A note regarding Gram-Schmidt states on $T^2$

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Abstract

An efficient procedure for generating Gram-Schmidt states on a toroidal surface $T^2$ is presented. As an application of the method, low-lying eigenvalues and wave functions for an electron on $T^2$ subjected to a constant magnetic field are determined.

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Toroidal systems are relevant to fusion [1], heat transfer [2, 3], vibrational [4, 5, 6, 7], electromagnetic [8] and, recently, nanostructure physics [9, 10, 11, 12]. For problems restricted to the neighborhood of a toroidal surface, i.e., to those on or near toroidal shells, Gram-Schmidt (GS) functions on $T^2$ could potentially prove useful. As noted elsewhere, the calculation of higher order GS states may be time consuming and oftentimes subject to numerical error [6] when performed in a black-box fashion, particularly when trigonometric functions are employed as the primitive basis set and integrations are performed over a non-trivial integration measure. In this note we show that there exists a simple algorithm for constructing higher order GS functions on $T^2$ that eliminates these difficulties and proceed to apply the functions to the problem of an electron on $T^2$ in a magnetic field directed along the $z$-axis.

The geometry adopted here parameterizes a toroidal surface of major radius $R$ and minor radius $a$ in terms of cylindrical coordinate unit vectors by

$$r(\theta, \phi) = W(\theta)\rho + a \sin \theta k$$

with $W = R + a \cos \theta$. Applying $d$ to Eq.(1) gives

$$dr = a d\theta \, \theta + W d\phi \phi$$

with $\theta = -\sin \theta \rho + \cos \theta k$. The metric elements $g_{ij}$ can be read off of

$$dr \cdot dr = a^2 d\theta^2 + W^2 d\phi^2$$

so that the integration measure is

$$\sqrt{g} dq_1 dq_2 \to a W d\theta d\phi.$$  

(4)

It will prove useful in what follows to write the Laplacian derived from Eq. (3); it is [13]

$$\nabla^2 = \frac{1}{a^2} \frac{\partial^2}{\partial \theta^2} - \frac{\sin \theta}{aW} \frac{\partial}{\partial \theta} + \frac{1}{W^2} \frac{\partial^2}{\partial \phi^2}.$$  

(5)

The solutions of the Schrödinger equation derived from Eq. (5) can be taken of the form $\psi_n(\theta)e^{i\nu\phi}$ with $\nu \equiv$ integer. A procedure for determining free particle surface wave functions $\psi_n(\theta)$ has been given elsewhere [13] and extended to several special cases in [14, 15, 16]. However, if an arbitrary potential $V(\theta, \phi)$ is included in the Hamiltonian, many $\theta, \phi$ states may be necessary in a basis set expansion to achieve suitable convergence for the eigenvalues and wave functions of $H(\theta, \phi)$.

The $\theta \to -\theta$ symmetry of the Laplacian allows the solutions of the Schrödinger equation to be split into even and odd functions, and the primitive basis set can be taken to possess this property,

$$u_n(\theta) = \frac{1}{\sqrt{\pi}} \cos [n\theta], \quad v_n(\theta) = \frac{1}{\sqrt{\pi}} \sin [n\theta].$$  

(6)

Here for the sake of brevity, we will consider only the even functions in detail and later comment briefly on the simple modification needed for the odd functions. Setting $\alpha = a/R$
and \( F(\theta) = 1 + \alpha \cos \theta \), the simple but key point in what follows is the integrals encountered in the GS procedure (irrelevant factors of \( R \) and \( a \) are dropped)

\[
t_{n\bar{n}} = \int_{0}^{2\pi} u_n(\theta)u_{\bar{n}}(\theta)F(\theta)d\theta
\]

are non-zero only for

\[
t_{00} = 2, \quad t_{01} = \alpha;
\]

\[
t_{nn} = 1, \quad t_{n,n+1} = \alpha/2, \quad n > 0.
\]

