

Coupling curvature to a uniform magnetic field: An analytic and numerical study

M. Encinosa*

Florida A&M University, Department of Physics, Tallahassee, Florida 32307, USA

(Received 13 October 2005; published 9 January 2006)

The Schrödinger equation for a spinless electron near an azimuthally symmetric curved surface Σ in the presence of an arbitrary uniform magnetic field \mathbf{B} is developed. A thin-layer quantization procedure is implemented to bring the particle onto Σ , leading to the well-known geometric potential $V_C \propto \hbar^2 - k$ and a second potential that couples A_N , the component of \mathbf{A} normal to Σ to mean surface curvature, as well as a term dependent on the normal derivative of A_N evaluated on Σ . Numerical results in the form of ground-state energies as a function of the applied field in several orientations are presented for a toroidal model.

DOI: [10.1103/PhysRevA.73.012102](https://doi.org/10.1103/PhysRevA.73.012102)

PACS number(s): 03.65.Ge, 73.22.Dj

I. INTRODUCTION

Nanostructures with novel geometries have become the subject of a large body of experimental and theoretical work [1–23]. Many of the fabricated structures exhibit curvature on the nanoscale, making once purely theoretical investigations of quantum mechanics on curved and reduced dimensionality surfaces relevant to device modeling. Because magnetic field effects prove important to Aharonov-Bohm and transport phenomena, the interplay of an applied field with the curved regions of a nanostructure [1,4,5,8,12,14,20,24,25] (particularly if the structure has holes) may be critical to a complete understanding of the physics of a nanodevice element.

In a previous work [5] the Schrödinger equation for a spinless electron on a toroidal surface T^2 in an arbitrary static magnetic field was developed and numerical results obtained. There, however, the particle was restricted *ab initio* to motion on T^2 , which precluded the appearance of the well-known geometric potential $V_C \propto (\hbar^2 - k)$ [26–42], with h and k the mean and Gaussian curvatures, that arises via thin-layer quantization [43]. Furthermore, if the degree of freedom normal to Σ (labeled q in everything to follow) is included, then the component of the vector potential A_N normal to Σ couples to the normal part of the gradient. Given that V_C is generated from differentiations in q and the requirement of conservation of the norm, it is not surprising that other curvature effects would follow from inclusion of \mathbf{A} . This work is concerned with determining the effective potential that arises from the $A_N \partial / \partial q$ operator and, through numerical calculation with a simple but realistic model, gauging its influence on the single-particle spectra and wave functions as a function of field strength and orientation.

The remainder of this paper is organized as follows: Sec. II develops the Schrödinger equation

$$\frac{1}{2m} \left(\frac{\hbar}{i} \nabla + e\mathbf{A} \right)^2 \Psi = E\Psi \quad (1)$$

for a spinless electron allowed to move in the neighborhood Σ . In an earlier, unpublished version of this work [44] dif-

ferential forms were employed to represent Eq. (1), but here more conventional language is used. Section III briefly reviews the procedure by which V_C is derived and uses a similar but not identical methodology to reduce the $A_N \partial / \partial q$ operator to an effective potential expressed entirely in surface variables. Section IV employs the formalism presented in Sec. III to calculate spectra and wave functions as a function of field strength and orientation for a toroidal structure, and Sec. V is reserved for conclusions.

II. CURVED-SURFACE SCHRÖDINGER EQUATION

The development of the Schrödinger equation in three dimensions on an arbitrary manifold generally yields a cumbersome expression. To remove some complexity in what ensues, an azimuthally symmetric surface Σ with q the coordinate that gives the distance from Σ will be adopted.

Let \mathbf{e}_ρ , \mathbf{e}_ϕ , and \mathbf{e}_z be cylindrical-coordinate-system unit vectors. Parametrize $\Sigma(\rho, \phi)$ by the Monge form

$$\mathbf{r}(\rho, \phi) = \rho \mathbf{e}_\rho + S(\rho) \mathbf{e}_z, \quad (2)$$

with $S(\rho)$ the shape of the surface. Points near the surface $S(\rho)$ are then described by

$$\mathbf{x}(\rho, \phi, q) = \mathbf{r}(\rho, \phi) + q \mathbf{e}_n(\rho, \phi), \quad (3)$$

with \mathbf{e}_n everywhere normal to the surface and to be defined momentarily below. The differential line element of Eq. (3) is

$$d\mathbf{x} = d\mathbf{r} + dq \mathbf{e}_n + q d\mathbf{e}_n. \quad (4)$$

After some manipulation along with a list of expressions to be defined below, Eq. (4) can be rewritten as (the subscript on S denotes differentiation with respect to ρ)

$$\begin{aligned} d\mathbf{x} &= Z(1 + k_1 q) \mathbf{e}_1 d\rho + \rho(1 + k_2 q) \mathbf{e}_\phi d\phi + dq \mathbf{e}_n \\ &\equiv Z f_1 \mathbf{e}_1 d\rho + \rho f_2 \mathbf{e}_\phi d\phi + dq \mathbf{e}_n, \end{aligned} \quad (5)$$

with

$$Z = \sqrt{1 + S_\rho^2}, \quad (6)$$

$$\mathbf{e}_1 = \frac{1}{Z} (\mathbf{e}_\rho + S_\rho \mathbf{e}_z), \quad (7)$$

