

Exact analytical propagators for anisotropic quantum dots under magnetic field with atomic spin-orbital coupling

CHEN Yin, GUO Wei, PAN Xiaoyin *

(School of Physical Science and Technology, Ningbo University, Ningbo 315211, China)

Abstract: In quantum mechanics, there are very few systems whose propagators can be obtained exactly, especially in the case of taking spin-orbital coupling (SOC) effects into account. Using the group theoretical method in phase space, we start with deriving exact analytical expressions for the propagators of anisotropic quantum dots with atomic spin-orbital coupling (ASOC). As an example of application, the evolution of spin-dependent Gaussian wave packets is calculated using the propagator, along with which the corresponding probability densities, the effects of ASOC and magnetic field on the expectations of the distances are also investigated.

Key words: path-integral method; spin-orbital coupling; quantum dot; magnetic field

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1 Introduction

In the past decades, due to the progress in semiconductor technology, electronic systems such as quantum dots^[1-5], antidots^[6-8], well wires^[9], and quantum rings^[10] under perpendicular magnetic fields have revealed many interesting physical phenomena and attracted much research interest. In particular, two-dimensional electron gas (2DEG) in quantum dots (QDs) under perpendicular magnetic fields have drawn a great deal of experimental and theoretical attention because all their parameters such as size, number of electrons, strength and shape of the confining potential, the coupling between dots, as well as external parameters such as temperature and magnetic electric fields can be varied in a controlled way. Confinement in electrostatic QDs is usually achieved by laterally restraining a 2D electron gas by an artificial potential. As a first

approximation, those artificial potentials are often described by parabolic potentials. In the simpler case when the QDs are isotropic, namely the confinement has circular symmetry with $\omega_x = \omega_y$, i.e., the same confining frequencies in the x and y directions, the full rotation symmetry of a circular dot leads to the most prominent shell structure and well-defined physical pictures^[3]. Under perpendicular magnetic fields, the isotropic QDs can be described by the well known exact solvable Fock-Darwin (FD) model^[11-12], which has wide applications in the studies of quantum Hall effects^[13-15].

However, because the presence of asymmetry in the confining potential is experimentally more realistic, there exist lots of works on the anisotropic QDs with the broken rotational symmetry, thereby altered electronic and dynamical properties^[3,16-20]. In order to study the magnetic properties of such QDs, the FD model has also been generalized to the elliptical parabolic potential case

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第一作者: 陈寅(1990-), 男, 浙江宁海人, 在读硕士研究生, 主要研究方向: 量子器件相关理论计算. E-mail: 15336698809@163.com

*通信作者: 潘孝胤(1974-), 男, 浙江宁海人, 研究员, 主要研究方向: 凝聚态理论. E-mail: panxiaoyin@nbu.edu.cn

and been solved exactly^[21]. Consequently, various physical properties, such as the quantization of the conductance^[22] and the electronic properties, can be studied^[23]. Moreover, this model also can be used to study rotating droplets of electrons trapped in quasi-two-dimensional quantum dots and rotating Bose-Einstein condensates^[24].

On the other hand, the SOC which couples the internal and orbital degrees of freedom was originally discovered in the fine structure of atomic spectra (henceforth referred to as ASOC), and later introduced to explain the nuclear structure. The form of ASOC is given in the form of $H_{\text{SO}}^a = \frac{-\hbar}{4m^*c^2} \vec{\sigma} \cdot [\hat{p} \times \nabla V]$, with V being the confining potential and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, where the vector of Pauli spin matrices can be derived from the non-relativistic approximation to the Dirac equation. Usually in semiconductors, in addition to the ASOC arising from the confining potential, there exist two other SOC mechanisms. The first one is Rashba SOC^[25-27], which is the signature of structure inversion asymmetry present in 2D materials. This SOC exists intrinsically and is responsible for the quantum spin-Hall-effect^[28-29]. The second one is Dresselhaus SOC^[30] which originates in bulk inversion asymmetry. By employing the above SOC mechanisms, the spin degree of freedom of the electron is exploited to improve the functionality of electronic devices. This active field of research is now known as spintronics^[25].

Hence, it will be interesting to understand the spin-dependent evolution of wave packets for electrons confined in quantum dots under a perpendicular magnetic field with ASOC. In order to get a better handle on the evolution of the corresponding physical systems, the propagator method^[31-32] is regarded as a powerful tool and shall be a good choice. It is well known in quantum mechanics that the propagator as a Green's function of the Schrödinger equation contains all the information about the system and plays a central role in Feynman's path integral approach^[31-32] to solve non-relativistic quantum mechanical problems. However, due to the difficulty of obtaining the analytical expressions for the

propagators, to our knowledge there are very few such investigations and are solely limited to the isotropic cases^[33]. To study the more interesting anisotropic case with broken rotational symmetry, in the present work we derive analytical expressions for the propagator of such systems using the group theoretical method on phase space^[34], then the effects of the ASOC and magnetic field on the evolution of the spin-dependent wave packets and the expectations of distances for spin-up and down components are investigated as an example of application.

2 The Hamiltonian

Consider a 2D system of an electron of charge $q = -e$, $e > 0$ and effective mass m^* confined in an anisotropic QD, under a perpendicular constant magnetic field B along the z -direction. Then the Hamiltonian takes the form,

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{SO}} + g\mu_B\sigma_z/2, \quad (1)$$

where

$$\hat{H}_0 = \frac{1}{2m^*} \left(\hat{p} + \frac{e}{c} \mathbf{A} \right)^2 + V(x, y) \quad (2)$$

is the Hamiltonian for the electron in the anisotropic QD with $V(x, y) = m^*(\omega_x^2 x^2 + \omega_y^2 y^2)/2$ being the lateral confining potential, and

$$\hat{H}_{\text{SO}} = \frac{-\hbar}{4m^{*2}c^2} \vec{\sigma} \cdot \left[\left(\hat{p} + \frac{e}{c} \mathbf{A} \right) \times \nabla V \right] \quad (3)$$

is the spin-orbital interaction, the last term on the r. h. s of Eq. (1) is the Zeeman coupling. Working in the symmetric gauge $\mathbf{A} = B(-y, x)/2$, and noticing that the system is 2D, then the Hamiltonian of Eq. (2) can be recast into the following form,

$$\begin{aligned} \hat{H} = & \frac{1}{2m^*} (\hat{p}_x^2 + \hat{p}_y^2) + \frac{m^*}{2} (\tilde{\omega}_x^2 x^2 + \tilde{\omega}_y^2 y^2) + \\ & \Gamma_x x \hat{p}_y - \Gamma_y y \hat{p}_x + \frac{1}{2} g\mu_B\sigma_z, \end{aligned} \quad (4)$$

