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One-dimensional ring in the presence of Rashba spin-orbit interaction: Derivation of the correct Hamiltonian

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We describe in detail the procedure for obtaining the correct one-dimensional Hamiltonian of electrons moving on a ring in the presence of Rashba spin-orbit interaction. The subtlety of this seemingly trivial problem has not been fully appreciated so far and it has led to some ambiguities in the existing literature. Our work illustrates the origin of these ambiguities and solves them.

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The effect of Rashba spin-orbit (SO) interaction¹ on electrons moving in a mesoscopic ring has been studied in several contexts, such as magnetoconductance oscillations,^{2,3} Peierls transition,^{4,5} and persistent current.^{6,7} Essentially all these theoretical studies have employed one-dimensional (1D) model Hamiltonians. Since different Hamiltonians have been used by different authors some ambiguity currently exists with regard to the correct form of the 1D Hamiltonian. For instance, Aronov and Lyanda-Geller, who studied the effect of Rashba SO interaction on the Aharonov-Bohm conductance oscillations,² used a non-Hermitean operator as Hamiltonian.⁸ Zhou, Li, and Xue⁹ noticed this fact and derived a different (Hermitean) Hamiltonian operator. However, in their Hamiltonian the Rashba SO term originates from an electric field pointing in the radial direction and not in the direction perpendicular to the plane of the ring. This is physically not correct. Subsequently others^{3,5,7,10} have employed a now commonly used 1D Hamiltonian for electrons on a ring, without explicitly discussing its derivation.

The purpose of this short paper is to identify the origin of the existing ambiguity and to discuss in detail the procedure to obtain the correct 1D Hamiltonian operator for electrons moving on a ring in the presence of Rashba SO interaction. We will show that the subtlety of this seemingly trivial problem has not been fully appreciated so far.

The “conventional” way to obtain the Hamiltonian for a 1D ring from the Hamiltonian in two dimensions consists of two steps. First the Hamiltonian operator is transformed into cylindrical coordinates r and ϕ . Then r is set to a constant and all terms proportional to derivatives with respect to r are discarded (i.e., set to 0). This procedure works correctly in simple cases, such as free electrons or electrons in the presence of a (uniform or textured¹¹) magnetic field. However, it does not work in the presence of Rashba SO interaction, as we will illustrate below.

The (2D) Hamiltonian for a (single) electron in the presence of Rashba spin-orbit interaction and a magnetic field is given by

$$\hat{H} = \frac{1}{2m} (\mathbf{p} - e\mathbf{A})^2 + \alpha \hat{\sigma} \cdot \mathbf{E} \times (\mathbf{p} - e\mathbf{A}) + \mu \hat{\sigma} \cdot \mathbf{B}, \quad (1)$$

where \mathbf{A} is the vector potential, α is the SO constant, \mathbf{E} and \mathbf{B} are pointing in the \hat{z} direction (perpendicular to the plane). In cylindrical coordinates, with $x = r \cos \phi$ and $y = r \sin \phi$, this operator reads

$$\begin{aligned} \hat{H}(r, \phi) = & -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{1}{r^2} \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right)^2 \right] \\ & - \frac{\alpha}{r} (\cos \phi \sigma_x + \sin \phi \sigma_y) \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right) \\ & + i\alpha (\cos \phi \sigma_y - \sin \phi \sigma_x) \frac{\partial}{\partial r} + \frac{\hbar \omega_B}{2} \sigma_z \quad (2) \end{aligned}$$

with Φ is the magnetic flux through the ring, $\Phi_0 = h/e$, and $\hat{\sigma}_{x,y,z}$ are the usual Pauli spin matrices. Notice also that we have redefined α ($\alpha \rightarrow \hbar E_z \alpha$). If we now set r to a constant value ($r = a$) and neglect the derivative terms, we obtain

$$\begin{aligned} \hat{H}(\phi) = & -\frac{\hbar^2}{2ma^2} \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right)^2 + \frac{\hbar \omega_B}{2} \sigma_z \\ & - \frac{\alpha}{a} (\cos \phi \sigma_x + \sin \phi \sigma_y) \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right). \quad (3) \end{aligned}$$

This operator, used by Aronov and Lyanda Geller,² is not Hermitean, as can be easily shown by calculating its matrix elements in any complete basis (i.e., the “conventional” procedure fails).

In order to find the correct form for the 1D Hamiltonian we go back to the full (2D) Hamiltonian [Eq. (2)]. To this Hamiltonian we add a potential $V(r)$, which forces the electron wave functions to be localized on the ring in the radial direction. Specifically $V(r)$ is small in a narrow region around $r = a$ and large outside this region. For a narrow ring (steep confining potential) the confining energy in the radial direction is much larger than the SO energy, the Zeeman energy, and the kinetic energy in the azimuthal direction. This allows us to solve the Hamiltonian for the radial wave function first and treat \hat{H}_{SO} , \hat{H}_{Zeeman} , and $\hat{H}_{\text{kin}}(\phi)$ as a perturbation. Specifically we write $\hat{H} = \hat{H}_0 + \hat{H}_1$, where

$$\hat{H}_0 = -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right] + V(r) \quad (4)$$

and the perturbation Hamiltonian \hat{H}_1 is given by

$$\begin{aligned} \hat{H}_1 = & \frac{\hbar^2}{2mr^2} \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right)^2 + \frac{\hbar \omega_B}{2} \sigma_z - \frac{\alpha}{r} (\cos \phi \sigma_x \\ & + \sin \phi \sigma_y) \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right) + i \alpha (\cos \phi \sigma_y - \sin \phi \sigma_x) \frac{\partial}{\partial r}. \end{aligned} \quad (5)$$

The eigenfunctions of \hat{H}_0 are separable in r and ϕ , i.e., $\Psi(r, \phi) = R(r)\Phi(\phi)$, since \hat{H}_0 does not depend on ϕ . In the limit of a very narrow (1D) ring all electrons will be in the lowest radial mode $R_0(r)$. We then have an infinitely degenerate set of states $\Psi_n(r, \phi) = R_0(r)\Phi_n(\phi)$ over which we have to diagonalize \hat{H}_1 [here, the $\Phi_n(\phi)$ denote a complete set of spinors in the ϕ direction].

