On the geometric potential derived from Hermitian momenta on a curved surface

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A geometric potential $V_C$ depending on the mean and Gaussian curvatures of a surface $\Sigma$ arises when confining a particle initially in a three-dimensional space $\Omega$ onto $\Sigma$ when the particle Hamiltonian $H_\Omega$ is taken proportional to the Laplacian $L$ on $\Omega$. In this work rather than assume $H_\Omega \propto L$, momenta $P_\eta$ Hermitian over $\Omega$ are constructed and used to derive an alternate Hamiltonian $H_\eta$. The procedure leading to $V_C$, when performed with $H_\eta$, is shown to yield $V_C = 0$. To obtain a measure of the difference between the two approaches, numerical results are presented for a toroidal model.

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1. INTRODUCTION

The study of quantum mechanics on curved surfaces has been a subject of theoretical effort for decades [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20]. The approach as pioneered in [1, 2, 3, 4] first defines a surface $\Sigma(u, v)$ and employs a coordinate $q$ to describe excursions at any point normal to $\Sigma$. The Hamiltonian appropriate to the three dimensional coordinate system $\Omega$ characterized by a metric $g_{ij}$ is then defined by $H_\Omega \equiv -\frac{1}{2} \nabla^2$ with

$$\nabla^2 = g^{-\frac{1}{2}} \frac{\partial}{\partial q^i} \left[ g^{ij} \frac{\partial}{\partial q^j} \right].$$

(1)

As will be briefly reviewed below, Eq.(1), along with imposing conservation of the norm in the limiting case where the particle is constrained to motion on $\Sigma$, leads to a geometric potential $V_C$. This paper with is concerned with how $V_C$ is modified when instead of defining $H_\Omega$ through Eq.(1), another choice of Hamiltonian, one for which surface and normal momenta are required to be Hermitian over $\Omega$ is adopted.

The remainder of this paper is organized as follows: in section 2 the geometric potential is derived from Eq.(1) for a cylindrically symmetric geometry $\Omega_c$. This material has appeared other places, but is included here to keep this work as self contained as possible and to establish some notation. A symmetric geometry was chosen for ease of presentation; the salient points for more general cases remain intact. In section 3 the classical Hamiltonian for a particle in $\Omega_c$ is written, Hermitian momenta on $\Omega_c$ are found, and standard quantum mechanical rules employed to write the first quantized Hamiltonian. Finally, using the limiting procedure detailed in section 2, the geometric potential is re-derived. Section 4 presents numerical calculations for a toroidal system, and section 5 is reserved for conclusions.

2. THE GEOMETRIC POTENTIAL; A BRIEF REVIEW.

The derivation of $V_C$ will be performed for a cylindrically symmetric geometry $\Omega_c$ with $H_\Omega \propto L$. The extension to the general case is straightforward and the central results below will be not be affected by the restriction to azimuthal symmetry.

Let $e_\rho, e_\phi$ be cylindrical coordinate system unit vectors defined through

$$e_\rho = \cos \phi \, i + \sin \phi \, j$$

(2)

$$e_\phi = -\sin \phi \, i + \cos \phi \, j$$

(3)

and let a cylindrically symmetric surface $\Sigma_c$ be described by

$$r(\rho, \phi) = \rho e_\rho + S(\rho) k.$$
$S(\rho)$ gives the shape of the surface. Any point near $\Sigma_c$ may be reached by travelling normal to $\Sigma_c$ up (or down) a distance $q$ via

$$x(\rho, \phi, q) = r(\rho, \phi) + q e_n$$

with $e_n$ everywhere normal to the surface. The metric near the surface derived from Eq. (5) is

$$ds^2 = Z^2 \left[ 1 - \frac{q S_{\rho \rho}}{Z^2} \right] d\rho^2 + \rho^2 \left[ 1 - \frac{q S_{\phi \phi}}{Z^2} \right] d\phi^2 + dq^2$$

(6)

$$\equiv Z^2 \left[ 1 + \frac{1}{2} (h^2 - k) \right] d\rho^2 + \rho^2 \left[ 1 + \frac{1}{2} (h^2 - k) \right] d\phi^2 + dq^2$$

(7)

with $Z = \sqrt{1 + S_{\rho \rho}}$. The Laplacian can be found straightforwardly from Eq. (7) but is not essential to the main arguments that follow.