where the coefficients are matrices,

$$\tilde{\omega}_x^2 = \omega_x^2 + \frac{\omega_c^2}{4} + \Gamma\omega_c\omega_x^2, \Gamma_x = \Gamma\omega_x^2 + \frac{\omega_c}{2}, \quad (5)$$

$$\tilde{\omega}_y^2 = \omega_y^2 + \frac{\omega_c^2}{4} + \Gamma\omega_c\omega_y^2, \Gamma_y = \Gamma\omega_y^2 + \frac{\omega_c}{2}, \quad (6)$$

with $\Gamma = \frac{\hbar}{4m^*c^2}\sigma_z$, $\omega_c = \frac{eB}{m^*c}$ being the cyclotron frequency. Since σ_z is diagonal, alternatively the Hamiltonian can be rewritten into a diagonal matrix form as

$$\hat{H} = \begin{pmatrix} \hat{H}_\uparrow & 0 \\ 0 & \hat{H}_\downarrow \end{pmatrix}, \quad (7)$$

where $\hat{H}_{\uparrow,\downarrow}$ are obtained by setting the values of σ_z in the coefficients of Eq. (5) and (6) to be ± 1 , namely $\hat{H}_{\uparrow,\downarrow}|_{\sigma_z=\pm 1}$. In the following calculations, one should treat σ_z as a number whose value is 1 for $\hat{H}_\uparrow$, or -1 for $\hat{H}_\downarrow$. This Hamiltonian is an asymmetric generalization of the one used by Bernevig et al^[35] to study the quantum spin Hall effect for strained materials with symmetric quantum well parabolic confinement.

3 Calculations of the exact analytical propagator

In this section we calculate the exact analytical propagator by using the group theoretical method on phase space developed in Ref. [34], where the representation of the Lie group $Sp(2N, R) \otimes N(N)$ on the phase space associated with standard ordering was considered and the calculation of the quantum mechanical propagator for a general N -dimensional system with Hamiltonian quadratic in the position and momentum variables may be reduced to the calculation of the propagator for a “free particle”. We refer the readers to Ref. [34] for more details. The key step of this method is to solve the equations of motion (EOM). To do so, we first ignore the Zeeman coupling term in Eq. (4) since it is merely a constant and will not affect the dynamics. Denoting the 2D position vector $\mathbf{r} = (x, y)^T$, $\mathbf{p} = (p_x, p_y)^T$, where T stands for transpose, the EOM can be written as,

$$\frac{d\mathbf{r}}{dt} = \begin{pmatrix} 0 & -\Gamma_y \\ \Gamma_x & 0 \end{pmatrix} \mathbf{r} + \frac{\mathbf{p}}{m^*}, \quad (8)$$

$$\frac{d\mathbf{p}}{dt} = -m^* \begin{pmatrix} \tilde{\omega}_x^2 & 0 \\ 0 & \tilde{\omega}_y^2 \end{pmatrix} \mathbf{r} + \begin{pmatrix} 0 & -\Gamma_x \\ \Gamma_y & 0 \end{pmatrix} \mathbf{p}, \quad (9)$$

or in matrix form as

$$\frac{d}{dt} \begin{pmatrix} \mathbf{r} \\ \mathbf{p} \end{pmatrix} = \mathcal{A} \begin{pmatrix} \mathbf{r} \\ \mathbf{p} \end{pmatrix}, \quad (10)$$

where the matrix

$$\mathcal{A} = \begin{pmatrix} 0 & -\Gamma_y & \frac{1}{m^*} & 0 \\ \Gamma_x & 0 & 0 & \frac{1}{m^*} \\ -m^*\tilde{\omega}_x^2 & 0 & 0 & -\Gamma_x \\ 0 & -m^*\tilde{\omega}_y^2 & \Gamma_y & 0 \end{pmatrix}, \quad (11)$$

whose eigenvalues are $\pm i\lambda_\pm$ with

$$\lambda_\pm = \frac{1}{\sqrt{2}} \left[(\tilde{\omega}_x^2 + \tilde{\omega}_y^2 + 2\Gamma_x\Gamma_y) \pm ((\tilde{\omega}_x^2 - \tilde{\omega}_y^2)^2 + 4\Gamma_x\Gamma_y(\tilde{\omega}_x^2 + \tilde{\omega}_y^2) + 4\Gamma_x^2\tilde{\omega}_y^2 + 4\Gamma_y^2\tilde{\omega}_x^2)^{\frac{1}{2}} \right]^{\frac{1}{2}}. \quad (12)$$

The EOM of Eq. (10) is hard to solve directly. However, note that $\pm i\lambda_\pm$ are the eigenvalues of the matrix $\mathcal{A}$, hence its solution must be a linear combination of $e^{\pm i\lambda_\pm t}$, or $\sin \lambda_\pm t$ and $\cos \lambda_\pm t$. Thus the solution to Eq. (10) can be written as

$$\begin{aligned} \mathbf{r} &= \mathbf{c}_1 \sin \lambda_+ t + \mathbf{c}_2 \sin \lambda_- t + \mathbf{c}_3 \cos \lambda_+ t + \mathbf{c}_4 \cos \lambda_- t, \\ \mathbf{p} &= \mathbf{d}_1 \sin \lambda_+ t + \mathbf{d}_2 \sin \lambda_- t + \mathbf{d}_3 \cos \lambda_+ t + \mathbf{d}_4 \cos \lambda_- t, \end{aligned} \quad (13)$$

where the coefficients $\mathbf{c}_i$ and $\mathbf{d}_i$ ($i=1, 2, 3, 4$) can be obtained after some algebraic manipulations as