*Electronic address: encinosa@cennas.nhmfl.gov

$$\mathbf{e}_n = \frac{1}{Z}(-S_\rho \mathbf{e}_\rho + \mathbf{e}_z) \quad (8)$$

and the principal curvatures

$$k_1 = -\frac{S_{\rho\rho}}{Z^3}, \quad (9)$$

$$k_2 = -\frac{S_\rho}{\rho Z}. \quad (10)$$

The metric elements can be read off of

$$dx^2 = Z^2 f_1^2 d\rho^2 + \rho^2 f_2^2 d\phi^2 + dq^2, \quad (11)$$

from which the Schrödinger equation can be determined, but since the minimal prescription will be employed as per Eq. (1), it proves convenient to use the gradient

$$\nabla = \frac{1}{f_1 Z} \mathbf{e}_1 \frac{\partial}{\partial \rho} + \frac{1}{f_2 \rho} \mathbf{e}_\phi \frac{\partial}{\partial \phi} + \mathbf{e}_n \frac{\partial}{\partial q} \quad (12)$$

instead. Equation (1) can be rearranged as

$$\begin{aligned} \frac{1}{2} \left[\frac{1}{Z^2 f_1^2} \frac{\partial^2}{\partial \rho^2} + \frac{1}{f_1 f_2 Z} \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{f_1 f_2 \rho^2} \frac{\partial^2}{\partial \phi^2} + \left(\frac{k_1}{f_1} + \frac{k_1}{f_1} \right) \frac{\partial}{\partial q} + \frac{\partial^2}{\partial q^2} \right. \\ \left. - \left(\frac{\rho k_1 k_2}{f_1^2} + \frac{k_1}{f_1} + \frac{q k_{1\rho}}{Z^2 f_1^3} \right) \frac{\partial}{\partial \rho} + 2\lambda i \left(\frac{A_1}{f_1 Z} \frac{\partial}{\partial \rho} + \frac{A_\phi}{f_2 \rho} \frac{\partial}{\partial \phi} \right. \right. \\ \left. \left. + A_N \frac{\partial}{\partial q} \right) - \lambda^2 (A_1^2 + A_\phi^2 + A_N^2) + \frac{2Em}{\hbar^2} \right] \Psi = 0, \quad (13) \end{aligned}$$

with $\lambda = e/\hbar$ and $A_j = \mathbf{A} \cdot \mathbf{e}_j$.

While Eq. (13) describes the general case for an azimuthally symmetric geometry, it can be simplified substantially when considering the $q \rightarrow 0$ limit or, as dubbed by Golovnev [43], with thin-layer quantization. The procedure entails first performing all q differentiations in accordance with the intuitive notion that the kinetic energy in a thin layer is large, then setting $q=0$ everywhere. Equation (13), leaving the q differentiations intact and setting $q=0$ everywhere save the A_N term, cleans up to

$$\begin{aligned} \frac{1}{2} \left[\frac{1}{Z^2} \frac{\partial^2}{\partial \rho^2} + \frac{1}{Z} \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + 2h \frac{\partial}{\partial q} + \frac{\partial^2}{\partial q^2} - k_1 (\rho k_2 + 1) \frac{\partial}{\partial \rho} \right. \\ \left. + 2\lambda i \left(\frac{A_1}{Z} \bigg|_{q=0} \frac{\partial}{\partial \rho} + \frac{A_\phi}{\rho} \bigg|_{q=0} \frac{\partial}{\partial \phi} + A_N \frac{\partial}{\partial q} \right) \right. \\ \left. - \lambda^2 (A_1^2 + A_\phi^2 + A_N^2) \bigg|_{q=0} + \frac{2Em}{\hbar^2} \right] \Psi = 0, \quad (14) \end{aligned}$$