Write

\[
\psi_n = \sum_{m=0}^{n} c_{nm}u_m,
\]

and use Eqs. (7) - (9) in the standard GS procedure; the first few GS states are sufficient to illustrate the general pattern that emerges (\( \beta = \alpha/2 \)),

\[
\psi_0 = u_0/\sqrt{2} \equiv N_0u_0
\]

\[
\psi_1 = N_1[u_1 - N_0\beta N_0u_0]
\]

\[
\psi_2 = N_2[u_2 - N_1\beta N_1u_1 + N_1\beta N_1N_0\beta N_0u_0]
\]

\[
\psi_3 = N_3[u_3 - N_2\beta N_2u_2 + N_2\beta N_2N_1\beta N_1u_1 - N_2\beta N_2N_1\beta N_1N_0\beta N_0u_0]
\]

\[\vdots\]

from which it is apparent that

\[
c_{nm} = (-)^{n+m}N_1(N_{n-1}\beta N_{n-1})(N_{n-2}\beta N_{n-2})...(N_m\beta N_m).
\]

To obtain the \( c_{nm} \) the normalization factors must be determined. Consider the \( k^{th} > 1 \) unnormalized state \( \Phi_k \); it is easy to establish \( N_k \) from

\[
<\Phi_k|\Phi_k> = 1 - N_{k-1}\beta N_{k-1}
\]

since all \( <u_i|u_{i+j}> \) vanish for \( j > 1 \). Starting then from \( N_1^2 = (1 - 2\beta^2)^{-1} \), for \( k > 1 \) the squared normalization for a given \( \Phi_k \) is

\[
N_{k+1}^2 = \frac{1}{1 - \beta^2 N_k^2}.
\]

In summary, Eq. (17) serves to generate all normalization factors and Eq. (15) the GS coefficients. The sinusoidal function coefficients may be obtained by the method employed above by starting with \( c_{11} \) rather than \( c_{00} \) and letting \( N_1 = 1 \).
It is worth noting that from Eq. (15) the ratio of successive coefficients within a given
\((n, m)\) series
\[
c_{n,m} / c_{n,m+1} = -N_m \beta N_m
\]  
allows for truncation approximations to be made for certain problems. To illustrate this
point, write Eq. (17) in continued fraction form; taking for example \(N_4\) (which is the largest
\(N_k\) that can be comfortably typeset),
\[
N_4^2 = \frac{1}{1 - \frac{\beta^2}{1 - \frac{\beta^2}{1 - \frac{\beta^2}{1 - 2\beta^2}}}} .
\]  
Any symbolic algebra program can be utilized to evaluate this expression, but once known
to a given order of \(\alpha = 2\beta\) it need not be evaluated any further. To \(O(\alpha^8)\) which occurs at
\(N_5\),
\[
N_5^2 = 1 + \frac{\alpha^2}{4} + \frac{\alpha^4}{8} + \frac{5\alpha^6}{64} + \frac{7\alpha^8}{128} + O(\alpha^{10}) + ..., \quad (20)
\]
and a final \(\frac{2}{3}\) factor multiplies the expression of Eq. (20) to establish right hand side of
Eq. (18). Since \(\alpha < 1\), concatenating several \(N_\beta N\) factors causes the series to converge
rapidly for larger \(n\) and smaller \(m\). For quantum mechanical applications, the kinetic energy
operator yields an \(m^2\) factor for each term in the expansion given by Eq. (10), making it
possible to truncate higher states at say, three terms for sufficiently large \(n\) (as set by the
particular problem)
\[
\psi_n(\theta) = c_{nn} \cos n\theta + c_{n,n-1} \cos (n - 1)\theta + c_{n,n-2} \cos (n - 2)\theta . \quad (21)
\]
An obvious immediate application for the GS states of relevance to nanoscience \[9, 11, 12\]
is the problem of an electron on \(T^2\) in the constant magnetic field
\[
B = B_0 k . \quad (22)
\]
In the Coulomb gauge \(\nabla \cdot A = 0\) the vector potential \(A(\theta, \phi) = \frac{1}{2}B \times r\) as expressed in
surface variables is
\[
A(\theta, \phi) = \frac{B_0 RF}{2} \phi . \quad (23)
\]
The Schrödinger equation (here the spin splitting is neglected)
\[
H = \frac{1}{2m} \left( \frac{\hbar}{i} \nabla + qA \right)^2 \Psi = E\Psi \quad (24)
\]
is more simply expressed if we first define
\[
\gamma_0 = B_0 \pi R^2 \quad \gamma_N = \frac{\pi \hbar}{q}
\]
\[ \tau_0 = \frac{\gamma_0}{\gamma_N} \]
\[ \varepsilon = \frac{2m_e E a^2}{\hbar^2} \]

