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Electron wave functions on T^2 in a static magnetic field of arbitrary direction

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Abstract

A basis set expansion is performed to find the eigenvalues and wave functions for an electron on a toroidal surface T^2 subject to a constant magnetic field in an arbitrary direction. The evolution of several low-lying states as a function of field strength and field orientation is reported, and a procedure to extend the results to include two-body Coulomb matrix elements on T^2 is presented.

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1. Introduction

Quantum dots with novel geometries have spurred considerable experimental and theoretical interest because of their potential applications to nanoscience. Ring and toroidal structures in particular have been the focus of substantial effort because their topology makes it possible to explore Ahranov–Bohm and interesting transport phenomena [1–4]. Toroidal InGaAs devices have been fabricated [5–8] and modelled, [9] and toroidal carbon nanotube structures studied by several groups [4,10,11].

This work is concerned with the evolution of one-electron wave functions on T^2 in response to a static magnetic field in an arbitrary direction. The problem of toroidal states in a magnetic field has been studied with various levels of mathematical sophistication. Onofri [12] has employed the holomorphic gauge to study Landau levels on a torus defined by a strip with appropriate boundary conditions and Narnhofer has analyzed the same in the context of Weyl algebras [13]. Here, the aim is to do the problem with standard methodology: develop a Schrödinger equation inclusive of surface curvature, evaluate the vector potential on that surface, and proceed to diagonalize the resulting Hamiltonian matrix.

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As noted in Ref. [14], ideally one would like to solve the N-electron case, but the single particle problem is generally an important first step, and while the N electron system on flat and spherical surfaces has been studied [15–20], the torus presents its own difficulties. In an effort to partially address this issue, the evaluation of Coulombic matrix elements on T^2 is also discussed here.

This paper is organized as follows: in Section 2, the Schrödinger equation for an electron on a toroidal surface in the presence of a static magnetic field is derived. In Section 3, a brief exposition on the basis set employed to generate observables is presented. Section 4 gives results. Section 5 develops the scheme by which this work can be extended to the two-electron problem on T^2, and Section 6 is reserved for conclusions.

2. Formalism

The geometry of a toroidal surface of major radius R and minor radius a may be parameterized by

$$\mathbf{r}(\theta, \phi) = W(\theta)\boldsymbol{\rho} + a \sin\theta \boldsymbol{k} \tag{1}$$

with

$$W = R + a\cos\theta, \tag{2}$$

$$\boldsymbol{\rho} = \cos\phi \mathbf{i} + \sin\phi \mathbf{j}. \tag{3}$$

The differential of Eq. (1)

$$\mathrm{d}\mathbf{r} = a\,\mathrm{d}\theta\boldsymbol{\theta} + W\,\mathrm{d}\phi\boldsymbol{\phi} \tag{4}$$

with $\boldsymbol{\theta} = -\sin\theta\boldsymbol{\rho} + \cos\theta\mathbf{k}$ yields for the metric elements g_{ij} on T^2

$$g_{\theta\theta} = a^2, \tag{5}$$

$$g_{\phi\phi} = W^2. \tag{6}$$

The integration measure and surface gradient that follow from Eqs. (5) and (6) become

$$\sqrt{g}\,\mathrm{d}q^1\,\mathrm{d}q^2 \to aW\,\mathrm{d}\theta\,\mathrm{d}\phi \tag{7}$$

and

$$\nabla = \boldsymbol{\theta}\frac{1}{a}\frac{\partial}{\partial\theta} + \boldsymbol{\phi}\frac{1}{W}\frac{\partial}{\partial\phi}. \tag{8}$$

The Schrödinger equation with the minimal prescription for inclusion of a vector potential $\mathbf{A}$ is

$$H = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla + q\mathbf{A}\right)^2 \Psi = E\Psi. \tag{9}$$

The magnetic field under consideration will take the form

$$\mathbf{B} = B_1\mathbf{i} + B_0\mathbf{k}, \tag{10}$$

which by symmetry comprises the general case. In the Coulomb gauge, the vector potential $\mathbf{A}(\theta, \phi) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ expressed in surface variables reduces to

$$\begin{aligned}\mathbf{A}(\theta, \phi) = \tfrac{1}{2}[&B_1(W\sin\phi\cos\theta + a\sin^2\theta\sin\phi)\boldsymbol{\theta} \\ &+ (B_0 W - B_1 a\sin\theta\cos\phi)]\boldsymbol{\phi} \\ &+ B_1(F\sin\phi\sin\theta - a\cos\theta\sin\theta\sin\phi)\mathbf{n}\end{aligned} \tag{11}$$

with $\mathbf{n} = \boldsymbol{\phi} \times \boldsymbol{\theta}$. The normal component of $\mathbf{A}$ contributes a quadratic term to the Hamiltonian but leads to no differentiations in the coordinate normal to the surface as per Eq. (8). There is a wealth of literature concerning curvature effects when a particle is constrained to a two-dimensional surface in three-space [21–38], including some dealing with the torus specifically [39], but the scope of this work will remain restricted to study of the Hamiltonian given by Eq. (9).

The Schrödinger equation (spin splitting will be neglected throughout this work) is more simply expressed by first defining

$$\alpha = a/R,$$

$$F = 1 + \alpha\cos\theta,$$

$$\gamma_0 = B_0\pi R^2,$$

$$\gamma_1 = B_1\pi R^2,$$

$$\gamma_N = \frac{\pi\hbar}{q},$$

$$\tau_0 = \frac{\gamma_0}{\gamma_N},$$

$$\tau_1 = \frac{\gamma_1}{\gamma_N},$$

$$\varepsilon = -\frac{2mEa^2}{\hbar^2},$$