The matrix elements of \hat{H}_1 are

$$a_{mn} = \langle \Phi_m(\phi) | \langle R_0(r) | \hat{H}_1(r, \phi) | R_0(r) | \Phi_n(\phi) \rangle, \quad (6)$$

from which we can read the correct 1D Hamiltonian $\hat{H}(\phi)$ directly

$$\hat{H}_{1D}(\phi) = \langle R_0(r) | \hat{H}_1(r, \phi) | R_0(r) \rangle. \quad (7)$$

In order to obtain the 1D Hamiltonian explicitly, we have to calculate the lowest radial mode for a given confining potential. If we assume without loss of generality (since we will consider the limit of a truly 1D ring) a harmonic confining potential [$V(r) = 1/2K(r-a)^2$], we have to solve

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 R(r)}{\partial r^2} + \frac{1}{r} \frac{\partial R(r)}{\partial r} \right] + \frac{1}{2} K(r-a)^2 R(r) = ER(r). \quad (8)$$

In the limit of a 1D ring we may neglect the $(1/r) \times (\partial/\partial r)$ term in comparison to the $\partial^2/\partial r^2$ term and obtain the harmonic-oscillator equation.¹² The lowest energy normalized solutions is then given by

$$R_0(r) = \left(\frac{\gamma}{a\sqrt{\pi}} \right)^{1/2} e^{-(1/2)\gamma^2(r-a)^2}, \quad (9)$$

where $\gamma^4 = mK/\hbar^2$ (the 1D limit is achieved by letting γ go to infinity).

From Eqs. (5) and (7) we can now derive the 1D Hamiltonian explicitly. Since \hat{H}_1 contains terms dependent on r and derivatives with respect to r we have to calculate their expectation value. We obtain

$$\langle R_0(r) | \frac{1}{r} | R_0(r) \rangle = \int_0^\infty R_0^2(r) dr = \frac{1}{a} \quad (10)$$

and the expectation value of $\partial/\partial r$ is given by

$$\langle R_0(r) | \frac{\partial}{\partial r} | R_0(r) \rangle = \int_0^\infty R_0(r) \frac{\partial R_0(r)}{\partial r} r dr = -\frac{1}{2a}. \quad (11)$$

From this we conclude that we cannot safely disregard the $\partial/\partial r$ term in order to obtain the correct 1D Hamiltonian.

It is worth stressing that it is not essential to choose a harmonic potential, nor to make any approximation as we have done above for simplicity, in order to obtain these results. To show this, let $|\rho_0(r)\rangle$ be the lowest radial mode for an arbitrarily given confining potential. We define $|\rho'_0(r)\rangle = (1/\sqrt{r})|\rho_0(r)\rangle$. From direct calculations it follows that $\langle \rho_0 | (1/2r) + (\partial/\partial r) | \rho_0 \rangle = \langle \rho'_0 | (1/r) (\partial/\partial r) | \rho'_0 \rangle = 1/2 \rho_0'^2|_0^\infty = 1/2r \rho_0^2|_0^\infty = 0$. We then obtain $\langle \rho_0 | \partial/\partial r | \rho_0 \rangle = -\langle \rho_0 | 1/2r | \rho_0 \rangle$. Therefore for the lowest radial mode in the 1D limit we always get $\langle \rho_0 | \partial/\partial r | \rho_0 \rangle = -(1/2a)$, independent of the precise form of $|\rho_0(r)\rangle$ and thus of the precise shape of the radial confining potential that is used in the calculation.

Having established the generality of our result, we can now write the 1D Hamiltonian explicitly. From Eqs. (7) and (10) we get

$$\begin{aligned} \hat{H}_{1D}(\phi) = & \frac{\hbar^2}{2ma^2} \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right)^2 + \frac{\hbar \omega_B}{2} \sigma_z - \frac{\alpha}{a} (\cos \phi \sigma_x \\ & + \sin \phi \sigma_y) \left(i \frac{\partial}{\partial \phi} + \frac{\Phi}{\Phi_0} \right) - i \frac{\alpha}{2a} (\cos \phi \sigma_y \\ & - \sin \phi \sigma_x). \end{aligned} \quad (12)$$

This is the correct form of the 1D Hamiltonian for electrons on a ring, in the presence of Rashba SO interaction.

The last term in Eq. (12) is neglected if we follow the ‘‘conventional’’ procedure. It is only recovered by following the procedure described above. In the simple cases mentioned earlier (e.g., free electrons), there are no terms present in the Hamiltonian proportional to both $\partial/\partial r$ and some function of ϕ (i.e., the two-dimensional Hamiltonian is separable). In these cases the ‘‘conventional’’ procedure produces the correct result. In all other cases it is necessary to take into account properly the confinement of the wave function in the radial direction as we have shown in this paper in order to obtain the correct 1D Hamiltonian on a ring.

In short, what we have described in this paper is a formally correct procedure to project the original Hamiltonian [Eq. (1)] defined on the Hilbert space of spinors in two dimensions on a restricted Hilbert subspace, spanned by the complete set of spinors $\Phi_n(\phi)$, which are function of the ϕ coordinate only.

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