Curvature induced toroidal bound states
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Abstract
Curvature induced bound state \((E < 0)\) eigenvalues and eigenfunctions for a particle constrained to move on the surface of a torus are calculated. A limit on the number of bound states a torus with minor radius \(a\) and major radius \(R\) can support is obtained. A condition for mapping constrained particle wave functions on the torus into free particle wave functions is established.

Pacs number(s): 03.65Ge, 68.65.-k

1. Introduction.

The physics of nanostructures [1,2] and quantum waveguides [3-7] may make questions concerning curved surfaces in quantum theory increasingly relevant to device modelling. Many workers have investigated with varying levels of formal machinery the existence of bound states of quantum systems on curved strips, tubes and hypervolumes [8-12]. The common thread through much of the work described in [8-12] is the existence of an attractive potential that appears in the Schrodinger equation as a consequence of constraining a particle from higher to lower dimensional manifolds. (In the majority of work the dimensionality is reduced from three to two, but see [11] for the generalization to other cases.) This potential, called here the curvature potential \(V_C\), has been shown sufficient to cause bound states in model systems. In this work \(V_C\) for a particle constrained to the surface of a torus is derived and bound state surface toroidal wavefunctions (STWs) are calculated.

This brief report is organized as follows: in section 2 the method by which \(V_C\) is derived is concisely described for a symmetric but non-trivial geometry. The method is then applied to the torus. In section 3 a brief description of the procedure used to solve the Hamiltonian found in section 2 is given and some low-lying bound state eigenvalues and STWs shown. Conclusions appear in section 4.

2. Derivation of \(V_C\).

In the interest of clarity the derivation of \(V_C\) will be performed for a cylindrically symmetric surface. The extension to the general case is straightforward and the salient points still obtain.

Let \(e_\rho, e_\phi, e_z\) be standard cylindrical coordinate system unit vectors. A cylindrically symmetric surface may be described by the Monge form

\[
r(\rho, \phi) = \rho e_\rho + S(\rho) e_z. \tag{1}
\]

\(S(\rho)\) gives the shape of the surface. Points near the surface \(S(\rho)\) may be described by

\[
x(\rho, \phi, q) = r(\rho, \phi) + q e_n \tag{2}
\]
with \( \mathbf{e}_n \) everywhere normal to the surface. The metric near the surface \( S \) is

\[
ds^2 = Z^2 \left[ 1 - \frac{q S_{\rho \phi}}{Z^3} \right]^2 d\rho^2 + \rho^2 \left[ 1 - \frac{q S_{\rho \rho}}{\rho^2 Z} \right]^2 d\phi^2 + dq^2
\]

\[
\equiv Z^2 [1 + qk_1]^2 d\rho^2 + \rho^2 [1 + qk_2]^2 d\phi^2 + dq^2
\]

with subscripts indicating differentiation and \( Z = \sqrt{1 + S^2_\rho} \). The Laplacian can be found straightforwardly from

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

but there is no advantage to writing the the Laplacian explicitly until the constraint that places the particle on the surface is effected.

Consider a situation where a large confining potential everywhere normal to \( S \) acts to restrict the particle to \( S \). This potential, called \( V_n(q) \) here, could take a hard wall or oscillator form, but however chosen it causes \( q \to 0 \). In this limit the wave function is expected to decouple into surface and normal parts, or in the language of [13], into “fast” and “slow” functions

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

Conservation of the norm in the decoupled limit implies [11,14,15]

\[
|\Psi|^2 W dS dq = |\chi_s|^2 |\chi_n|^2 dS dq
\]

where \( W = 1 + 2qH + q^2K \) and \( dS \) the surface measure. \( H, K \) are the mean and Gaussian curvatures given by

\[
H = \frac{1}{2} (k_1 + k_2),
\]

\[
K = k_1 k_2.
\]

Write

\[
\Psi = \frac{\chi_s \chi_n}{\sqrt{W}}
\]

and insert the right hand side of equation (10) into the time independent Schrödinger equation. Performing the differentiations and taking \( q \to 0 \) gives the pair of equations

\[
- \frac{1}{2} \left[ \frac{1}{Z^2} \frac{\partial^2}{\partial \rho^2} + \frac{1}{Z \rho} \frac{\partial}{\partial \rho} - \frac{Z \rho}{Z^3} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + (H^2 - K) \right] \chi_s = E_s \chi_s
\]