Now consider a situation where a large confining potential $V_n(q)$ everywhere normal to $\Sigma_c$ acts to restrict the particle to the surface. The derivation of the geometric potential is independent of its specific form [21], but however chosen it causes the particle to sit on $\Sigma_c$. In this limit the wave function decouples into surface and normal parts [1, 2, 3, 4]

$$\Psi(\rho, \phi, q) \to \chi_s(\rho, \phi) \chi_n(q).$$

(8)

Conservation of the norm in the decoupled limit is imposed by insisting upon the condition

$$|\Psi|^2 F d\Sigma dq = |\chi_s|^2 |\chi_n|^2 d\Sigma dq$$

(9)

with $F = 1 + 2qh + q^2k$ and $d\Sigma$ the surface measure. $h$ and $k$ are the mean and Gaussian curvatures given by

$$h = \frac{1}{2} (k_1 + k_2),$$

$$k = k_1k_2.$$  

(10, 11)

Inserting the expression given by Eq. (8)

$$\Psi = \frac{\chi_s \chi_n}{\sqrt{F}}$$

(12)

into the time independent Schrodinger equation $-\frac{1}{2} \nabla^2 \Psi = E \Psi$, and taking the $q \to 0$ limit after performing all $q$ differentiations, yields the pair of equations ($h = m = 1$)

$$-\frac{1}{2} \left[ \frac{1}{Z^2} \frac{\partial}{\partial \rho} \right]^2 + \frac{1}{Z^2} \frac{\partial}{\partial \rho} - \frac{Z_{\rho}}{Z^3} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial}{\partial \phi}^2 + (h^2 - k) \right] \chi_s = E_s \chi_s$$

(13)

$$-\frac{1}{2} \frac{\partial^2 \chi_n}{\partial q^2} + V_n(q) \chi_n = E_n \chi_n.$$  

(14)

The curvature potential $V_C$ is

$$V_C = -\frac{1}{2} [k^2 - k];$$

(15)

seeing specifically how $V_C$ is generated will prove important in the following section. It arises from the $q \to 0$ limit of the

$$\left( \frac{\partial^2}{\partial q^2} + 2h \frac{\partial}{\partial q} \right) \chi_s(\rho, \phi) \chi_n(q) F^{-1/2}$$

(16)

term in the full Laplacian. The $Z$ dependence appearing in the kinetic energy operator given by Eq. (13) occurs independently of the $q$ degree of freedom. The effect on the spectra of some simple systems due to metric factors in the operator was shown to be small in [15, 16] for some parameterizations of $S(\rho)$, but it is also possible for the effects to be large [22].
3. THE HAMILTONIAN WITH HERMITIAN MOMENTA

In this section a Hamiltonian $H_\eta$ quadratic in momenta $P_\eta$ Hermitian over $\Omega_c$ is developed. The procedure followed comprises standard quantum mechanical rules, to wit:

a. the classical Lagrangian is written

b. the canonical momenta are determined
c. the classical momenta are replaced with their first quantized form $\hat{P}_\eta$ Hermitian on $\Omega_c$.

The Lagrangian for a particle in a geometry described by Eq. (6) is

$$L = \frac{1}{2} (Z^2 [1 + k_1 q]^2 \dot{\rho}^2 + \rho^2 [1 + k_2 q]^2 \dot{\phi}^2 + \dot{q}^2).$$ (17)

With $P_\eta = \partial L/\partial \dot{q}_\eta$, the classical Hamiltonian for this geometry is

$$H = \frac{1}{2} \left(\frac{P_\rho^2}{Z^2 [1 + k_1 q]^2} + \frac{P_\phi^2}{\rho^2 [1 + k_2 q]^2} + P_\eta^2\right).$$ (18)

To proceed with first quantization via $P_\eta \rightarrow \hat{P}_\eta$, it is necessary to produce momentum operators Hermitian on a geometry described by $g_{ij}$. The required relation is

$$\hat{P}_\eta = \frac{1}{i} \left(\frac{\partial}{\partial q_\eta} + \frac{1}{2} \frac{\partial}{\partial q_\eta} \ln \sqrt{g}\right).$$ (19)