with the mean curvature h above given by

$$h = \frac{1}{2}(k_1 + k_2). \quad (15)$$

The Gaussian curvature which will appear later is

$$k = k_1 k_2. \quad (16)$$

III. DERIVATION OF GEOMETRIC POTENTIALS

The geometric potential $V_C(\rho)$ is found by reducing Eq. (13) further by the well-known procedure of assuming a suitable confining potential $V_n(q)$ in the normal direction and demanding conservation of the norm in the $q \rightarrow 0$ limit. The latter requirement is generally imposed via assuming a separation of variables in the surface and normal parts of the total wave function [26–30,39–41]

$$\Psi(\rho, \phi, q) \rightarrow \chi_S(\rho, \phi) \chi_N(q) \quad (17)$$

and imposing conservation of the norm through

$$|\Psi(\rho, \phi, q)|^2 (1 + 2qh + q^2 k) d\Sigma dq \rightarrow |\chi_S(\rho, \phi)|^2 |\chi_N(q)|^2 d\Sigma dq, \quad (18)$$

or, equivalently,

$$\Psi = \chi_S \chi_N (1 + 2qh + q^2 k)^{-1/2} \equiv \chi_S \chi_N G^{-1/2}. \quad (19)$$

Inserting the rightmost term in Eq. (19) into Eq. (13) and subsequently taking $q \rightarrow 0$ reduces the q differentiations there to

$$2h \frac{\partial}{\partial q} + \frac{\partial^2}{\partial q^2} \rightarrow \frac{\partial^2}{\partial q^2} + h^2 - k. \quad (20)$$

Separability of the surface and normal variables in the non-magnetic part of the Hamiltonian is manifest.

Since A_N can be a function of q while h is not, it is not immediately apparent that separability of the Schrödinger equation in the surface and normal variables is preserved by the $A_N(\rho, \phi, q) \partial/\partial q$ operator. Rather than apply the method above or that employed in [45] to this term, instead integrate out any q dependence with some reasonable ansatz for $\chi_N(q)$ —say, a normalized hard-wall form $\chi_N(q) = \sqrt{2/L} \sin \pi q/L$. While equivalent to the method summarized in Eqs. (17)–(20), this procedure assists in establishing conditions on A_N that will prove useful later, and previous work [46] has demonstrated that to a good approximation the procedure is justified even for a particle not strongly confined to a region near Σ .

Write

$$I = \int_0^L \frac{\chi_N(q)}{G^{-1/2}} A_N(\theta, \phi, q) \left[\frac{\partial}{\partial q} \frac{\chi_N(q)}{G^{-1/2}} \right] G dq, \quad (21)$$

which is equivalent to

$$\begin{aligned} I = - \int_0^L \chi_N^2(q) (h + qk) G^{-1} A_N(\rho, \phi, q) dq \\ + \int_0^L \chi_N(q) A_N(\rho, \phi, q) \chi_N'(q) dq. \quad (22) \end{aligned}$$

Consider the left-hand integral I_L , and assume (suppressing

surface arguments) $A_N(q) \sim a_0 + a_1 q + \dots$; expanding out the arguments and noting that each power of q when integrated picks up a power of L that will vanish as $L \rightarrow 0$, the result in this limit is

$$I_L^0 \cong -hA_N(\rho, \phi, 0) \int_0^L \chi_N^2(q) dq; \quad (23)$$

i.e., the effective potential arising from I_L is proportional to $-hA_N(\rho, \phi, 0)$.

Turning to the second integral I_R , write $\chi_N(q)\chi_N'(q)$ as $\partial/\partial q[\chi_N^2(q)/2]$ and perform an integration by parts. The surface term vanishes so that

$$I_R = -\frac{1}{2} \int_0^L \chi_N^2(q) \frac{\partial A_N(\rho, \phi, q)}{\partial q} dq. \quad (24)$$

Again taking $A_N(q) \sim a_0 + a_1 q + \dots$ allows Eq. (24) to be expressed in the $q \rightarrow 0$ limit as

$$I_R^0 \cong -\frac{1}{2} \int_0^L \chi_N^2(q) \left. \frac{\partial A_N(\rho, \phi, q)}{\partial q} \right|_{q=0} dq. \quad (25)$$

Equations (23) and (25) combine to give an effective surface potential (with constants appended)

$$V_N^{\text{mag}}(\rho, \phi) = \frac{ie\hbar}{m} \left[h(\rho)A_N(\rho, \phi, 0) + \frac{1}{2} \left. \frac{\partial A_N(\rho, \phi, q)}{\partial q} \right|_{q=0} \right]. \quad (26)$$

There are two points that should be addressed with further explanation. First, assuming a nonsingular series expansion for A_N is reasonable since $A_N(\rho, \phi, 0)$ is the value of the vector potential on the surface; it should certainly be physically well behaved there but need not vanish. Second, while a hard-wall form has been assumed for the trial wave function (a Gaussian works as well), it is a reasonable conjecture that the arguments made above are independent of the choice of $\chi_N(q)$ as long as there is negligible mixing among states in the q degree of freedom.

