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Effect of symmetry on the electronic properties of arbitrarily shaped quantum rings in a magnetic field

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HIGHLIGHTS

- One-dimensional model of a quantum ring with an arbitrary contour is formulated.
- Analytical solutions are found for three rings with different orders of symmetry.
- The structure of the energy gaps is shown to be dependent on the order of symmetry.
- Asymmetry of a quantum ring causes some chaos in widths of the energy gaps.

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ABSTRACT

The energy states and persistent current oscillations considered here are formulated in a one-dimensional model for a quantum ring with a nearly circular arbitrary contour. Using conformal mapping, the curvature of the ring is introduced into the Schrodinger equation via the Lamé coefficient of the conformal mapping. Asymptotic methods were employed in order to derive analytical solutions. Energy levels and current oscillations were studied for three cases of the possible non-circular QR symmetries: a QR with two axes of symmetry (ellipse), a QR with one axis of symmetry and also on QRs with no axes of symmetry, i.e. asymmetric shapes. We obtain explicit expressions for the periodic energy and the energy gaps opened at the half-integer and integer values of the flux. The spectrum behavior is found to be dependent on the order of symmetry. In particular, small asymmetries of the QR cause some perceptible chaos in the width of the gaps.

1. Introduction

The properties of quantum rings (QRs) in external magnetic fields, together with their potential applications in quantum information processing and low-dimensional semiconductor optoelectronic devices, place these systems among the topics attracting attention of researchers [1–6]. The electronic properties of QRs are not only of fundamental interest, but are also important due to their potential applications. The increasing development of advanced epitaxial growth techniques makes it possible to form various novel-shaped quantum rings [7–11].

Although electronic properties of perfect circular QRs in the presence of a magnetic flux are well studied theoretically, distorted QRs are typically treated mainly for specific shapes of the contour by using numerical methods. The energy states and persistent current in a non-circular QR were studied numerically in Ref. [12] and later in Ref. [13] for a two-dimensional (2D) elliptical ring of non-constant width. Narrow elliptical rings were considered in certain asymptotic models in Refs. [14,15] for a constant width ring, and in Refs. [16,17] for an elliptical ring of non-constant width. Asymptotic equations were also suggested for QRs of arbitrary shapes where several examples of such were given [16,17]. Specific effects arising from a very specially distorted contour that consists of constant-curvature segments were studied in Refs. [2,18]. The persistent current in a narrow 2D QR on a surface of constant negative curvature was considered in Ref. [19]. We also mention Ref. [20] in which an interesting asymptotic treatment procedure is suggested for 2D narrow quantum rings. The two lowest quantum energy states of an elliptical QR were studied numerically in Ref. [21] with the one-dimensional (1D) model.

In this paper, we formulate the relations of the energy states and persistent current oscillations of electrons confined to a QR of arbitrary shape in the framework of the 1D model describing an electron with delta-shaped potential along a contour (Sections 1 and 2). We ignore the electron's spin and treat only its spatial degree of freedom. Based on these relations, the dependence of the

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spectrum and persistent current on the geometric properties of the contour is demonstrated using analytical calculations for quantum rings that are distorted circles with various orders of symmetry. In particular, an elliptical QR (two axes of symmetry) is treated in Section 3. The instances of a QR with one axis of symmetry (Section 4) and an asymmetric QR (Section 5) are similarly studied. Conclusions are given in Section 6.

2. General theory

For narrow rings, in which we are especially interested, the electron energy levels stemming from the different radial eigenfunctions are far apart. The energy bands arising from the azimuthal structure of the ring do not depend (to leading order) on the ring width. The effect of ring width is completely contained within a prefactor to the one-dimensional energy levels. Hence, the structure of the energy levels of a 2D ring threaded by a flux tube can be quantitatively described by a 1D ring with certain effective parameters that captures the azimuthal structure.

To directly evaluate the effect of curvature symmetry on the properties of electron spectrum and its persistent current, we consider the motion of a single electron with delta-function potential in a planar infinitely narrow QR. Under this assumption, a general relationship between the path curvature and the electronic properties of a free particle confined to the 1D closed contour will be derived below.