$$\begin{aligned} \mathbf{c}_1 &= \frac{\lambda_+}{D(t)} \left[\begin{pmatrix} 0 & \frac{\lambda_-^2 \Gamma_x}{\Gamma_x^2 - \tilde{\omega}_x^2} - \Gamma_y \\ \Gamma_x - \frac{\lambda_-^2 \Gamma_y}{\Gamma_y^2 - \tilde{\omega}_y^2} & 0 \end{pmatrix} \mathbf{r}_0 + \begin{pmatrix} \frac{\lambda_-^2}{\Gamma_x^2 - \tilde{\omega}_x^2} + 1 & 0 \\ 0 & \frac{\lambda_-^2}{\Gamma_y^2 - \tilde{\omega}_y^2} + 1 \end{pmatrix} \frac{\mathbf{p}_0}{m^*} \right], \\ \mathbf{c}_2 &= \frac{\lambda_-}{D(t)} \left[\begin{pmatrix} 0 & -\frac{\lambda_+^2 \Gamma_x}{\Gamma_x^2 - \tilde{\omega}_x^2} + \Gamma_y \\ -\Gamma_x + \frac{\lambda_+^2 \Gamma_y}{\Gamma_y^2 - \tilde{\omega}_y^2} & 0 \end{pmatrix} \mathbf{r}_0 - \begin{pmatrix} \frac{\lambda_+^2}{\Gamma_x^2 - \tilde{\omega}_x^2} + 1 & 0 \\ 0 & \frac{\lambda_+^2}{\Gamma_y^2 - \tilde{\omega}_y^2} + 1 \end{pmatrix} \frac{\mathbf{p}_0}{m^*} \right], \end{aligned}$$

$$\begin{aligned}
c_3 &= \frac{1}{D(t)} \left[\begin{pmatrix} \tilde{\omega}_x^2 - \lambda_-^2 + \Gamma_x \Gamma_y & 0 \\ 0 & \tilde{\omega}_y^2 - \lambda_-^2 + \Gamma_x \Gamma_y \end{pmatrix} r_0 + \right. \\
&\quad \left. \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (\Gamma_x + \Gamma_y) \frac{p_0}{m^*} \right], \\
c_4 &= \frac{1}{D(t)} \left[\begin{pmatrix} \lambda_+^2 - \tilde{\omega}_x^2 - \Gamma_x \Gamma_y & 0 \\ 0 & \lambda_+^2 - \tilde{\omega}_y^2 - \Gamma_x \Gamma_y \end{pmatrix} r_0 - \right. \\
&\quad \left. \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (\Gamma_x + \Gamma_y) \frac{p_0}{m^*} \right], \quad (14)
\end{aligned}$$

and

$$\begin{aligned}
d_1 &= \frac{\lambda_+}{D(t)} \left[\begin{pmatrix} \tilde{\omega}_x^2 + \frac{\lambda_-^2 \tilde{\omega}_y^2}{\Gamma_y^2 - \tilde{\omega}_y^2} & 0 \\ 0 & \tilde{\omega}_y^2 + \frac{\lambda_-^2 \tilde{\omega}_x^2}{\Gamma_x^2 - \tilde{\omega}_x^2} \end{pmatrix} m^* r_0 + \right. \\
&\quad \left. \begin{pmatrix} 0 & \frac{\lambda_-^2 \Gamma_y}{\Gamma_y^2 - \tilde{\omega}_y^2} - \Gamma_x \\ -\frac{\lambda_-^2 \Gamma_x}{\Gamma_x^2 - \tilde{\omega}_x^2} + \Gamma_y & 0 \end{pmatrix} p_0 \right], \\
d_2 &= \frac{\lambda_-}{D(t)} \left[\begin{pmatrix} \tilde{\omega}_x^2 + \frac{\lambda_+^2 \tilde{\omega}_y^2}{\Gamma_y^2 - \tilde{\omega}_y^2} & 0 \\ 0 & \tilde{\omega}_y^2 + \frac{\lambda_+^2 \tilde{\omega}_x^2}{\Gamma_x^2 - \tilde{\omega}_x^2} \end{pmatrix} m^* r_0 - \right. \\
&\quad \left. \begin{pmatrix} 0 & \frac{\lambda_+^2 \Gamma_y}{\Gamma_y^2 - \tilde{\omega}_y^2} - \Gamma_x \\ -\frac{\lambda_+^2 \Gamma_x}{\Gamma_x^2 - \tilde{\omega}_x^2} + \Gamma_y & 0 \end{pmatrix} p_0 \right], \\
d_3 &= \frac{1}{D(t)} \left[\begin{pmatrix} 0 & -\Gamma_y \tilde{\omega}_x^2 - \Gamma_x \tilde{\omega}_y^2 \\ \Gamma_y \tilde{\omega}_x^2 + \Gamma_x \tilde{\omega}_y^2 & 0 \end{pmatrix} m^* r_0 + \right. \\
&\quad \left. \begin{pmatrix} -\lambda_-^2 + \tilde{\omega}_x^2 + \Gamma_x \Gamma_y & 0 \\ 0 & -\lambda_-^2 + \tilde{\omega}_y^2 + \Gamma_x \Gamma_y \end{pmatrix} p_0 \right], \\
d_4 &= \frac{1}{D(t)} \left[\begin{pmatrix} 0 & \Gamma_y \tilde{\omega}_x^2 + \Gamma_x \tilde{\omega}_y^2 \\ -\Gamma_y \tilde{\omega}_x^2 - \Gamma_x \tilde{\omega}_y^2 & 0 \end{pmatrix} m^* r_0 + \right. \\
&\quad \left. \begin{pmatrix} \lambda_+^2 - \tilde{\omega}_x^2 - \Gamma_x \Gamma_y & 0 \\ 0 & \lambda_+^2 - \tilde{\omega}_y^2 - \Gamma_x \Gamma_y \end{pmatrix} p_0 \right], \quad (15)
\end{aligned}$$

with $D(t) = \lambda_+^2 - \lambda_-^2$. Substitution of Eq. (14)–(15) into (13) yields

$$r = A_1 p_0 - A_2 r_0, \quad p = M_1 p_0 - M_2 r_0, \quad (16)$$

where the matrix elements for A_1, A_2 are

$$(A_1)_{11} = \frac{1}{m^* (\lambda_+^2 - \lambda_-^2)} \left[\frac{\lambda_+ \sin \lambda_+ t (\Gamma_x^2 - \tilde{\omega}_x^2 + \lambda_-^2)}{\Gamma_x^2 - \tilde{\omega}_x^2} - \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t (\Gamma_x^2 - \tilde{\omega}_x^2 + \lambda_+^2)}{\Gamma_x^2 - \tilde{\omega}_x^2} \right],$$

$$(A_1)_{12} = -(A_1)_{21} = \frac{(\Gamma_x + \Gamma_y)(\cos \lambda_+ t - \cos \lambda_- t)}{m^* (\lambda_+^2 - \lambda_-^2)},$$