IV. NUMERICS

The formalism developed above is now applied to calculate the spectrum and eigenfunctions for a toroidal structure in a uniform magnetic field of arbitrary orientation inclusive of geometric potentials.

A convenient choice to parametrize points near a toroidal surface T^2 of major radius R and minor radius a is [47]

$$\mathbf{x}(\theta, \phi) = W(\theta)\mathbf{e}_\rho + a \sin \theta \mathbf{e}_z + q\mathbf{e}_n, \quad (27)$$

with

$$W = R + a \cos \theta \quad (28)$$

and

$$\mathbf{e}_n = \cos \theta \mathbf{e}_\rho + \sin \theta \mathbf{e}_z. \quad (29)$$

The differential line element is

$$\begin{aligned} d\mathbf{x} &= a(1 + k_1^T q)\mathbf{e}_\rho d\theta + W(\theta)(1 + k_2^T q)\mathbf{e}_\phi d\phi + \mathbf{e}_n dq \\ &\equiv a_q(q)\mathbf{e}_\rho d\theta + W_q(\theta, q)\mathbf{e}_\phi d\phi + \mathbf{e}_n dq, \end{aligned} \quad (30)$$

with $\mathbf{e}_\theta = -\sin \theta \mathbf{e}_\rho + \cos \theta \mathbf{e}_z$ and the toroidal principle curvatures

$$k_1^T = \frac{1}{a}, \quad (31)$$

$$k_2^T = \frac{\cos \theta}{W(\theta)}. \quad (32)$$

The gradient that follows from Eq. (30) is

$$\nabla = \mathbf{e}_\theta \frac{1}{a_q(q)} \frac{\partial}{\partial \theta} + \mathbf{e}_\phi \frac{1}{W_q(\theta, q)} \frac{\partial}{\partial \phi} + \mathbf{e}_n \frac{\partial}{\partial q}. \quad (33)$$

The symmetry of the torus allows an arbitrary static magnetic field to be taken as

$$\mathbf{B} = B_1 \mathbf{i} + B_0 \mathbf{k}. \quad (34)$$

In the Coulomb gauge the vector potential $\mathbf{A}(\theta, \phi) = \frac{1}{2} \mathbf{B} \times \mathbf{r}$ expressed in the geometry of Eq. (27) is

$$\begin{aligned} \mathbf{A}(\theta, \phi, q) &= \frac{1}{2} [B_1 \sin \phi (R \cos \theta + a_q) \mathbf{e}_\theta \\ &\quad + (B_0 W_q - B_1 a_q \sin \theta \cos \phi) \mathbf{e}_\phi \\ &\quad + B_1 R \sin \phi \sin \theta \mathbf{e}_n]. \end{aligned} \quad (35)$$

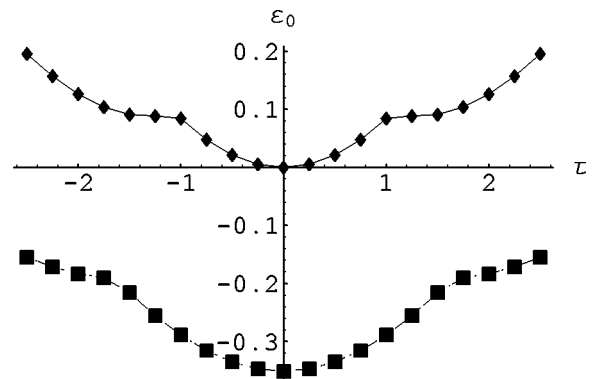


FIG. 1. ε_0 as a function of τ for $\mathbf{B} = B_0 \mathbf{k}$. Diamonds correspond to $V_C = V^{\text{mag}} = 0$, stars to $V_C \neq 0$, $V^{\text{mag}} = 0$, and squares to $V_C \neq 0$, $V^{\text{mag}} \neq 0$.