after which Eq. (24) may be put in the form

\[
\left( \frac{\partial^2}{\partial \theta^2} - \frac{\alpha}{F} \sin \theta \frac{\partial}{\partial \theta} + \frac{\alpha^2}{F^2} \frac{\partial^2}{\partial \phi^2} + i \tau_0 \alpha^2 \frac{\partial}{\partial \phi} - \frac{\tau_0^2 \alpha^2 F^2}{4} + \varepsilon \right) \Psi = 0
\]

(25)

\[ \equiv (H_\tau + \varepsilon) \Psi = 0. \]  

(26)

The basis expansion functions are taken as per Eqs. (11) - (14) with azimuthal eigenfunctions appended (the magnetic field term considered here does not cause even (+) and odd (-) functions to mix),

\[
\psi_{n\nu}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} \sum_m c_{nm}^{\pm} \begin{pmatrix} u_m(\theta) \\ v_m(\theta) \end{pmatrix} e^{i\nu\phi}. \]  

(27)

The matrix

\[ H_{\tau n\bar{n}} = \langle \bar{n} | H_\tau | n \rangle \]  

(28)

is then easily constructed since the matrix elements can all be written in closed form, and the eigenvalues and eigenvectors determined with a six-state expansion for each \( \theta \)-parity [17] (no truncations were performed).

Table 1 gives the even function ground and first excited state energy eigenvalues and wave functions for several values of \( \nu \) and \( \tau_0 \). Table 2 gives the same for the odd functions [18]. Three decimal place accuracy was achieved for the eigenvalues/wave functions for four of the six states generated from \( H_{\tau n\bar{n}} \) when \( \tau_0 = 10 \), which corresponds to a field of 2.6 \( T \) for a torus with \( R = 50 \) nm. Although a large scale treatment of this problem was considered outside the scope of this work, it should be noted that because the basis states are so simple to generate the only inherent limitation to such a treatment is the matrix inversion. Additionally, the matrix elements of the Hamiltonian for an off-axis magnetic field that comprises the general case

\[ \mathbf{B} = B_x \mathbf{i} + B_z \mathbf{k} \]  

(29)

can also be done in closed form given sufficient patience [10].

In conclusion, we have presented an algebraic method to derive GS states on \( T^2 \) with very little effort. The ability to obtain these functions rapidly may prove of use to problems in the areas mentioned in the opening paragraph of this note. As an example of their utility, we have used them to calculate the spectra of an electron on the surface of a torus in the presence of a magnetic field.

Acknowledgments

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[18] Parity here has only referred to the evenness/oddness of the basis functions; in general the quantum mechanical parity will depend on the azimuthal quantum number.

