Wave functions in the neighborhood of a toroidal surface; hard vs. soft constraint

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The curvature potential arising from confining a particle initially in three-dimensional space onto a curved surface is normally derived in the hard constraint $q \to 0$ limit, with $q$ the degree of freedom normal to the surface. In this work the hard constraint is relaxed, and eigenvalues and wave functions are numerically determined for a particle confined to a thin layer in the neighborhood of a toroidal surface. The hard constraint and finite layer (or soft constraint) quantities are comparable, but both differ markedly from those of the corresponding two dimensional system, indicating that the curvature potential continues to influence the dynamics when the particle is confined to a finite layer. This effect is potentially of consequence to the modelling of curved nanostructures.

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I. INTRODUCTION

The existence of a potential $V_C$ in the Schrodinger equation which stems from constraining a particle to a one or two-dimensional surface embedded in three dimensions has a long history [1, 2, 3, 4, 5, 6]. The manifestations of $V_C$ have been investigated through formal and numerical means [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17], motivated recently in part by the sophistication with which nanostructures can be fabricated. The physics of objects with novel geometries is increasingly relevant to the modelling of real devices, hence substantial effort has been directed towards understanding the physics of bent tubes and wires, as well as more complicated shapes [18, 19, 20, 21, 22, 23, 24].

Consider a surface $\Sigma(u,v)$ with $(u,v)$ surface coordinates and define $q$ as the coordinate labelling the degree of freedom normal to $\Sigma(u,v)$. Generally $V_C$ (as detailed in the following section) is derived by imposing a hard constraint on the particle wherein a $q \to 0$ limit is taken along with a wave function re-scaling such that the norm is preserved. Here, rather than imposing a hard constraint, the particle will be confined to a thin layer in the neighborhood of a toroidal surface. The extent to which the hard constraint mirrors the more physically realizable soft constraint is then determined by calculating some low-lying eigenvalues and eigenfunctions of the system.

There are several reasons to investigate these ideas with a toroidal structure:

1. The symmetry of the torus reduces computational intensiveness, but, because a torus has non-trivial mean and Gaussian curvatures, curvature effects remain important [25].

2. The spectrum and eigenfunctions for a particle on a toroidal surface have been determined [26], so comparisons can be made between the finite layer system and the two dimensional system both with and without $V_C$ present.

3. Toroidal structures have been fabricated and calculations addressing their transport [27, 28, 29, 30] and magnetic [31] properties performed. Toroidal structures are novel because unlike a bulk sample, conductivity through the device is anticipated to be dominated by azimuthal modes.

The remainder of this paper is organized as follows: in section II, $H_q$, the Hamiltonian for a particle near a toroidal surface is derived. The hard constraint $q \to 0$ limit of that Hamiltonian is then taken; under the requirement that the norm of the wave function be preserved, $H_C$ obtains. Finally, the ab initio Hamiltonian $H_0$ is written. In section III the computational method employed to generate eigenvalues and wave functions is presented. Section IV gives results and section V is reserved for conclusions.

II. THE TOROIDAL SCHRODINGER EQUATIONS

To restate, there are three Hamiltonians relevant to this work:

1. $H_q$ will be the Hamiltonian for a particle allowed to move in a thin layer normal to $T^2$, where again the normal degree of freedom will be labelled by $q$.

2. $H_C$ will be the Hamiltonian derived from $H_q$ after imposing the $q \to 0$ hard constraint, and

3. $H_0$ the Hamiltonian for a particle restricted ab initio to $T^2$, i.e., $q = 0$ at the onset of the derivation of $H_0$.

It is best to begin with the most general case, that of $H_0$, and later take the appropriate limits to obtain $H_C$ and $H_0$.

Points near a toroidal surface of major radius $R$ and minor radius $a$ may be parameterized in terms of cylindrical coordinate unit vectors and a vector $\hat{n}$ normal to the surface by

$$\mathbf{r}(\theta, \phi, q) = (R + a \cos \theta) \hat{\rho} + a \sin \theta \hat{\phi} + q \hat{n}. \quad (1)$$

The curvature potential $V_C$ in the hard constraint $q \to 0$ limit, with $q$ the degree of freedom normal to $\Sigma(u,v)$. Generally $V_C$ has been investigated through formal and numerical means [7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17], motivated recently in part by the sophistication with which nanostructures can be fabricated. The physics of objects with novel geometries is increasingly relevant to the modelling of real devices, hence substantial effort has been directed towards understanding the physics of bent tubes and wires, as well as more complicated shapes [18, 19, 20, 21, 22, 23, 24].