Anticipating the $q \to 0$ limit, it is useful to note the differentiations done by the surface momenta will pass over any appearances of the $q$ variable, making it possible to set $q = 0$ in both of them without affecting the final result. The momenta in this limit are

$$\hat{P}_\rho = \frac{1}{i} \left(\frac{\partial}{\partial \rho} + \frac{1}{2} \frac{\partial Z}{\partial \rho} \right),$$ (20)

$$\hat{P}_\phi = \frac{1}{i} \frac{\partial}{\partial \phi},$$ (21)

$$\hat{P}_q = \frac{1}{i} \left(\frac{\partial}{\partial q} + \frac{1}{F} [h + qk]\right).$$ (22)

$H_\eta$ is straightforward to obtain from the three momenta listed above, but it is Eqs. (16) and (22) that will be focused upon to generate the central result of this paper. Write

$$-\hat{P}_q^2 = \frac{\partial^2}{\partial q^2} + \frac{2}{F} (h + qk) \frac{\partial}{\partial q} + \frac{1}{F} \left(\frac{\partial h}{\partial q} + k\right) - \frac{1}{F^2} \frac{\partial F}{\partial q} (h + qk) + \frac{1}{F^2} (h + qk)^2;$$ (23)

upon taking the $q \to 0$ limit the result is

$$-\hat{P}_q^2 = \frac{\partial^2}{\partial q^2} + 2h \frac{\partial}{\partial q} + k - h^2.$$ (24)

The key point is simple; Eq.(24) includes the operator that appears in the Laplacian formulation of the problem as shown in Eq.(16). It eventually yields $\frac{\partial^2}{\partial q^2} + h^2 - k$, from which it is trivially seen that the geometric potential cancels in the Hermitian formulation.

4. A NUMERICAL EXAMPLE

In this section the spectra and wave functions of the Schrödinger equation for a particle on a toroidal surface $T^2$ of major radius $R$ and minor radius $a$ will be compared using the two formalisms detailed above. There are good reasons to choose such a system, not the least being calculating system observables is tractable. Additionally, toroidal
nanostructures of varied types have been fabricated so there is some relevance to real devices, a point which will be elaborated upon in the conclusions section below.

The surface of a doughnut shaped torus has may be parameterized by

\[ x(\theta, \phi, q) = (R + a \cos \theta) e_p + a \sin \theta k + q e_n. \]

(25)

Applying \( d \) to Eq.(25) gives

\[ dx = (a + q) d\theta e_\theta + [R + (a + q) \cos \theta] d\phi e_\phi + dq e_n, \]

(26)

with \( e_\theta = -\sin \theta e_p + \cos \theta k \) and \( e_n \equiv e_\phi \times e_\theta \).

Let \( \alpha = a/R, \beta = 2Ea^2 \); applying the formalism described in section 2 and making the standard separation ansatz for the azimuthal part of the wave function \( \Psi(\theta, \phi) = \psi(\theta) \exp[i\nu \phi] \) yields the Schrödinger equation with \( V_C \) present

\[ \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\alpha \sin \theta}{[1 + \alpha \cos \theta]} \frac{\partial \psi}{\partial \theta} - \frac{(\nu^2 \alpha^2 - \frac{1}{4})}{[1 + \alpha \cos \theta]^2} \psi + \beta \psi = 0. \]

(27)

The method of section 3 gives the Schrödinger equation

\[ \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\alpha \sin \theta}{[1 + \alpha \cos \theta]} \frac{\partial \psi}{\partial \theta} - \frac{\nu^2 \alpha^2 + \frac{1}{4}(\alpha^2 - 1)}{[1 + \alpha \cos \theta]^2} \psi + (\beta - \frac{1}{4} \psi) = 0. \]

(28)

Even before consideration of the solutions of Eq. (27) and (28), there is an immediate distinction between the two. The cancellation of the azimuthal kinetic energy term at discrete values of \( \alpha \) occurs in the former at values of

\[ \alpha = \frac{1}{2\nu}, \]

(29)

and in the latter at

\[ \alpha = \sqrt{\frac{1}{1 + 4\nu^2}}. \]

(30)

The ramifications of Eq.(29) and by implication Eq.(30) have been discussed elsewhere. Here it need be noted that while there appears a term in the Hermitian formalism that is identical to \( V_C \) derived from the Laplacian method, it is an artifact of the high degree of symmetry of the torus and may take a very different form in the general case.

Numerical solutions of Eqs. (27) and (28) were determined by a basis set expansion in Gram-Schmidt functions on \( T^2 \).