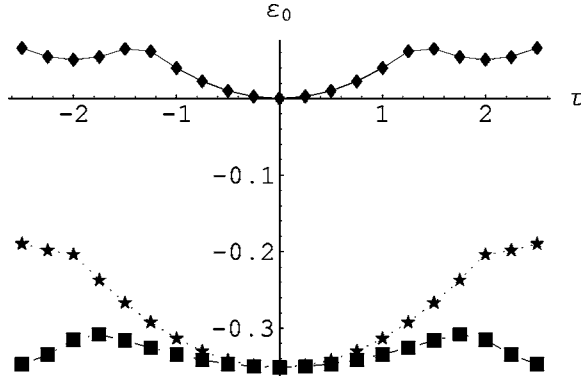


FIG. 2. $\varepsilon_0(\tau)$ for $\mathbf{B}=B_0(\mathbf{i}+\mathbf{k})/\sqrt{2}$. Diamonds correspond to $V_C=V^{mag}=0$, stars to $V_C \neq 0$, $V^{mag}=0$, and squares to $V_C \neq 0$, $V^{mag} \neq 0$.

In this case $\partial A_N / \partial q = 0$, so only the first term in Eq. (26) will contribute to $V_N^{mag}(\theta, \phi)$. The Schrödinger equation in the $q \rightarrow 0$ limit inclusive of geometric potentials can be written (spin will be neglected) in a compact form by first defining

$$\alpha = a/R,$$

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

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

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

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

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

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

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

after which Eq. (1) may be written

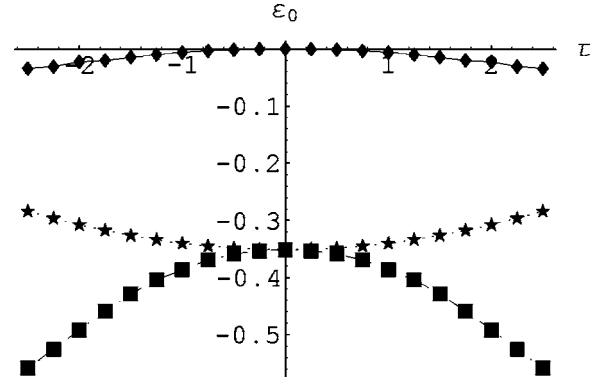


FIG. 3. $\varepsilon_0(\tau)$ for $\mathbf{B}=B_1\mathbf{i}$. Diamonds correspond to $V_C=V^{mag}=0$, stars to $V_C \neq 0$, $V^{mag}=0$, and squares to $V_C \neq 0$, $V^{mag} \neq 0$.

$$\left[\frac{\partial^2}{\partial \theta^2} - \frac{\alpha \sin \theta}{F(\theta)} \frac{\partial}{\partial \theta} + \frac{\alpha^2}{F^2(\theta)} \frac{\partial^2}{\partial \phi^2} + \frac{1}{4F^2(\theta)} \right. \\ \left. + \frac{i\alpha\tau_1}{2} \sin \theta \sin \phi \frac{1 + 2\alpha \cos \theta}{F(\theta)} \right. \\ \left. + i \left(\tau_0 \alpha^2 - \frac{\tau_1 \alpha^3}{F(\theta)} \sin \theta \cos \phi \right) \frac{\partial}{\partial \phi} \right. \\ \left. + i\alpha\tau_1 \sin \phi (\alpha + \cos \theta) \frac{\partial}{\partial \theta} - \frac{\tau_0^2 \alpha^2 F^2(\theta)}{4} \right. \\ \left. - \frac{\tau_1^2 \alpha^2 F^2(\theta)}{4} \left(\sin^2 \phi + \frac{\alpha^2 \sin^2 \theta}{F^2(\theta)} \right) \right. \\ \left. + \frac{\tau_0 \tau_1 \alpha^3 F(\theta)}{2} \sin \theta \cos \phi \right] \Psi = \varepsilon \Psi, \quad (36)$$

$$\Rightarrow H_\tau \Psi = \varepsilon \Psi, \quad (37)$$

with the fourth and fifth terms of Eq. (36) being proportional to V_C and V_C^{mag} .

To obtain solutions of Eq. (36) a basis-set expansion orthogonal over the integration measure $d^2J(\theta) = F(\theta)d\theta d\phi$ may be employed for a given α . Here R will be set to 500 Å in accordance with fabricated structures [16,23,48,49] (for an $R=500$ Å torus $\tau \equiv \sqrt{\tau_0^2 + \tau_1^2} = 0.263 \sqrt{B_0^2 + B_1^2}$). With $a=250$ Å, $\alpha=1/2$, a value which serves as a compromise between smaller α where the solutions tend towards simple trigonometric functions and larger α which are less likely to be physically realistic.