We study the effect of a magnetic field, $\mathbf{B}(0,0,H(x,y))$, that acts perpendicular to the plane of motion of an electron $z=0$, where (x,y,z) are the Cartesian coordinates. The electron is confined to a smooth closed 1D contour, $F(x,y)=0$, $z=0$, which is the boundary of the flat inner domain S. Thus we start with the Hamiltonian

$$\mathcal{H}=\frac{1}{2m_e}\left(\widehat{\mathbf{p}}_\tau-\frac{e}{c}\mathbf{A}_\tau\right)^2 \tag{1}$$

which describes the motion of an electron confined to a flat closed 1D contour, where m_e is the effective mass of the electron; τ is the tangential direction to the contour; $\widehat{\mathbf{p}}_\tau$ and $\mathbf{A}_\tau$ are, respectively, tangential projections of the electron momentum operator $\widehat{\mathbf{p}}$ and the vector potential $\mathbf{A}$ for the given magnetic field configuration, which are taken along the contour.

In order to write the corresponding Schrödinger equation explicitly, we introduce new curved orthogonal coordinates (ξ,η,z)

$$\begin{aligned} &z=z, \quad x+iy=f(\omega), \quad \omega=\xi+i\eta, \\ &f(\omega)=u(\xi,\eta)+iv(\xi,\eta), \end{aligned} \tag{2}$$

with the basic unit vectors $\mathbf{a}_\xi$, $\mathbf{a}_\eta$, $\mathbf{a}_z$, and such that the line $F(x,y)=0$ turns into the unit circle $|\omega|=1$. Here the function $f(\omega)$ conformally maps a certain domain of the plane $\omega=\xi+i\eta$ containing the unit circle onto a domain of the $(x,y)-$plane containing the line $F(x,y)=0$ and preserves the positive orientation of the contour ($\mathbf{a}_\xi\times\mathbf{a}_\eta=\mathbf{a}_z$). It is known (see Ref. [22]) that at least one mapping function $f(\omega)$ always exists.

It is natural now to use "polar" coordinates $\omega=\rho e^{i\theta}$. Then $x+iy=f(\rho e^{i\theta})$ and the basic unit vectors of this orthogonal coordinate system are $\mathbf{a}_\rho$, $\mathbf{a}_\theta$, $\mathbf{a}_z$, where $\mathbf{a}_\theta$ is tangential to the contour. Along the contour, the impulse $\widehat{\mathbf{p}}_\tau$ and the tangential vector potential $\mathbf{A}_\tau$ on the contour are equal, respectively, to the projections of the operator $\widehat{\mathbf{p}}$ and the vector potential $\mathbf{A}$ onto the direction $\mathbf{a}_\theta$ when $\rho=1$, i.e. $\mathbf{A}_\tau=A_\theta(1,\theta)\mathbf{a}_\theta(1,\theta)$. The vector transformation is achieved through the Lamé coefficients $h_z=1$, $h_\rho(\rho,\theta)$ and $h_\theta(\rho,\theta)=\rho h_\rho(\rho,\theta)$, where, in the polar coordinate system

$$h_\rho(\rho,\theta)=\sqrt{\left(\frac{\partial u}{\partial\rho}\right)^2+\left(\frac{\partial v}{\partial\rho}\right)^2}=\left|\frac{df(\omega)}{d\omega}\right|_{\omega=\rho e^{i\theta}}.$$

Along the contour $\rho=1$, the vector relations in the curvilinear coordinates lead to the Schrödinger equation $H\psi(\theta)=E\psi(\theta)$ with the Hamiltonian

$$H=\frac{\hbar^2}{2m_e g^2(\theta)}\left(-i\frac{d}{d\theta}-\frac{eg(\theta)}{c\hbar}A_\theta(1,\theta)\right)^2, \tag{3}$$

where $g(\theta)=h_\rho(\rho=1,\theta)$. The wave function $\psi(\theta)$ should be single-valued, i.e. satisfies the boundary conditions $\psi(\theta)=\psi(\theta+2\pi)$ and $d\psi(\theta)/d\theta=d\psi(\theta+2\pi)/d\theta$.