The results indicate clearly that the two Hamiltonians can differ, particularly at the “magic” \( \alpha \) given by Eq. (29) or Eq. (30), and when the torus fattens to values of \( \alpha \sim 2/3 \).

5. CONCLUSIONS

This work demonstrated that a Hamiltonian quadratic in momenta Hermitian on a curved surface and consistent with standard quantum mechanical rules leads to a vanishing geometric potential \( V_C \). It is interesting that Golovnev has recently employed an alternate (Dirac quantization) procedure for which \( V_C = 0 \) on a sphere; however, it is not clear to the author how the DQ method could be easily implemented on \( T^2 \).

Numerical results were presented to show the differences in spectra and wave functions between the two Hamiltonians discussed here can be substantial. It is possible to speculate as to whether advances in nanostructure fabrication may perhaps allow for experimental determination of which (if either) Hamiltonian studied here is the more correct description of curved surface nanophysics. Given that toroidal structures have been fabricated and are “clean” with respect to curvature effects (in that there is enough symmetry to make the problem interesting but not so much to make it trivial), it is conceivable that existing devices may be employed to settle the very fundamental issue of what is the appropriate Hamiltonian for a particle constrained to a surface.

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TABLE 1: Eigenvalues and wave functions corresponding to the solutions of Eqs. (27) and (28) for $\alpha = \frac{1}{3}$ (the $(2\pi)^{-\frac{1}{2}}$ normalization from the $\phi$ dependence is omitted.) Terms not shown are at least an order of magnitude smaller than those listed.

| $\beta$ | $\alpha = \frac{1}{3}$ $V_C \neq 0$ | $\alpha = \frac{1}{3}$ $V_C = 0$ |
|---------|---------------------------------|--------------------------------|
| -.2834  | $\Psi_0 = .4082 - 0.0776 \cos \theta$ | $\Psi_0 = -.4075 - 0.0686 \cos \theta$ |
| -.1528  | $\Psi_1 = [.4049 - 0.0421 \cos \theta] e^{\pm \phi}$ | $\Psi_1 = [.4038 - 0.0335 \cos \theta] e^{\pm \phi}$ |
| +.1968  | $\Psi_2 = [.4000 - 0.0525 \cos \theta] e^{\pm 2\phi}$ | $\Psi_2 = [.3869 - 0.0593 \cos \theta] e^{\pm 2\phi}$ |

TABLE 2: As per table 1 with $\alpha = \frac{1}{2}$. The middle state is qualitatively very different due to $\alpha = \frac{1}{2}$ defining a “magic radius” when $V_C = 0$.

| $\beta$ | $\alpha = \frac{1}{2}$ $V_C \neq 0$ | $\alpha = \frac{1}{2}$ $V_C = 0$ |
|---------|---------------------------------|--------------------------------|
| -.3511  | $\Psi_0 = .4230 - 0.1470 \cos \theta$ | $\Psi_0 = .4191 - 0.1072 \cos \theta$ |
| 0       | $\Psi_1 = e^{\pm \phi}$ | $\Psi_1 = [.3912 + 0.0293 \cos \theta] e^{\pm \phi}$ |
| +.6288  | $\Psi_2 = [.3293 - 0.1935 \cos \theta] e^{\pm 2\phi}$ | $\Psi_2 = [.3289 - 0.2008 \cos \theta] e^{\pm 2\phi}$ |

TABLE 3: As per table 1 with $\alpha = \frac{2}{3}$. The second excited state for the case when $V_C = 0$ becomes a negative parity function in $\theta$.

| $\beta$ | $\alpha = \frac{2}{3}$ $V_C \neq 0$ | $\alpha = \frac{2}{3}$ $V_C = 0$ |
|---------|---------------------------------|--------------------------------|
| -3.410^{-1} | $\Psi_0 = 0.4597 - 0.3406 \cos \theta - 0.1000 \cos 2\theta$ | $\Psi_0 = -0.4369 + 0.1516 \cos \theta$ |
| +.2924  | $\Psi_1 = [0.3570 + 0.1079 \cos \theta] e^{\pm \phi}$ | $\Psi_1 = [0.3405 + 0.1446 \cos \theta] e^{\pm \phi}$ |
| +.4377  | $\Psi_2 = 0.5930 \cos \theta - 0.1363 \cos 2\theta$ | $\Psi_2 = -0.5888 \sin \theta - 0.0992 \sin 2\theta$ |