$$(A_1)_{22} = \frac{1}{m^* (\lambda_+^2 - \lambda_-^2)} \left[\frac{\lambda_+ \sin \lambda_+ t (\Gamma_y^2 - \tilde{\omega}_y^2 + \lambda_-^2)}{\Gamma_y^2 - \tilde{\omega}_y^2} - \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t (\Gamma_y^2 - \tilde{\omega}_y^2 + \lambda_+^2)}{\Gamma_y^2 - \tilde{\omega}_y^2} \right],$$

$$(A_2)_{11} = \frac{-1}{(\lambda_+^2 - \lambda_-^2)} \left[(\tilde{\omega}_x^2 - \lambda_-^2 + \Gamma_x \Gamma_y) \cos \lambda_+ t - \right.$$

$$(\tilde{\omega}_x^2 - \lambda_+^2 + \Gamma_x \Gamma_y) \cos \lambda_- t \left. \right],$$

$$(A_2)_{12} = \frac{-1}{(\lambda_+^2 - \lambda_-^2)} \left[\frac{\lambda_+ \sin \lambda_+ t [\lambda_-^2 \Gamma_x - \Gamma_y (\Gamma_x^2 - \tilde{\omega}_x^2)]}{\Gamma_x^2 - \tilde{\omega}_x^2} + \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t [(-\lambda_+^2 \Gamma_x + \Gamma_y) (\Gamma_y^2 - \tilde{\omega}_y^2)]}{\Gamma_y^2 - \tilde{\omega}_y^2} \right],$$

$$(A_2)_{21} = \frac{-1}{(\lambda_+^2 - \lambda_-^2)} \left[\frac{\lambda_+ \sin \lambda_+ t [\Gamma_x (\Gamma_y^2 - \tilde{\omega}_y^2) - \lambda_-^2 \Gamma_y]}{\Gamma_y^2 - \tilde{\omega}_y^2} + \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t [\lambda_+^2 \Gamma_y - \Gamma_x (\Gamma_x^2 - \tilde{\omega}_x^2)]}{\Gamma_x^2 - \tilde{\omega}_x^2} \right],$$

$$(A_2)_{22} = \frac{-1}{(\lambda_+^2 - \lambda_-^2)} \left[(\tilde{\omega}_y^2 - \lambda_-^2 + \Gamma_x \Gamma_y) \cos \lambda_+ t - \right.$$

$$(\tilde{\omega}_y^2 - \lambda_+^2 + \Gamma_x \Gamma_y) \cos \lambda_- t \left. \right], \quad (17)$$

the matrix elements for M_1 and M_2 are

$$(M_1)_{11} = \frac{1}{\lambda_+^2 - \lambda_-^2} \left[(\tilde{\omega}_x^2 - \lambda_-^2 + \Gamma_x \Gamma_y) \cos \lambda_+ t - \right.$$

$$(\tilde{\omega}_x^2 - \lambda_+^2 + \Gamma_x \Gamma_y) \cos \lambda_- t \left. \right],$$

$$(M_1)_{12} = \frac{1}{\lambda_+^2 - \lambda_-^2} \left[\frac{\lambda_+ \sin \lambda_+ t [\lambda_-^2 \Gamma_y - \Gamma_x (\Gamma_y^2 - \tilde{\omega}_y^2)]}{\Gamma_y^2 - \tilde{\omega}_y^2} - \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t [(\lambda_+^2 \Gamma_y - \Gamma_x) (\Gamma_y^2 - \tilde{\omega}_y^2)]}{\Gamma_y^2 - \tilde{\omega}_y^2} \right],$$

$$(M_1)_{21} = \frac{1}{\lambda_+^2 - \lambda_-^2} \left[\frac{\lambda_+ \sin \lambda_+ t [\Gamma_y (\Gamma_x^2 - \tilde{\omega}_x^2) - \lambda_-^2 \Gamma_x]}{\Gamma_x^2 - \tilde{\omega}_x^2} + \right.$$

$$\left. \frac{\lambda_- \sin \lambda_- t [\lambda_+^2 \Gamma_x - \Gamma_y (\Gamma_x^2 - \tilde{\omega}_x^2)]}{\Gamma_x^2 - \tilde{\omega}_x^2} \right],$$

$$(M_1)_{22} = \frac{1}{\lambda_+^2 - \lambda_-^2} \left[(\tilde{\omega}_y^2 - \lambda_-^2 + \Gamma_x \Gamma_y) \cos \lambda_+ t - \right.$$

$$(\tilde{\omega}_y^2 - \lambda_+^2 + \Gamma_x \Gamma_y) \cos \lambda_- t \left. \right], \quad (18)$$

$$(M_2)_{11} = \frac{-m^*}{\lambda_+^2 - \lambda_-^2} \left[\frac{-\lambda_+ \sin \lambda_+ t [(\Gamma_y^2 - \tilde{\omega}_y^2) \tilde{\omega}_x^2 + \lambda_-^2 \tilde{\omega}_y^2]}{\Gamma_y^2 - \tilde{\omega}_y^2} + \right.$$

$$\begin{aligned}
 & \frac{\lambda_- \sin \lambda_- t [\tilde{\omega}_x^2 (\Gamma_y^2 - \tilde{\omega}_y^2) + \lambda_+^2 \tilde{\omega}_y^2]}{\Gamma_y^2 - \tilde{\omega}_y^2} \Bigg], \\
 (\mathbf{M}_2)_{12} = -(\mathbf{M}_2)_{21} = & \frac{m^*}{\lambda_+^2 - \lambda_-^2} \times \\
 & \left[(\Gamma_x \tilde{\omega}_y^2 + \Gamma_y \tilde{\omega}_x^2) (\cos \lambda_+ t - \cos \lambda_- t) \right], \\
 (\mathbf{M}_2)_{22} = & \frac{-m^*}{\lambda_+^2 - \lambda_-^2} \left[\frac{-\lambda_+ \sin \lambda_+ t [(\Gamma_x^2 - \tilde{\omega}_x^2) \tilde{\omega}_y^2 + \lambda_-^2 \tilde{\omega}_x^2]}{\Gamma_x^2 - \tilde{\omega}_x^2} + \right. \\
 & \left. \frac{\lambda_- \sin \lambda_- t [\tilde{\omega}_x^2 (\Gamma_y^2 - \tilde{\omega}_y^2) + \lambda_+^2 \tilde{\omega}_y^2]}{\Gamma_y^2 - \tilde{\omega}_y^2} \right]. \quad (19)
 \end{aligned}$$

Since $\mathbf{r}$ and $\mathbf{p}$ must obey the same commutative relationships as those of r_0 and p_0 , it should be mentioned that the 2×2 matrices $\mathbf{A}_1, \mathbf{A}_2, \mathbf{M}_1, \mathbf{M}_2$ must satisfy the following identities,

$$\begin{aligned}
 \mathbf{A}_1 \mathbf{A}_2^T &= \mathbf{A}_2 \mathbf{A}_1^T, \\
 \mathbf{M}_1 \mathbf{M}_2^T &= \mathbf{M}_2 \mathbf{M}_1^T, \\
 \mathbf{A}_1 \mathbf{M}_2^T + \mathbf{A}_2 \mathbf{M}_1^T &= -\mathbf{I}.
 \end{aligned} \quad (20)$$

These identities shall be useful later on.