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$$\mathbf{r}(\theta, \phi, q) = (R + a \cos \theta) \hat{\rho} + a \sin \theta \hat{\phi} + q \hat{n}. \quad (1)$$
Applying $d$ to Eq. (2) gives
\[ d\mathbf{r} = (a + q) d\theta \hat{j} + (R + (a + q) \cos \theta)d\phi \hat{k} + dq \hat{i} \]  
(2)
with $\hat{n} \equiv \hat{\phi} \times \hat{j}$, and $\hat{\Theta} = -\sin \theta \hat{\rho} + \cos \theta \hat{k}$. The metric elements $g_{ij}$ can be read off of
\[ d\mathbf{r} \cdot d\mathbf{r} = (a + q)^2 d\theta^2 + (R + (a + q) \cos \theta)^2 d\phi^2 + dq^2 \]  
(3)
and the Laplacian derived from
\[ \nabla^2 = g^{-\frac{1}{2}} \frac{\partial}{\partial q^i} \left[ g^{ij} \frac{\partial}{\partial q^j} \right]. \]  
(4)
Setting $a_q = a + q$ and $F_q = R + (a + q) \cos \theta$ yields the $H_q$ Schrodinger equation
\[ \frac{1}{a_q^2} \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\sin \theta}{a_q F_q} \frac{\partial \psi}{\partial \theta} + \frac{1}{F_q^2} \frac{\partial^2 \psi}{\partial \phi^2} + 2\hbar \frac{\partial \psi}{\partial q} + \frac{\partial^2 \psi}{\partial q^2} - 2V_n(q) + 2E \psi = 0 \]  
(5)
Making the standard ansatz for the azimuthal part of the eigenfunction $\chi(\phi) = \exp[im\phi]$ reduces Eq. (11) to
\[ \frac{\partial^2 \psi}{\partial \theta^2} - \frac{\alpha \sin \theta}{1 + \alpha \cos \theta} \frac{\partial \psi}{\partial \theta} + \frac{m^2 \alpha^2 - 1}{1 + \alpha \cos \theta} \psi + \beta \psi = 0. \]  
(14)
Eq. (14) is the Schrodinger equation that corresponds to $H_C$. It is the analog to Eq. (5) wherein the $q$ dependence has decoupled from the the angular part of the kinetic energy operator and a curvature potential $V_C$ results from insisting upon conservation of the norm.

The Hamiltonian $H_0$ for a particle that lives on the surface may be obtained by the method employed to derive $H_q$ by setting $q = 0$ in Eq. (1) from which
\[ d\mathbf{r} \cdot d\mathbf{r} = a^2 d\theta^2 + (R + a \cos \theta)^2 d\phi^2. \]  
(15)
The resulting expression is simple; $H_0$ is Eq. (11) with $V_C$ omitted. It should be emphasized that for more complicated surfaces the kinetic energy operator will have terms depending on the surface curvature not present here because of the azimuthal symmetry of the torus. The normalization of an eigenfunction is determined by
\[ \int_{q_1}^{q_2} \int_0^{2\pi} \int_0^{2\pi} \psi^* (q, \theta, \phi) \psi(q, \theta, \phi) M(\theta, q) d\theta d\phi dq = 1. \]  
(16)
with
\[ M(\theta, q) = a_q F_q \]  
(17)
when $q \neq 0$. Wave functions obtained from $H_{0,C}$ are normalized with $M(\theta, 0)$ and the $q$ integration omitted.

### III. Computational Method

The goal is to obtain eigenvalues/functions of $H_q$ that can be compared to those of $H_C$ and $H_0$. A procedure for determining the low-lying eigenvalues and eigenfunctions of $H_0$ has been given in [20] and applied to $H_C$ in [23] so the focus here may be placed on the method employed for
solving Eq. (5). In the $q \to 0$ limit the surface solutions are independent of the specific choice of $V_n(q)$, but for finite $q$ a form or forms for $V_n(q)$ must be settled upon. Two convenient choices are hard wall confinement with the walls at $\pm L/2$ and an oscillator potential $V_n(q) = \omega^2 q^2/2$.

The main complication in solving Eq. (5) ensues from the integration measure for the geometry described by Eq. (3), which precludes adopting a simple basis set of trigonometric functions in $\theta$ since they are not in general orthogonal over $M(\theta, q)$. It should also be noted that for finite $q$ it is not possible to recover orthogonality by rescaling the basis states because the resulting Hamiltonian matrix is not Hermitian. These difficulties can be avoided if one performs a two-variable Gram-Schmidt procedure.

Because the interest here is focused on issues other than generating a large number of eigenfunctions, two basis functions in $q$ and three in $\theta$ were used. This is a reasonable ansatz; the $q$ motion will produce an energy spectrum with much larger spacing than the $\theta, \phi$ motion, so two functions in $q$ are sufficient to insure nothing is missed. Additionally, it has been shown previously \[26\] that only a few trigonometric functions in general are necessary to accurately describe an eigenfunction on $T^2$.