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

The curvature potential \( V_C \) is

\[
V_C = - \frac{1}{2} [H^2 - K].
\]

The surface given by equation (1) was chosen to illustrate that there are modifications to the Laplacian (aside from the appearance of \( V_C \)) even for surfaces possessing symmetry. In
[16] it was shown that kinetic energy modifications for some parameterizations of $S(\rho)$ can be small, but it is easy to conceive of cases where the contrary would be true.

Now apply the above procedure to the torus. Let $F = R + a \cos \theta$. Points near the surface of the torus may be parameterized as

$$\mathbf{x}(\theta, \phi, q) = F \mathbf{e}_\rho + a \sin \theta \mathbf{e}_z + q \mathbf{e}_n.$$  \hfill (14)

Proceeding as above gives the constraint and curvature modified Hamiltonian

$$H = -\frac{1}{2} \left[ \frac{1}{a^2 \partial \theta^2} + \frac{\sin \theta}{aF} \frac{\partial}{\partial \theta} + \frac{1}{F^2 \partial \phi^2} + \frac{R^2}{a^2} \frac{1}{4F^2} \right]$$

$$\quad = H_0 - \frac{R^2}{a^2} \frac{1}{8F^2} \equiv H_0 + V_C.$$ \hfill (15)

In equation (16), $H_0$ is identical to $-\frac{1}{2} \nabla^2$ derived from eq. (14) with $q = 0$; it is the Hamiltonian for particle on a toroidal surface subject to no other potential [17] (it proves convenient to refer to the zero potential case as the free system). In contrast to the operator that appears in equation (11), no surface dependent prefactors, i.e. $Z(\rho)$ or additional terms modifying $H_0$ are present. It is interesting to compare equation (15) to the corresponding operator for spherical and cylindrical surfaces; for those surfaces the constraint procedure gives a coordinate independent $V_C$ behaving as $\sim -1/R^2$ [18] and again no modifications to $H_0$. This point will be discussed further in section 4.

3. Solution method; results.

Setting $\alpha = \frac{a}{R}, \beta = 2Ea^2$ and making the standard ansatz for the azimuthal eigenfunction $\chi(\phi) = \exp[im\phi]$ in equation (15) gives

$$\frac{\partial^2 \psi}{\partial \theta^2} - \frac{\alpha \sin \theta}{[1 + \alpha \cos \theta]} \frac{\partial \psi}{\partial \theta} - \frac{(m^2a^2 - \frac{1}{4})}{[1 + \alpha \cos \theta]^2} \psi + \beta \psi = 0.$$ \hfill (17)

Equation (17) can be solved numerically, but it is convenient to have approximate analytic representations of its eigenfunctions. Recently a method was found for obtaining closed form solutions for zero energy states and for surface potentials $V_S(\theta)$ which satisfy an auxiliary condition derivable from $H_0$ [19]. However, the $V_S(\theta) = 0$ case is no more easily solved with the method given in [19] than the method employed below.

Solutions of equation (17) can be found by defining $z = \exp[i\theta]$ and writing

$$\psi(z) = \sum_{n=-\infty}^{\infty} c_n z^n.$$ \hfill (18)

The Hamiltonian given by equation (15) is invariant under $\theta \to -\theta$, so the solutions of equation (17) can be split into odd and even parity eigenfunctions, yielding a series in sines for negative parity states and cosines for positive parity states. Computing the eigenvalues and eigenfunctions of equation (17) follows from a method given in detail in [17].
Table 1 shows eigenvalues and wave functions for $\alpha = 3/4, 1/2, 1/4, 1/20$ for those $m$ values which yield $\beta < 0$ states (only three states are given for $\alpha = 1/20$; there are nine total). No negative parity states appear in table 1. In table 2 wave functions for states corresponding to those in table 1 with $V_C$ shut off are given. As evidenced in table 2, the ground state $m = 0$ wave function of $H_0$ for any $\alpha$ is a constant. A natural question is: Should the $V_C \neq 0$ ground state wave function be compared to the constant wave function or the lowest $\beta \neq 0$ wave function? Here the constant wave function was chosen on the grounds that it is the state actually altered from its constant value by $V_C$.