Having obtained the solutions for EOM, we can obtain the propagator directly by the group theoretical method on phase space^[34],

$$\begin{aligned}
 K(\mathbf{x}_b, t; \mathbf{x}_a, 0) &= [\det(-\mathbf{A}_2)]^{\frac{1}{2}} \exp \left\{ \frac{i}{2\hbar} \mathbf{x}_b^T \mathbf{M}_2 \mathbf{A}_2^{-1} \mathbf{x}_b \right\} \times \\
 & K_F \left(-\frac{1}{2} \mathbf{A}_2^{-1} \mathbf{A}_1; -\mathbf{A}_2^{-1} \mathbf{x}_b, t; \mathbf{x}_a, 0 \right), \quad (21)
 \end{aligned}$$

where the second term on the r. h. s of above equation is defined as

$$\begin{aligned}
 K_F(A(t); \mathbf{x}, t; \mathbf{x}_a, 0) &= \frac{1}{4\pi i \hbar} [\det A(t)]^{\frac{1}{2}} \times \\
 & \exp \left\{ \frac{i}{4\hbar} [(\mathbf{x} - \mathbf{x}_a)^T A(t)^{-1} (\mathbf{x} - \mathbf{x}_a)] \right\}. \quad (22)
 \end{aligned}$$

Recovering the contribution $e^{\frac{ig\mu_B\sigma_z t}{2\hbar}}$ from the Zeeman coupling term, the propagator finally can be recast into the following form,

$$\begin{aligned}
 K(\mathbf{x}_b, t; \mathbf{x}_a, 0) &= \begin{pmatrix} K_\uparrow(\mathbf{x}_b, t; \mathbf{x}_a, 0) & 0 \\ 0 & K_\downarrow(\mathbf{x}_b, t; \mathbf{x}_a, 0) \end{pmatrix} = \\
 & \exp \left\{ \frac{i}{2\hbar} \mathbf{x}_b^T [\mathbf{M}_2 \mathbf{A}_2^{-1} - (\mathbf{A}_1 \mathbf{A}_2^T)^{-1}] \mathbf{x}_b - \frac{ig\mu_B\sigma_z t}{2\hbar} \right\} \\
 & \frac{1}{2\pi i \hbar (\det \mathbf{A}_1)^{1/2}} \times \\
 & \exp \left\{ -\frac{i}{2\hbar} [\mathbf{x}_a^T (\mathbf{A}_1^{-1} \mathbf{A}_2) \mathbf{x}_a + 2\mathbf{x}_a^T \mathbf{A}_1^{-1} \mathbf{x}_b] \right\}. \quad (23)
 \end{aligned}$$

It can be readily verified that the propagator of Eq.

(23) can reduce to various special cases in the literature.

For instances, in the isotropic case namely when $\omega_x = \omega_y = \omega_0$, denoting $\Gamma_x = \Gamma_y = \Gamma_0 = \Gamma\omega_0^2 + \omega_c/2$, $\tilde{\omega}_x^2 = \tilde{\omega}_y^2 = \tilde{\omega}_0^2 = \omega_0^2 + \omega_c^2/4 + \Gamma\omega_c\omega_0^2$, then we have

$$\mathbf{A}_1 = \frac{\mathbf{M}_2}{(m^* \tilde{\omega}_0)^2} = \begin{pmatrix} \sin \tilde{\omega}_0 t \\ m^* \tilde{\omega}_0 \end{pmatrix} \cdot e^{-J\Gamma_0 t}, \quad (24)$$

$$-\mathbf{A}_2 = \mathbf{M}_1 = \cos \tilde{\omega}_0 t \cdot e^{-J\Gamma_0 t},$$

where $\mathbf{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Substitution of Eq. (24) into (23)

yields the propagator for the isotropic case,

$$\begin{aligned}
 K(\mathbf{x}_b, t; \mathbf{x}_a, 0) &= \frac{-B(t)}{\pi} \exp \{ B(t) [(\mathbf{x}_b^2 + \mathbf{x}_a^2) \cos \tilde{\omega}_0 t - \\
 & 2(x_a x_b + y_a y_b) \cos \Gamma_0 t - \\
 & 2(x_a y_b - x_b y_a) \sin \Gamma_0 t] \}, \quad (25)
 \end{aligned}$$

with $B(t) = \frac{im^* \tilde{\omega}_0}{2\hbar \sin \tilde{\omega}_0 t}$. It is evident that in the absence

of the external magnetic field, then the above propagator reduces to that studied in Ref. [33]. If one further neglects the effect of the ASOC, the propagator can further reduce to that of an isotropic 2D harmonic oscillator^[32].

4 The ASOC effects on the evolution of spin-dependent wave packets

As an example of application, next let us consider the evolution of a 2D Gaussian wave packet that has the following form initially at $t=0$,

$$\Psi_0(\mathbf{r}, 0) = \frac{1}{\sqrt{\pi d}} \exp \left(-\frac{\mathbf{r}^2}{2d^2} \right) (\chi |\uparrow\rangle + \xi |\downarrow\rangle), \quad (26)$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are up and down spin states in the z -direction with constant coefficients χ, ξ chosen to satisfy $|\chi|^2 + |\xi|^2 = 1$. Applying the Feynman path-integral approach, we can calculate the wave packet at time t as,

$$\begin{aligned}
 \Psi(\mathbf{r}_b, t) &= \int K(\mathbf{r}_b, t; \mathbf{r}_a, 0) \Psi_0(\mathbf{r}_a) d\mathbf{r}_a = \\
 & \int \begin{pmatrix} K_\uparrow(\mathbf{x}_b, t; \mathbf{x}_a, 0) & 0 \\ 0 & K_\downarrow(\mathbf{x}_b, t; \mathbf{x}_a, 0) \end{pmatrix} \Psi_0(\mathbf{r}_a) d\mathbf{r}_a. \quad (27)
 \end{aligned}$$