For hard walls the basis functions with $n = (0, 1, 2)$ are

$$\Phi_{hw}^{0n} = \cos\left(\frac{\pi q}{L}\right)\cos(n\theta) \quad (18)$$
$$\Phi_{hw}^{1n} = \sin\left(\frac{2\pi q}{L}\right)\cos(n\theta) \quad (19)$$

and for oscillator confinement

$$\Phi_{osc}^{0n} = e^{-\omega q^2} \cos(n\theta) \quad (20)$$
$$\Phi_{osc}^{1n} = e^{-\omega q^2} H_1(\sqrt{\omega q})\cos(n\theta) \quad (21)$$

For each case the six states computed from the Gram-Schmidt procedure are employed to construct the matrix

$$H_{hw, osc}^{i j m n} = \langle \Phi_{hw, osc}^{i m}| H_q | \Phi_{hw, osc}^{j n}\rangle \quad (22)$$

that yields eigenvalues and wave functions.

**IV. RESULTS**

Toroidal radii $R = 500\text{\,Å}$ and $a = 250\text{\,Å}$ were chosen on the order of structures that have been synthesized \[34, 35\], and surface layer widths as set by $L, \omega$ within realistic values for confinement regions. It should be emphasized that the results which follow are very representative; the trends exhibited below were found to obtain for larger values of $R, a$, and $L$ as well as for $m \neq 0$ and negative parity states.

In Table I the spectra for hard wall and oscillator confinement potentials with $L = 25, 10 \text{\,Å}$ and $\omega = .05, .1$ A$^{-2}$ respectively are shown. The dimensionless eigenvalues $\beta_i$ are found from subtracting the $q$ degree of freedom energy ($\pi^2/2L^2$ or $\omega/2$) from the eigenvalues found from the Hamiltonian matrix defined through Eq. (22) and multiplying by $2a^2$. The $\beta_i$ are compared to those found in \[25\] where $V_C$ was included in $T^2$ Hamiltonian and in \[26\] where it was not. These results indicate the soft constraint quantities are relatively insensitive to differing $L$ and $\omega$, and are better matched by the spectra of \[25\]. In tables II and III the ground and first excited state wave functions for the six cases described above are shown. The results illustrate that hard constraint eigenvalues and eigenfunctions are very good approximations to the physically realistic soft constraint values, at least for cases where the length scale that determines the surface energies of the system is near the curvature length scale of the device. Here that scale is set by the minor radius $a$; however, in general as the length scale that sets local curvature becomes small, $V_C$ increases such that $\langle \Phi| V_C | \Phi\rangle$ matrix elements may become comparable to the largest energy in the system. For a disc or strip structure the scales can be very different. In the case of a disk for example, the energy scale is set by the radius of the disk, but a bump or ripples can be placed on the disc at much smaller scales \[16, 17\]. Although the results here are relatively independent of whether hard wall or oscillator confinement was used, it was found that some care must be taken with the choice of $V_n(q)$. If instead of using hard walls at $\pm L/2$, the walls are placed at $0$ and $L$, agreement with the hard constraint spectrum is lessened, though by only of order ten percent in both the eigenvalues and wave function expansion coefficients. A possible explanation for this is the $\sin(n\pi q/L)$ functions always vanish on the $q = 0$ surface so that some terms that multiply curvature functions are zero there.

The basis set expansion employed here comprises two functions in the $q$ degree of freedom; for the sake of brevity, only angular eigenvalues/eigenfunctions which belong to the $q$ ground state wave function have been reported. The surface states that correspond to excited normal modes lie much higher in energy than the low-lying surface excitations dealt with here, but may prove important to device modelling as the $q$-motion becomes more diffusive.

**V. CONCLUSIONS**

The main result of this paper is the good agreement between the low-lying spectra and eigenfunctions resulting from $H_0$ and those that emerge from $H_q$ and, as importantly, the relative disagreement that the eigenfunctions of $H_q$ display when contrasted to those of $H_0$. If a two-dimensional approximation is to be adopted for curved nanostructures, the results here indicate that for cases where the normal excitations are unimportant the physics would be better captured with $H_0 + V_C$ than with $H_0$. 