4. Conclusions.

In this brief report wave functions for bound states of a particle constrained to the surface of a torus were obtained for several values of $\alpha = a/R$. Constraint and curvature effects were shown to alter the angular dependence of the free particle STWs.

An interesting consequence of equation (17) is manifested by the results presented in table 1. For $m \neq 0$, $\alpha = \frac{1}{2m}$ provides a cutoff for the existence of bound states. It follows that there are no $m \neq 0$ bound states for $\alpha > 1/2$. Additionally $\alpha = 1/2m$ provides a series of magic radii for which an $m \neq 0$ state of the constrained system maps exactly into the $m = 0$ state with the same $n$ and parity of the $V_C = 0$ free STW.

In section 2 it was stated that the torus shares with the sphere the property that constraint adds only a curvature potential to the Hamiltonian, leaving $\nabla^2$ on the surface unchanged. This comparable behavior is likely a consequence of the torus being the most symmetric compact genus one surface that can be embedded in $R^3$. It would be interesting to learn if there are higher genus surfaces embedded in $R^3$ for which $H = -\frac{1}{2} \nabla^2$ reduces to the lower dimensional operator $H_0$ plus a curvature potential upon imposing the condition given by equation (10). This question generalizes to $M < N$ dimensional surfaces embedded in $R^N$. 

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Acknowledgments

The authors would like to acknowledge useful discussions with Babak Etemadi. M.E. would like to thank Norman Melom for useful suggestions. Both authors received support from NASA grant NAG2-1439.

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Table 1: Eigenvalues and wave functions of equation (17) for four values of $\alpha$. Normalizations (not including the $(2\pi)^{-\frac{1}{2}}$ from the $\phi$ dependence) are in brackets proceeding the functions. Terms not shown are at least an order of magnitude smaller than those listed. There are no negative parity states with $\beta < 0$.

$$
\begin{array}{|c|c|c|}
\hline
\alpha & \beta & \Psi_{nm}(\theta); \ V_C \neq 0 \\
\hline
.75 & -1.0725 & \Psi_{10} = (.1298)[4.6072 - 5.2143 \cos \theta + 2.2465 \cos 2\theta - .9495 \cos 3\theta] \\
.50 & -0.3512 & \Psi_{10} = (.2455)[2.4509 - .9015 \cos \theta + .1921 \cos 2\theta] \\
.25 & -0.2673 & \Psi_{10} = (.3765)[2.1458 - .2916 \cos \theta + .0280 \cos 2\theta] \\
.25 & -0.1987 & \Psi_{11} = (.3826)[2.1069 - .2138 \cos \theta + .0197 \cos 2\theta] \\
.05 & -0.2506 & \Psi_{10} = (.8813)[2.0254 - .0508 \cos \theta] \\
.05 & -0.2481 & \Psi_{11} = (.8814)[2.0251 - .0507 \cos \theta] \\
.05 & -0.2406 & \Psi_{12} = (.8817)[2.0244 - .0487 \cos \theta] \\
\hline
\end{array}
$$

Table 2: Eigenvalues and wave functions of $H_0$ corresponding to those appearing in table 1.

$$
\begin{array}{|c|c|c|}
\hline
\alpha & \beta & \Psi_{nm}(\theta); \ V_C = 0 \\
\hline
.75 & 0.0000 & \Psi_{00} = .4607 \\
.50 & 0.0000 & \Psi_{00} = .5642 \\
.25 & 0.0000 & \Psi_{00} = .7979 \\
.25 & 0.0641 & \Psi_{11} = (.4073)[1.9676 + .0648 \cos \theta] \\
.05 & 0.0000 & \Psi_{00} = 1.7841 \\
.05 & 0.0025 & \Psi_{11} = (.8822)[1.9998 + .0005 \cos \theta] \\
.05 & 0.0010 & \Psi_{12} = (.8822)[1.9996 + .0002 \cos \theta] \\
\hline
\end{array}
$$