Inserting the expression for the propagator into above equation, and performing the integral we obtain

$$\Psi(\mathbf{r}, t) = \begin{pmatrix} \Psi_\uparrow(\mathbf{r}; t) \\ \Psi_\downarrow(\mathbf{r}; t) \end{pmatrix} = \frac{1}{2i\hbar \sqrt{\pi d} \sqrt{\det \mathbf{A}_1}} \times$$

$$\begin{aligned}
& \exp \left\{ \frac{i}{2\hbar} \mathbf{r}^T [\mathbf{M}_2 \mathbf{A}_2^{-1} - (\mathbf{A}_1 \mathbf{A}_2^T)^{-1}] \mathbf{r} \right\} \\
& \left[\left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right) \left(\frac{1}{2d} + \frac{i\mathcal{A}}{2\hbar} \right) + \frac{(\mathcal{B} + \mathcal{C})^2}{16\hbar^2} \right]^{1/2} \times \\
& \exp \left\{ -\frac{\left(\frac{F}{\hbar} \right)^2}{4 \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right)} \right\} \times \\
& \exp \left\{ -\frac{1}{4 \left[\left(\frac{1}{2d} + \frac{i\mathcal{A}}{2\hbar} \right) \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right) + \frac{(\mathcal{B} + \mathcal{C})^2}{16\hbar^2} \right]} \right\} \times \\
& \left[\left(\frac{E}{\hbar} \right)^2 \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right) - \frac{iEF(\mathcal{B} + \mathcal{C})}{2\hbar^3} - \right. \\
& \left. \frac{(\mathcal{B} + \mathcal{C})^2}{16\hbar^2} \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right) \left(\frac{F}{\hbar} \right)^2 \right] \left\{ \begin{pmatrix} \chi \\ \lambda \end{pmatrix} \right\}, \quad (28)
\end{aligned}$$

where E, F are functions of (x, y) , i.e.,

$$\begin{aligned}
E(x, y) &= \frac{(\mathbf{A}_1)_{22}x - (\mathbf{A}_1)_{12}y}{\det(\mathbf{A}_1)}, \\
F(x, y) &= \frac{(\mathbf{A}_1)_{12}x + (\mathbf{A}_1)_{11}y}{\det(\mathbf{A}_1)}, \quad (29)
\end{aligned}$$

and $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{D}$ are the elements of the matrix $\mathbf{A}_1^{-1} \mathbf{A}_2$,

$$\mathbf{A}_1^{-1} \mathbf{A}_2 = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{C} & \mathcal{D} \end{pmatrix}. \quad (30)$$

Note that in the isotropic case, $\sqrt{\det \mathbf{A}_1} = \frac{\sin \tilde{\omega}_0 t}{m^* \tilde{\omega}_0}$, $\mathcal{B} = \mathcal{C} = 0$, $\mathcal{A} = \mathcal{D} = -m^* \tilde{\omega}_0 \cot \tilde{\omega}_0 t$, and

$$\begin{aligned}
E(x, y) &= \frac{m^* \tilde{\omega}_0}{\sin \tilde{\omega}_0 t} (x \cos \Gamma_0 t + y \sin \Gamma_0 t), \\
F(x, y) &= \frac{m^* \tilde{\omega}_0}{\sin \tilde{\omega}_0 t} (y \cos \Gamma_0 t - x \sin \Gamma_0 t). \quad (31)
\end{aligned}$$

Thus, Eq. (28) reduces to

$$\begin{aligned}
\Psi(\mathbf{r}, t) &= \frac{m^* \tilde{\omega}_0 \exp \left\{ \frac{im^* \tilde{\omega}_0 \cot \tilde{\omega}_0 t}{2\hbar} \mathbf{r}^2 \right\}}{2i\hbar \sqrt{\pi d} \sin \tilde{\omega}_0 t \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right)} \times \\
& \exp \left\{ -\frac{\left(\frac{F}{\hbar} \right)^2 + \left(\frac{E}{\hbar} \right)^2}{4 \left(\frac{1}{2d} + \frac{i\mathcal{D}}{2\hbar} \right)} \right\} \begin{pmatrix} \chi \\ \lambda \end{pmatrix}, \quad (32)
\end{aligned}$$

and the spatial density is

$$\rho_i(\mathbf{r}, t) = \frac{e^{-\frac{r^2}{2\sigma_i^2(t)}}}{2\pi\sigma_i^2(t)}, \quad (33)$$

where $i = \uparrow, \downarrow$, and

$$\sigma_i(t) = \frac{\sqrt{\sin^2 \tilde{\omega}_0 t + (m^* \tilde{\omega}_0)^2 \cos^2 \tilde{\omega}_0 t}}{\sqrt{2} m^* \tilde{\omega}_0}. \quad (34)$$

This density is always a Gaussian distribution with a spin-dependent width $\sigma_i(t)$.

From Eq. (28) it is evident that due to the effect of ASOC, the wave packet splits into two components, one is for spin-up and one is for spin-down, with their evolutions being governed by $\hat{H}_\uparrow$ and $\hat{H}_\downarrow$ respectively. In other words, the evolution of the wave packet becomes spin-dependent. In order to see the differences between the evolution of the probability densities for spin-up and spin-down wave packets, we present the 3D graphs for $\rho_\uparrow(\mathbf{r}, t) = |\Psi_\uparrow(\mathbf{r}, t)|^2$ and $\rho_\downarrow(\mathbf{r}, t) = |\Psi_\downarrow(\mathbf{r}, t)|^2$ at time $t=5.0$ s and $\omega_c = 2\omega_0$ in Fig. 1. Set $\omega_x = \omega_0 \cos \beta$, $\omega_y = \omega_0 \sin \beta$ with $\beta = \pi/4$ for isotropic case and $\beta = \pi/6$ for an anisotropic case. The atomic units are employed, namely $\hbar = m^* = \omega_0 = 1$, and $d = 1$ in the initial wave packet. The spatial components for the initial wave packets are the same for spin-up and down components as described in Eq. (26). For comparison, we also give the plots at the same values of time for the isotropic cases in the same figure. From the graphs, it is clear that the heights and widths of the probability densities for the spin-up $\Psi_\uparrow(\mathbf{r}, t)$ and spin-down $\Psi_\downarrow(\mathbf{r}, t)$ wave packets evolve quite differently. The height of the probability densities increases faster in the anisotropic cases than those in the isotropic cases for the spin-up cases, while it is even faster in the spin-down cases. But the area of the corresponding cross-sections becomes smaller since the volumes of the probability densities are fixed to unit. Moreover, it should be pointed out that the cylinder symmetry is remained all the time in the isotropic cases as reflected in Eq. (33), while it is broken in the anisotropic cases. In the latter cases, though initially at $t=0$ the wave packets have cylinder symmetry, this symmetry is lost soon after $t>0$.