TABLE I: Ground, first and second excited state eigenvalues \( \beta \) for the six Hamiltonians relevant to this paper with \( R = 500 \, \text{Å} \) and \( a = 250 \, \text{Å} \).

| \( L = 25 \, \text{Å} \) | \( L = 10 \, \text{Å} \) | \( \omega = 0.5 \, \text{Å}^{-2} \) | \( \omega = 1 \, \text{Å}^{-2} \) | \( \text{Ref.} \) [25] | \( \text{Ref.} \) [26] |
|---|---|---|---|---|---|
| \( \beta_0 \) | -3.406 | -3.408 | -3.489 | -3.988 | -3.511 |
| \( \beta_1 \) | .6618 | .6610 | .6515 | .6446 | .6386 |
| \( \beta_2 \) | 4.0520 | 3.7886 | 3.7876 | 3.7919 | .3405 |

TABLE II: Ground state wave functions; coefficients are normalized to the constant term in the series to facilitate comparisons. Terms not shown are at least an order of magnitude smaller than those given.

| \( \psi_0(\theta, q) \) | \( L = 25 \, \text{Å} \) | \( (1 - 0.3676 \cos \theta + 0.0693 \cos 2\theta) \cos \frac{q}{2L} \) |
|---|---|---|
| \( L = 10 \, \text{Å} \) | \( (1 - 0.3675 \cos \theta + 0.0693 \cos 2\theta) \cos \frac{q}{2L} \) |
| \( \omega = 0.5 \, \text{Å}^{-2} \) | \( (1 - 0.3580 \cos \theta + 0.0669 \cos 2\theta) e^{-0.5q^2} \) |
| \( \omega = 1 \, \text{Å}^{-2} \) | \( (1 - 0.3567 \cos \theta + 0.0654 \cos 2\theta) e^{-0.5q^2} \) |

Ref. [25] 1 | Ref. [26] 1

TABLE III: First excited state wave functions; coefficients are normalized to the dominant \( \cos \theta \) term in the series to facilitate comparisons. Terms not shown are at least an order of magnitude smaller than those given.

| \( \psi_1(\theta, q) \) | \( L = 25 \, \text{Å} \) | \( (-0.0842 + \cos \theta - 0.1369 \cos 2\theta) \cos \frac{q}{2L} \) |
|---|---|---|
| \( L = 10 \, \text{Å} \) | \( (-0.0842 + \cos \theta - 0.1370 \cos 2\theta) \cos \frac{q}{10L} \) |
| \( \omega = 0.5 \, \text{Å}^{-2} \) | \( (-0.0879 + \cos \theta - 0.1358 \cos 2\theta) e^{-0.25q^2} \) |
| \( \omega = 1 \, \text{Å}^{-2} \) | \( (-0.0877 + \cos \theta - 0.1362 \cos 2\theta) e^{-0.5q^2} \) |

Ref. [25] | \( -0.0851 + \cos \theta - 0.1540 \cos 2\theta \) |

Ref. [26] | \( -0.2500 + \cos \theta - 0.0820 \cos 2\theta \) |

[1] H. Jensen and H. Koppe, Ann. of Phys. 63, 586 (1971).
[2] R. C. T. da Costa, Phys. Rev. A 23, 1982 (1981).
[3] R. C. T. da Costa, Phys. Rev. A 25, 2893 (1982).
[4] P. Exner and P. Seba, J. Math. Phys. 30, 2574 (1989).
[5] S. Matusani, J. Phys. Soc. Jap. 61, 55 (1991).
[6] M. Burgess and B. Jensen, Phys. Rev. A 48, 1861 (1993).
[7] P. Duclos and P. Exner, Rev. Math. Phys. 7, 73 (1995).
[8] J. Londergan, J. Carini, and D. Murdock, *Binding and scattering in two dimensional systems; applications to quantum wires, waveguides, and photonic crystals* (Springer-Verlag, Berlin, 1999).
[9] J. Goldstone and R. L. Jaffe, Phys. Rev. B 45, 14100 (1991).
[10] P. Ouyang, V. Mohta, and R. L. Jaffe, Ann. of Phys. 275, 297 (1998).
[11] I. Popov, Phys. Lett. A 269, 148 (2000).
[12] S. Midgley and J. Wang, J. Phys. A 53, 77 (2000).
[13] I. J. Clark and A. J. Bracken, J. Phys. A 29, 4527 (1996).
[14] P. C. Schuster and R. L. Jaffe, J. Phys. B 307, 132 (2003).
[15] M. Encinosa and B. Etemad, Phys. Rev. A 58, 77 (1998).
[16] M. Encinosa and B. Etemad, Physica B 266, 361 (1998).
[17] M. Encinosa, IEEE Trans. Elec. 47, 878 (2000).
[18] K. Lin and R. L. Jaffe, Phys. Rev. B 54, 5757 (1996).
[19] A. Chaplik and R. H. Blick, New J. Phys. 6, 33 (2004).
[20] S. Qu and M. Geller, Phys. Rev. B 70, 085414 (2004).
[21] B. Nilsson, cond-mat/0103029.
[22] L. Mott, M. Encinosa, and B. Etemad, quant-ph/0406074, accepted for publication in Physica E.