There are two options available for basis functions, one being

TABLE I. Ground-state wave functions for $\mathbf{B}=B_0\mathbf{k}$ at integer values of τ . The arguments in square brackets indicate if V_C/V^{mag} are switched off or on. Only the dominant terms are shown.

| | $\tau=0$ | $\tau=1$ | $\tau=2$ |
|----------------------------------|------------------------|------------------------|------------------------------------|
| $\chi_G[\text{off}, \text{off}]$ | 1 | ~ 1 | $(-0.969f_0 + 0.245f_1)e^{-i\phi}$ |
| $\chi_G[\text{on}, \text{off}]$ | $-0.968f_0 - 0.244f_1$ | $-0.957f_0 + 0.254f_1$ | $(0.987f_0 - 0.158f_1)e^{-i\phi}$ |
| $\chi_G[\text{on}, \text{on}]$ | $-0.968f_0 - 0.244f_1$ | $-0.957f_0 + 0.254f_1$ | $(0.987f_0 - 0.158f_1)e^{-i\phi}$ |

TABLE II. Ground-state wave functions for $\mathbf{B}=B_0(\mathbf{i}+\mathbf{k})/\sqrt{2}$ as per Table I. For this field configuration $A_N(\theta, \phi) \neq 0$.

| | $\tau=0$ | $\tau=1$ | $\tau=2$ |
|---------------------------|---------------------|---|---|
| $\chi_G[\text{off, off}]$ | 1 | $-0.989f_0-0.115g_1e^{-i\phi}$ | $(-0.928f_0+0.159f_1)e^{-i\phi}-g_1(0.287-0.145e^{-i\phi})$ |
| $\chi_G[\text{on, off}]$ | $0.968f_0-0.244f_1$ | $0.961f_0-0.252f_1$ | $0.932f_0-0.270f_1$ |
| $\chi_G[\text{on, on}]$ | $0.968f_0-0.244f_1$ | $(0.957f_0-0.232f_1)+g_1(0.094e^{i\phi}-0.127e^{-i\phi})$ | $f_0(0.909e^{-i\phi}-0.126)-g_1(0.173e^{-i\phi}-0.351)$ |

$$\chi_{n\nu}(\theta, \phi) = \frac{1}{\sqrt{2\pi}} F^{-1/2} e^{in\theta} e^{i\nu\phi} \quad (38)$$

and the other being

$$\chi_{n\nu}^{\pm}(\theta, \phi) = \begin{pmatrix} f_n(\theta) \\ g_n(\theta) \end{pmatrix} e^{i\nu\phi}, \quad (39)$$

with $f_n(\theta)$ and $g_n(\theta)$ even (odd) orthonormal functions labeled by $+$ ($-$), respectively, constructed by a Gram-Schmidt (GS) procedure [50] over $d^2J(\theta)$ using $\cos n\theta$, $\sin n\theta$ as primitives. Here the latter approach will be adopted in order to facilitate comparisons to a related work [5] and because of the ease by which the Hamiltonian matrix elements

$$H_{n\nu n'\nu'}^{\pi\pi} = \langle \chi_{n\nu}^{\pi} | H_{\tau} | \chi_{n'\nu'}^{\pi} \rangle \quad (40)$$

can be evaluated analytically. The basis comprises six GS functions of each θ parity and five azimuthal functions spanning $-2 \leq \nu \leq 2$ per θ function for a total of 60 basis states. The resulting 60×60 Hamiltonian matrix blocks schematically into

$$\begin{pmatrix} H^{++} & H^{+-} \\ H^{+} & H^{-} \end{pmatrix},$$

from which eigenvalues and eigenfunctions are determined. Since the concern here is with the ground-state eigenfunctions, only a few GS states prove relevant; they are $f_0(\theta)=0.3987$, $f_1(\theta)=0.6031 \cos \theta - 0.1508$, and $g_1(\theta)=0.5642 \sin \theta$.

Figures 1–3 plot the ground-state energy ε_0 as a function of the magnitude of flux τ for three field orientations. Each figure displays results for $\varepsilon_0(\tau)$ with V_C and/or V^{mag} switched on or off. In Fig. 1 the field is oriented along the z axis. In this case there is no component of \mathbf{A} normal to the surface, so only two curves are evidenced. The curves are qualitatively similar, and the effect of V_C is to smooth out the $V_C=0$ curve at $\tau_0 \approx 1$ and shift it downward by an overall

constant. It should be noted that although the curves are similar, persistent current effects depend on the smoothness and shape of the $\varepsilon(\tau)$ curves so that even fine details can prove important. Table I shows the evolution of the ground-state wave function $\chi_G(\theta, \phi)$ for several τ , because the field is oriented along the z axis, τ also measures the flux through the toroidal plane. Both V_C and V^{mag} are zero so that the evolution of $\chi_G(\theta, \phi)$ is due only to changes in field strength.