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TABLE 1: Even function (the (+) superscript has been suppressed) ground and first excited state energies and wave functions. GS state coefficients not shown in the table are much smaller than those given. $-\nu$ states are trivially obtained from those given below.

| $\nu$ | $\tau_0$ | $\varepsilon_0$ | $\psi_0$ | $\varepsilon_1$ | $\Psi_1$ |
|-------|----------|-----------------|----------|----------------|--------|
| 0     | 0        | 0               | $\psi_0$ | 1.122          | $.997\psi_1 - .082\psi_2 + .014\psi_3$ |
| 0     | 5        | .139            | $.840\psi_0 - .533\psi_1 + .099\psi_2 | 3.208 | $.531\psi_0 + .772\psi_1 - .345\psi_2$ |
| 0     | 10       | -.747           | $.744\psi_0 - .637\psi_1 + .198\psi_2 | 7.925 | $.466\psi_0 + .289\psi_1 - .751\psi_2$ |
| 1     | 0        | .249            | -.987\psi_0 - .162\psi_1 + .021\psi_2 | 1.1663 | -.162\psi_0 + .987\psi_1 + .006\psi_2 |
| 1     | 5        | 1.955           | $.882\psi_0 - .469\psi_1 + .052\psi_2 | 4.806 | $.462\psi_0 + .838\psi_1 - .289\psi_2$ |
| 1     | 10       | 2.429           | $.759\psi_0 - .627\psi_1 + .176\psi_2 | 10.927 | -.457\psi_0 - .327\psi_1 - .755\psi_2 - .333\psi_3 |
| 2     | 0        | .795            | $.931\psi_0 + .364\psi_1 - .018\psi_2 | 3.175 | -.342\psi_0 + .891\psi_1 + .296\psi_2 |
| 2     | 5        | 4.569           | $.973\psi_0 - .221\psi_1 - .068\psi_2 | 7.198 | $.217\psi_0 + .973\psi_1 - .063\psi_2 |
| 2     | 10       | 6.851           | -.803\psi_0 + .587\psi_1 - .105\psi_2 | 14.940 | $.423\psi_0 + .448\psi_1 - .7747\psi_2 + .247\psi_3 |

TABLE 2: Odd function (the (-) superscript has been suppressed) ground and first excited state energies and wave functions. GS state coefficients not shown in the table are much smaller than those given. $-\nu$ states are trivially obtained from those given below.

| $\nu$ | $\tau_0$ | $\varepsilon_0$ | $\psi_0$ | $\varepsilon_1$ | $\Psi_1$ |
|-------|----------|-----------------|----------|----------------|--------|
| 0     | 0        | .977            | $.996\psi_1 - .086\psi_2 | 4.033 | -.087\psi_1 - .991\psi_2 + .103\psi_3 |
| 0     | 5        | 2.510           | $.948\psi_1 - .316\psi_2 + .047\psi_3 | 5.834 | -.317\psi_1 - .914\psi_1 + .250\psi_3 |
| 0     | 10       | 5.749           | $.757\psi_1 - .617\psi_2 + .210\psi_3 | 11.128 | $.600\psi_1 + .530\psi_2 - .569\psi_3 |
| 1     | 0        | 1.264           | $.999\psi_1 - .037\psi_1 | 4.411 | -.036\psi_1 - .997\psi_2 + .067\psi_3 |
| 1     | 5        | 4.125           | $.963\psi_1 - .269\psi_2 + .026\psi_3 | 7.441 | -.268\psi_1 - .938\psi_2 + .218\psi_3 |
| 1     | 10       | 8.760           | $.776\psi_1 - .602\psi_2 + .186\psi_3 | 14.000 | -.581\psi_1 - .567\psi_2 + .558\psi_3 - .166\psi_4 |
| 2     | 0        | 2.041           | -.995\psi_1 + .069\psi_2 | 5.532 | $.088\psi_1 - .995\psi_2 - .046\psi_3 |
| 2     | 5        | 6.359           | $.991\psi_1 - .132\psi_2 - .022\psi_3 | 9.774 | $.129\psi_1 + .985\psi_2 - .113\psi_3 |
| 2     | 10       | 12.710          | -.829\psi_1 + .548\psi_2 - .115\psi_3 | 17.611 | $.518\psi_1 + .676\psi_2 - .513\psi_3 + .107\psi_4 |