We perform a unitary gauge transformation $H_0=UHU^{-1}$ by choosing

$$U(\theta)=\exp\left(-\frac{ie}{c\hbar}\int_0^\theta A_\theta(1,t)g(t)\,dt\right). \tag{4}$$

This transforms the Hamiltonian (3) into the field-free Hamiltonian

$$H_0=-\frac{\hbar^2}{2m_e g^2(\theta)}\frac{d^2}{d\theta^2} \tag{5}$$

while the wave function is given by the relation $\psi(\theta)=U^{-1}(\theta)\tilde{\psi}(\theta)$ in which $\tilde{\psi}(\theta)$ is an eigenfunction of a certain boundary value problem for

$$\frac{d^2\tilde{\psi}}{d\theta^2}+K_n^2g^2(\theta)\tilde{\psi}=0 \tag{6}$$

where ${K_n}^2$ and the electron energy E_n are related by $K_n^2=2m_eE_n/\hbar^2$. Denoting the quantum flux $\Phi_0=ch/e$, one might rewrite the boundary conditions as follows:

$$\tilde{\psi}(\theta)=\tilde{\psi}(2\pi+\theta)e^{i2\pi\nu}, \quad \frac{d\tilde{\psi}(\theta)}{d\theta}=\frac{d\tilde{\psi}(2\pi+\theta)}{d\theta}e^{i2\pi\nu}, \tag{7}$$

where the parameter ν, defined for $-1/2<\nu\le 1/2$, is a Φ_0-periodic function of the flux Φ:

$$\nu=\nu\left(\frac{\Phi}{\Phi_0}\right)=\begin{cases}\dfrac{\Phi}{\Phi_0}-\left[\dfrac{\Phi}{\Phi_0}\right] & \text{if } \dfrac{\Phi}{\Phi_0}-\left[\dfrac{\Phi}{\Phi_0}\right]\le\dfrac{1}{2} \\ \dfrac{\Phi}{\Phi_0}-\left[\dfrac{\Phi}{\Phi_0}\right]-1 & \text{if } \dfrac{\Phi}{\Phi_0}-\left[\dfrac{\Phi}{\Phi_0}\right]>\dfrac{1}{2}\end{cases}. \tag{8}$$

By virtue of the periodicity of $A_\theta(1,\theta)$ and $g(\theta)$, the flux

$$\Phi=\int_\theta^{2\pi+\theta}g(t)A_\theta(1,t)\,dt=\oint\mathbf{A}\,d\mathbf{l}=\iint_S H(x,y)\,dS$$

is the magnetic flux through S that is induced by the magnetic field $\mathbf{B}=H(x,y)\mathbf{a}_z$.

Due to the periodic coefficients, the dimensionless equation (6) can be treated with the Bloch theorem (or, equivalently, Floquet's theory) according to which such wave functions exist for any magnetic flux Φ and have the form $\tilde{\psi}_n(\theta)=\phi_n(\theta)\exp(-i\nu\theta)$, where $\phi_n(\theta)$ are the periodic functions. Except for the trivial case of the circular QR, the spectrum displays gaps that occur only at $\nu=0$ and $\nu=1/2$, i.e. at half-integer or integer Φ. Width of the n-th gap very quickly tends to zero as $n\to\infty$. Eigenfunctions are complex for $\nu\neq 0$, 1/2. Purely real eigenfunctions may arise only for $\nu=0$, 1/2 in which case the corresponding quantum spectrum is simple.

It is often convenient to represent the wave functions as

$$\tilde{\psi}_n(\theta)=\frac{1}{\Omega_n}\exp\left(i\int_0^\theta\varphi_n(t)\,dt\right), \tag{9}$$

where $\Omega_n=\int_0^{2\pi}g(\theta)\exp(-2\int_0^\theta \mathrm{Im}\varphi_n(t)\,dt)\,d\theta$ is the normalizing coefficient. Inserting Eq. (9) into Eq. (6) yields the nonlinear equation

$$i\frac{d\varphi_n(\theta)}{d\theta}-\varphi_n^2(\theta)+K_n^2g^2(\theta)=0 \tag{10}$$