It should also be noted that the probability density for spin-up and down wave packets behave quite differently as one can see from Fig. 1. This is not out of expectation, since $\Psi_{\uparrow}(\mathbf{r}, t)$ and $\Psi_{\downarrow}(\mathbf{r}, t)$ evolve according to Hamiltonian $\hat{H}_{\uparrow}$ and $\hat{H}_{\downarrow}$ of Eq. (7), respectively.

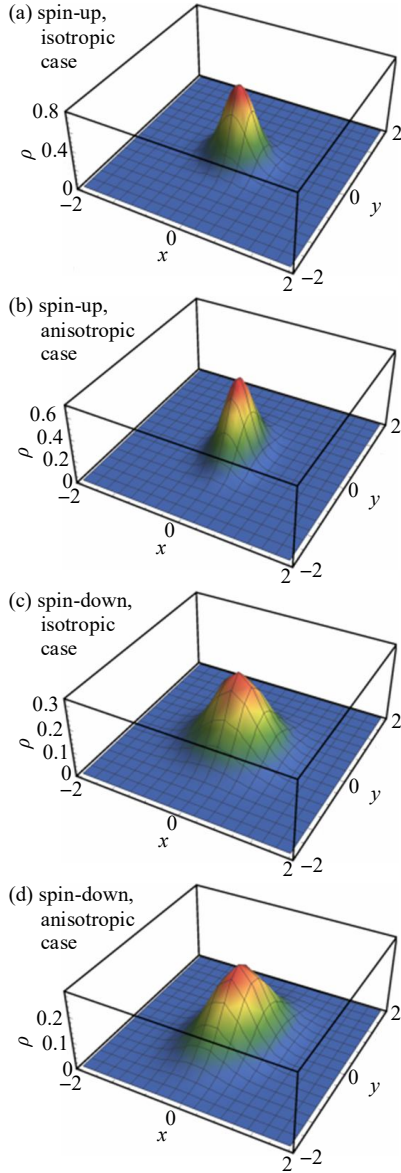


Fig. 1 The probability densities for the QD with $|\Gamma|=0.25$

Basically, with the expression of the wave functions Eq. (28) at hand, one is able to calculate various expectation values of the observables in quantum mechanics. To get a quantitative understanding, next we proceed to investigate the spin-dependent expectation of the distance $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$, which are defined for spin-up and -down component, i.e. $i=\uparrow$

and $\downarrow$, as

$$r_i(t) = \int \Psi_i^*(\mathbf{r}, t) r \Psi_i(\mathbf{r}, t) d\mathbf{r} = \int \rho_i(\mathbf{r}, t) r d\mathbf{r}. \quad (35)$$

In the isotropic cases, the substitution of Eq. (33) into (35) yields the following analytical expression,

$$r_i(t) = \sqrt{\frac{\pi}{2}} \sigma_i(t). \quad (36)$$

Together with Eq. (34), it is obvious that in the isotropic cases $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ are periodic functions of time, this is also clearly reflected in the left two panels of Fig. 2 below.

To see the ASOC effect on the expectations of the distance, in Fig. 2 we plot $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ of the quantum dot at fixed value of the strength of the magnetic field $\omega_c = 0.5\omega_0$ and three different values of the ASOC $|\Gamma| = 0, 0.25, 0.5$. For the spin-up case, the period and the average of the expectations decrease as the strength of the ASOC $|\Gamma|$ increases, while the period and the average of the expectations increase as the strength of the ASOC $|\Gamma|$ increases for the spin-down case. However, the amplitude of the expectations always increases as $|\Gamma|$ increases in both cases. In contrast to the right two panels of Fig. 2, the periodicity of the expectation is broken and the motion becomes quasi-periodic in the anisotropic case. But the average of the expectations has similar behaviors to the isotropic cases as the strength $|\Gamma|$ varies. In other words, the average of the expectations decreases for the spin-up case but increases for the spin-down case when the strength of the ASOC $|\Gamma|$ increases.

In order to study the effects of the magnetic field, in Fig. 3 we plot the $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ for the quantum dot at fixed strength of the ASOC $|\Gamma|=0.25$ but at three different values of the strength of the magnetic field. It is evident that in the isotropic case, $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ are constant in the absence of the magnetic field (this is because when $\omega_c = 0$, $\tilde{\omega}_0 = \omega_0 = 1$, and note that in the plots we choose $m^* = 1$, $m^* \tilde{\omega}_0 = 1$, and $\sigma_i(t) = 1/\sqrt{2}$). As one switches on the magnetic field, they become periodic functions of time. As the strength of the magnetic field increases, the period decreases. When $|\Gamma|=0.25$ as we choose in Fig. 3, (i) in the spin-up

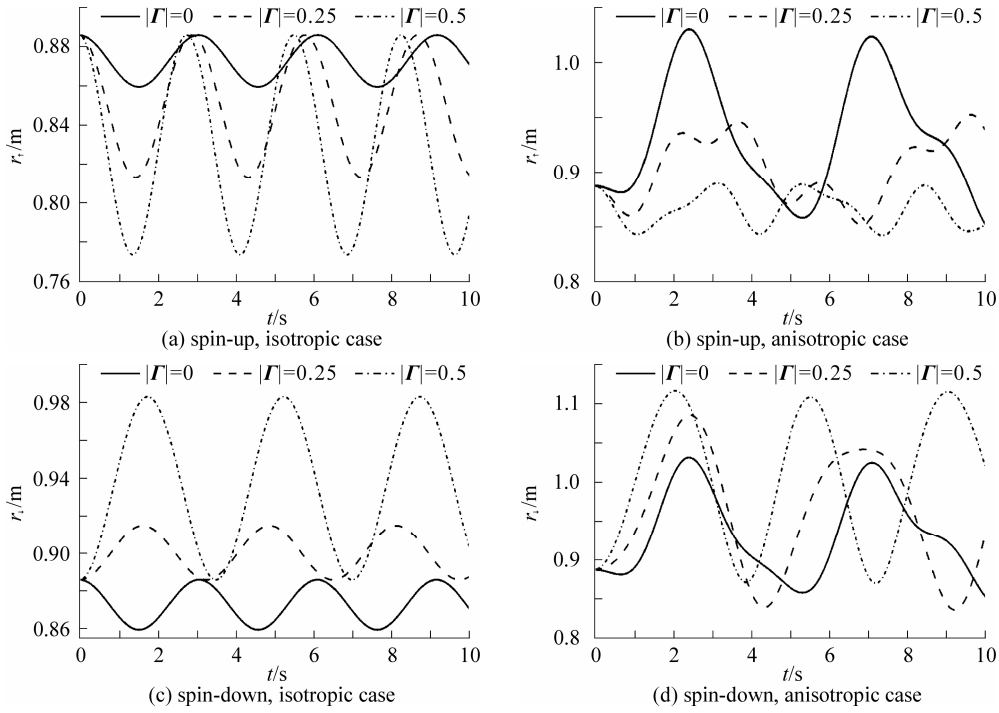


Fig. 2 $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ of the quantum dot at fixed strength of the magnetic field $\omega_c = 0.5$