Figure 2 shows results for a field orientation oriented tilted $\pi/4$ radians relative to the toroidal plane with the magnitude of τ plotted on the horizontal axis. The divergence of the two lower curves illustrates the influence of V^{mag} on the spectrum. The curve inclusive of V^{mag} begins to involve excited states in both the θ and azimuthal degrees of freedom (see Table II). While the admixture of excited states would tend to raise ε_0 , the interaction is strong enough to pull the $\varepsilon_0(\tau)$ down as the applied field increases.

In Fig. 3 the magnetic field is situated parallel to the toroidal plane along the x axis. As would be anticipated, there is no structure in the $V_C=V^{mag}=0$ curve since no flux penetrates the plane of the torus. This trend obtains also when $V_C, V^{mag} \neq 0$. The effect of V^{mag} becomes substantial very quickly both in $\varepsilon_0(\tau)$ and on $\chi_G(\theta, \phi)$ (Table III). In this case there is not even qualitative agreement between results with $V_C \neq 0$ with V^{mag} omitted compared to when it is included.

V. CONCLUSIONS

This work presents a method to reduce the $A_N \partial / \partial q$ term appearing in the Schrödinger equation for a spinless electron near a two-dimensional surface in an arbitrary static magnetic field to a geometric potential V^{mag} written entirely in terms of surface variables. This potential can appreciably modify energy versus magnetic flux curves as well as surface wave functions considered here.

In the context of real structures, the practical utility of deriving geometric potentials lies in reducing three-dimensional problems to two-dimensional ones. Earlier work

TABLE III. Ground-state wave functions for $\mathbf{B}=B_1\mathbf{i}$ at integer values of τ as per Table I. $A_N(\theta, \phi)$ is nonzero, and there is no flux through the toroidal plane.

| | $\tau=0$ | $\tau=1$ | $\tau=2$ |
|---------------------------|---------------------|--|---|
| $\chi_G[\text{off, off}]$ | $0.968f_0-0.244f_1$ | $0.978f_0+0.279ig_1 \sin \phi$ | $0.894f_0+0.133f_1-0.552ig_1 \sin \phi$ |
| $\chi_G[\text{on, off}]$ | $0.968f_0-0.244f_1$ | $0.964f_0-0.218f_1$ | $0.941f_0-0.132f_1+0.403ig_1 \sin \phi$ |
| $\chi_G[\text{on, on}]$ | $0.968f_0-0.244f_1$ | $-0.954f_0+0.178f_1+0.320ig_1 \sin \phi$ | $0.869f_0-0.250f_1 \cos \phi - 0.314ig_1 \sin \phi$ |

[46] on a simple nanoscale model has shown that solutions of an *ab initio* two-dimensional Schrödinger equation do not adequately approximate thin-layer three-dimensional solutions on a curved space unless V_C is included in the Schrödinger equation. From this perspective, geometric potentials of the form discussed here should be considered effective potentials that must be included in the modeling of

curved structures in order to achieve a complete description of the object.

ACKNOWLEDGMENT

The author would like to thank M. Jack for useful discussions.

