{4\pi m}{A(M)}, \text{ as } m \uparrow +\infty. \tag{24}$$

In order to better understand the above estimates we return to the harmonic oscillator example. Since the levels are  $(n+1)$ -fold degenerate,

$$N(\lambda_n) = \sum_{j=1}^n (j+1) = \frac{1}{2}n(n+1), \tag{25}$$

while from (23), using (20) for  $\lambda_n$  and  $A(M) = \pi E/\omega^2$ , we have

$$N(\lambda_n) \sim \frac{1}{2} \left(n + \frac{4}{3}\right)^2. \tag{26}$$

Weyl’s estimate is not bad considering the rather drastic approximations involved in obtaining estimate (20). Conversely from (24)

$$\lambda_m \sim 4\omega^2 m/E, \tag{27}$$

where  $m \sim \frac{1}{2}n(n+1)$ . Finally if we let  $\lambda=2E$ , we obtain the estimate

$$E_m \sim \omega \sqrt{2m} \sim \omega n. \tag{28}$$

We see that without detailed knowledge of the distribution and multiplicity of degenerate states, estimates (23) and (24) give us information on an “equivalent” *non-degenerate* spectrum reflecting certain qualitative features of the actual spectrum rather well, e.g., the variation of the density of states with coupling constant. Thus these estimates can be used as a rough quantization rule [11].

We shall illustrate these ideas with one further example, the Pullen–Edmonds potential [7], whose Hamiltonian is

$$H = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}\omega^2(x^2 + y^2) + \alpha x^2 y^2, \\ \alpha > 0. \quad (29)$$

This system has been the subject of several investigations both classically and quantum mechanically [7,12]. Classically, for  $\omega^2=1$ ,  $\alpha=0.05$ , the motion is almost wholly regular below energy  $E=15$ , while at energies above  $E=50$  the motion is almost entirely chaotic. Quantum mechanically, painstaking calculations [7,12] confirmed "energy level repulsion" for  $E$  in the chaotic regime; i.e., the distribution of the nearest-neighbor spacings is Wigner not Poisson. In order to examine the energy level fluctuations meaningfully, one has to decompose the given spectrum into secular variations and fluctuations. There are several "unfolding" procedures which map the original spectrum  $\{E_m\}$  onto a new spectrum  $\{\epsilon_m\}$ , which has on the average a constant mean spacing over the entire energy interval. This spacing is then taken as the energy unit. One such procedure makes use of Weyl's estimate (23) (with correction terms if applicable) to obtain  $\epsilon_m = N(\lambda_m = 2E_m)$  [13]. This particular procedure has been so far used only for systems with vertical wall potentials (Dirichlet boundary conditions). We are suggesting that in the semi-classical region it could be used for any two-dimensional potential which has only bound states.

System (29) has a Jacobi manifold  $M$  with  $K > 0$ ,  $\chi = 1$ , and area  $A(M)$  given by

$$A(M) = 32(r_0/3\gamma)^2 \sqrt{1+\gamma} \\ \times [(1 + \frac{3}{2}\gamma)K(k) - (1 + 2\gamma)E(k)], \quad (30)$$

where  $r_0^2 = E/\omega^2$ , and  $K(k)$ ,  $E(k)$  are complete elliptic integrals whose modulus  $k = [\gamma/(1+\gamma)]^{1/2}$  and  $\gamma = 4\alpha E/\omega^4$ . Estimates (23) and (24) give the approximate  $N(\lambda)$  and  $\lambda_m$  respectively, but we can easily go a little further. Apart from the overall factor of  $E$  coming from  $r_0^2$ ,  $A(M)$  depends only on the product  $\alpha E$  in  $\gamma$  (we let  $\omega^2=1$ ), thus we write  $A = E_m f(\alpha E_m)$ , and using (24) and  $\lambda_m = 2E_m$  we have the rough quantization rule

$$m \sim E_m^2 f(\alpha E_m) / 2\pi. \quad (31)$$

Every  $E_m$  that makes the r.h.s. of (31) an integer is an approximate energy eigenvalue (large  $m$ ) of the "split" spectrum.

As mentioned above the Gaussian curvature  $K > 0$ , and it turns out that the Ricci curvature satisfies the inequality

$$\text{Ric}(u, u) \geq \omega^2/E > 0, \quad (32)$$

$u$  being any unit tangent vector in TM. There exist in the literature several results giving lower and upper bounds on  $\lambda_m$ , and in particular on the lowest (nonzero) eigenvalue  $\lambda_1$ , for manifolds with  $\text{Ric}(u, u) \geq c$  where the constant  $c > 0$  as in (32) (e.g., refs. [4,5,14]). Although the low lying  $\lambda_m$  cannot be related to quantum mechanical energy eigenvalues, they are tightly controlled by the geometry of the manifold, and as Balazs and Voros [3] suggest, there may exist interesting connections between certain classical dynamical quantities characterizing chaos and the low lying  $\lambda_m$ .

The author wishes to thank Dr. T. Azzarelli, Professor R.T. Park, and Professor J. Zeitlin for stimulating and helpful discussions.

## References

- [1] V.I. Arnold, *Mathematical methods of classical mechanics* (Springer, Berlin, 1978).
- [2] R. Abraham and J.E. Marsden, *Foundations of mechanics* (Benjamin, Reading, 1978).
- [3] N.L. Balazs and A. Voros, *Phys. Rep.* 143 (1986) 109.
- [4] I. Chavel, *Eigenvalues in Riemannian geometry* (Academic Press, New York, 1984).
- [5] P.H. Bérard, *Spectral geometry: direct and inverse problems* (Springer, Berlin, 1986).
- [6] M. Hénon and C. Heiles, *Astron. J.* 69 (1964) 73.
- [7] R.A. Pullen and A.R. Edmonds, *J. Phys. A* 14 (1981) L477.
- [8] E.C. Kemble, *The fundamental principles of quantum mechanics* (Dover, New York, 1958).
- [9] H. Buchholz, *The confluent hypergeometric function* (Springer, Berlin, 1969).
- [10] M. Abramowitz and I. Stegun, eds., *Handbook of mathematical functions* (Dover, New York, 1965) eq. (13.5.19), p. 509.
- [11] M.V. Berry, in: *Quantum measurements and chaos*, eds. E.R. Pike and S. Sarkar (Plenum, New York, 1987) p. 81.
- [12] E. Haller, H. Köppel and L.S. Cederbaum, *Phys. Rev. Lett.* 52 (1984) 1665; H.-D. Meyer, E. Haller, H. Köppel and L.S. Cederbaum, *J. Phys. A* 17 (1984) L831; E.B. Bogomolnyi, *JETP Lett.* 41 (1985) 65; H.-D. Meyer, *J. Chem. Phys.* 84 (1986) 3147; Z. Deng and F.T. Hioe, *Phys. Lett. A* 115 (1986) 21.

- [13] O. Bohigas, M.J. Giannoni and C. Schmit, *Phys. Rev. Lett.* 52 (1984) 1.  
[14] R.C. Reilly, *Indiana Univ. Math. J.* 26 (1977) 459;  
P. Li and S.-T. Yau, in: *Am. Math. Soc. Proc. Symp. Pure*

*Math.* 36. *Geometry of the Laplace operator*, eds. R. Osserman and A. Weinstein (1980) p. 205;  
P. Li, in: *Seminar on differential geometry*, *Ann. Math. Stud.* 102 (1982) 73.