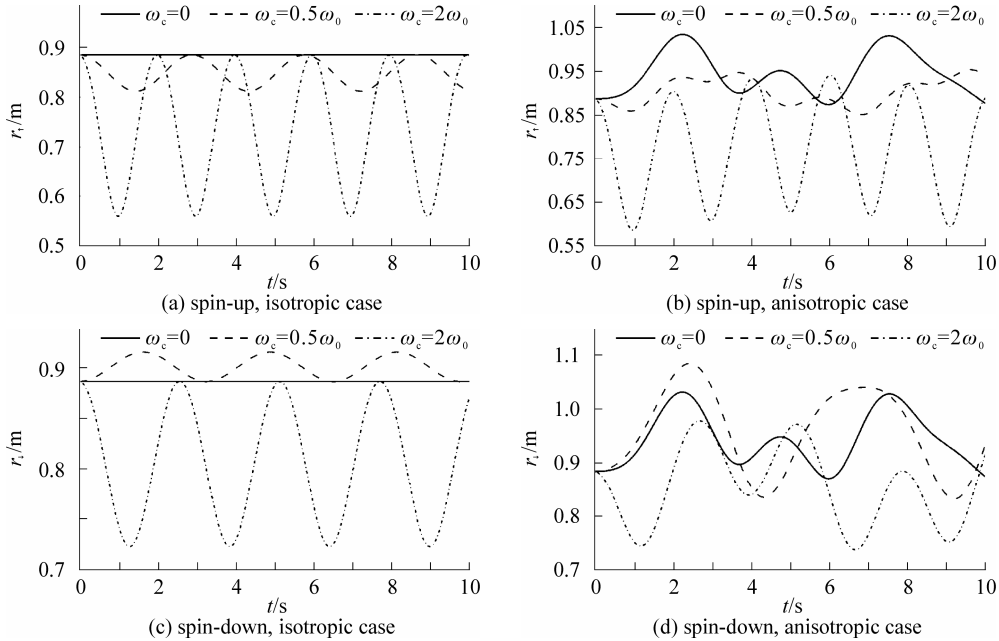


Fig. 3 $r_{\uparrow}(t)$ and $r_{\downarrow}(t)$ for the quantum dot at fixed strength of the ASOC $|\Gamma| = 0.25$

case $\tilde{\omega}_0 = \sqrt{\omega_0^2 + \omega_c^2/4 + |\Gamma|\omega_c\omega_0^2}$, $\tilde{\omega}_0$ increases monotonically as ω_c increases from 0 to $2\omega_0$, this leads the average of $r_{\uparrow}(t)$ decreases when ω_c increases as shown in Fig. 3(a), (ii) in the spin-down

case $\tilde{\omega}_0 = \sqrt{\omega_0^2 + \frac{\omega_c^2}{4} - |\Gamma|\omega_c\omega_0^2} = \sqrt{\frac{15}{16} + \frac{1}{4}\left(\omega_c - \frac{1}{2}\right)^2}$, it is obvious that $\tilde{\omega}_0$ decreases as ω_c increases from

0 to 1/2, then increases monotonically as ω_c increases from 1/2 to ∞ . This behavior of $\tilde{\omega}_0$ leads to the fact that the average of $r_{\uparrow}(t)$ at $\omega_c = 0$ is less than that at $\omega_c = 0$, but greater than that at $\omega_c = 2\omega_0$ as shown in Fig. 3(c). In the anisotropic cases, as shown in the right two panels of Fig. 3, similar behaviors of the averages of the expectations are observed except that the

expectations become quasi-periodic instead of periodic.

5 Conclusions

By employing the group theoretical method, we have obtained analytical expressions for the propagators of anisotropic quantum dots with atomic SOC, then as an example of application, the propagator is applied to calculate the evolution of spin-dependent Gaussian wave packets. Consequently, the corresponding probability densities, expectations of the distances are investigated for the anisotropic and isotropic cases. The wave packet splits into two components, one for spin-up and the other for spin-down, and they evolve differently. It is shown that in the isotropic cases, a Gaussian wave packet is always a Gaussian and the cylinder symmetry of the probability densities is kept all the time, and the expectations of the distances are periodic functions of time. While in the anisotropic case, this symmetry of the probability densities is broken and the expectations of the distances become quasi-periodic functions of time. Nevertheless, the strength of the ASOC and the magnetic field in the anisotropic case have similar effects on the averages of the expectations of the distances to those in the isotropic case. But their effects on spin-up component are quite different from those on spin-down one. It must be stressed that this group-theoretical method relies on the solutions to the quite complicated equation of motion of the system, and this may not be achieved for other forms of SOC like Rashba SOC or Dresselhaus SOC. Finally, it is worthy to mention that the propagator we obtained may also be applied to study the evolution of spin-dependent atomic wave packets in a harmonic magnetic trapping potential in the area of Bose-Einstein condensates^[36-37].

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磁场下有原子自旋轨道耦合的各向异性量子点的精确解析传播子

陈 寅, 郭 伟, 潘孝胤*

(宁波大学 物理科学与技术学院, 浙江 宁波 315211)

摘要: 量子力学中很少有系统能够精确地计算传播子, 特别是在考虑了自旋轨道耦合效应的情况下. 利用相空间的群论方法, 首先导出了有原子自旋轨道耦合的各向异性量子点传播子的精确解析表达式. 随后利用传播子来计算自旋高斯波包的演化与相应的概率密度, 并研究了原子自旋轨道耦合效应和磁场强度对距离期望值的影响.

关键词: 路径积分方法; 自旋轨道耦合; 量子点; 磁场

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