-
- [1] D. Bellucci, M. Rontani, G. Goldoni, F. Troiani, and E. Molinari, *Physica E (Amsterdam)* **26**, 327 (2005).
- [2] D. Bulaev, V. Geyler, and V. Margulis, *Physica B* **337**, 180 (1997).
- [3] Y. Y. Chou, G.-Y. Guo, L. Liu, C. S. Jayanthi, and S. Y. Wu, *J. Appl. Phys.* **96**, 2249 (2004).
- [4] W. Tian and S. Datta, *Phys. Rev. B* **49**, 5097 (1994).
- [5] M. Encinosa, *Physica E (Amsterdam)* **28**, 209 (2005).
- [6] I. Filikhin, E. Deyneka, and B. Vlahovic, *Modell. Simul. Mater. Sci. Eng.* **12**, 1121 (2004).
- [7] T. Heinzel, K. Ensslin, W. Wegscheider, A. Fuhrer, S. Lüscher, and M. Bichler, *Nature (London)* **413**, 822 (2001).
- [8] A. Goker and P. Norlander, *J. Phys.: Condens. Matter* **16**, 8233 (2004).
- [9] J. Gravesen, M. Willatzen, and L. L. Y. Voon, *Phys. Scr.* **72**, 105 (2005).
- [10] D. Gridin, A. T. I. Adamou, and R. V. Craster, *Phys. Rev. B* **69**, 155317 (2004).
- [11] S. Gylfadottir, M. Nita, V. Gudmundsson, and A. Manolescu, *Physica E (Amsterdam)* **27**, 209 (2005).
- [12] A. Ivanov and O. Lobanova, *Physica E (Amsterdam)* **23**, 61 (2003).
- [13] A. Latgé, C. G. Rocha, L. A. L. Wanderley, M. Pacheco, P. Orellana, and Z. Barticevic, *Phys. Rev. B* **67**, 155413 (2003).
- [14] S. Latil, S. Roche, and A. Rubio, *Phys. Rev. B* **67**, 165420 (2003).
- [15] A. Lorke, S. Bohm, and W. Wegscheider, *Superlattices Microstruct.* **33**, 347 (2003).
- [16] A. Lorke, R. J. Luyken, A. O. Govorov, J. P. Kotthaus, J. M. Garcia, and P. M. Petroff, *Phys. Rev. Lett.* **84**, 2223 (2000).
- [17] S. Mendach, O. Schumacher, C. Heyn, S. Schnull, H. Welsch, and W. Hansen, *Physica E (Amsterdam)* **23**, 274 (2004).
- [18] Y. Pershin and C. Piermarocchi, *Phys. Rev. B* **72**, 195340 (2005).
- [19] S. X. Qu and M. R. Geller, *Phys. Rev. B* **70**, 085414 (2004).
- [20] K. Sasaki, Y. Kawazoe, and R. Saito, *Phys. Lett. A* **321**, 369 (2004).
- [21] M. Sano, A. Kamino, J. Okamura, and S. Shinkai, *Science* **293**, 1299 (2004).
- [22] J. Tempere, I. F. Silvera, and J. T. Devreese, *Phys. Rev. B* **65**, 195418 (2002).
- [23] H. Zhang, S. W. Chung, and C. A. Mirkin, *Nano Lett.* **3**, 43 (2003).
- [24] C. Chryssomalakos, A. Franco, and A. Reyes-Coronado, *Eur. J. Phys.* **25**, 489 (2004).
- [25] K. Sasaki and Y. Kawazoe, *Prog. Theor. Phys.* **112**, 369 (2004).
- [26] M. Burgess and B. Jensen, *Phys. Rev. A* **48**, 1861 (1993).
- [27] H. Jensen and H. Koppe, *Ann. Phys. (N.Y.)* **63**, 586 (1971).
- [28] R. C. T. da Costa, *Phys. Rev. A* **23**, 1982 (1981).
- [29] R. C. T. da Costa, *Phys. Rev. A* **25**, 2893 (1982).
- [30] S. Matusani, *J. Phys. Soc. Jpn.* **61**, 55 (1991).
- [31] S. Matsutani, *Rev. Math. Phys.* **11**, 171 (1999).
- [32] P. Duclos and P. Exner, *Rev. Math. Phys.* **7**, 73 (1995).
- [33] 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).
- [34] I. Popov, *Phys. Lett. A* **269**, 148 (2000).
- [35] P. Ouyang, V. Mohta, and R. L. Jaffe, *Ann. Phys. (N.Y.)* **275**, 297 (1998).
- [36] S. Midgley and J. Wang, *Aust. J. Phys.* **53**, 77 (2000).
- [37] M. Encinosa and B. Etemadi, *Phys. Rev. A* **58**, 77 (1998).
- [38] M. Encinosa and B. Etemadi, *Physica B* **266**, 361 (1998).
- [39] J. Goldstone and R. L. Jaffe, *Phys. Rev. B* **45**, 14100 (1991).
- [40] P. Exner and P. Seba, *J. Math. Phys.* **30**, 2574 (1989).
- [41] P. C. Schuster and R. L. Jaffe, *Ann. Phys. (N.Y.)* **307**, 132 (2003).
- [42] I. J. Clark and A. J. Bracken, *J. Phys. A* **29**, 4527 (1996).
- [43] A. Golovnev, e-print quant-ph/0508044.
- [44] M. Encinosa and R. O'Neal, e-print quant-ph/9908087.
- [45] Y. V. Pershin and C. Piermarocchi, *Phys. Rev. B* **72**, 125348 (2005).
- [46] M. Encinosa, L. Mott, and B. Etemadi, *Phys. Scr.* **72**, 13 (2005).
- [47] M. Encinosa and B. Etemadi, *Found. Phys. Lett.* **16**, 403 (2003).
- [48] J. M. Garca, G. Medeiros-Ribeiro, K. Schmidt, T. Ngo, J. L. Feng, A. Lorke, J. Kotthaus, and P. M. Petroff, *Appl. Phys. Lett.* **71**, 2014 (1997).
- [49] A. Lorke, R. J. Luyken, A. O. Govorov, J. P. Kotthaus, J. M. Garcia, and P. M. Petroff, *Phys. Rev. Lett.* **84**, 2223 (2000).
- [50] M. Encinosa, e-print physics/0501161.