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Analytic propagators for spin–orbit interactions

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Abstract

We derive analytic expressions for propagators in spin–orbit coupled systems. In addition to their kinetic energy, these systems exhibit a potential energy that mixes position, momentum and spin operators. We consider Hamiltonians with limited noncommutativities: the confined spin–orbit coupled Hamiltonian $H_{\text{SO}}^c = \frac{\mathbf{p}^2}{2m} + \gamma \boldsymbol{\sigma} \cdot \mathbf{L} + \frac{1}{2}m\eta^2(x^2 + y^2)$, the confined Equal–Strength–Rashba–Dresselhaus Hamiltonian $H_{\text{ESRD}}^c = \frac{\mathbf{p}^2}{2m} + \frac{\alpha}{\hbar}(p_x + p_y)(\sigma_x - \sigma_y) + \frac{1}{2}m\eta^2(x^2 + y^2)$ and the confined Opposite–Strength–Rashba–Dresselhaus Hamiltonian $H_{\text{OSRD}}^c = \frac{\mathbf{p}^2}{2m} + \frac{\alpha}{\hbar}(p_x - p_y)(\sigma_x + \sigma_y) + \frac{1}{2}m\eta^2(x^2 + y^2)$. We use both a classical action method and an algebraic method in our derivations. We mention specific applications for these propagators and illustrate their significance with examples of wavepacket evolution.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The spin-orbit coupling (SOC) occurs in many areas of physics. Discovered in the fine structure of atomic spectra, later introduced to explain the nuclear structure, it is now also of great interest in condensed matter systems, such as graphene [1] and semiconducting materials with promising spintronics applications [2, 3]. It is also found in the physics of optical lattices mimicking condensed matter systems [4]. The SOC is characterized by interaction terms that contain position **r**, momentum **p** and spin operators **S**. In nuclear and atomic systems, the spin-orbit interaction is given in the form $H_{SO} = \gamma(r)\mathbf{S} \cdot \mathbf{L}$, where $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. The coupling strength γ is determined in atomic systems by the Coulomb potential V(r) such that

$$\gamma(r) \sim \frac{1}{r} \frac{\mathrm{d}V(r)}{\mathrm{d}r}.$$
(1)

 H_{SO} can be derived in the nonrelativistic approximation of relativistic electron-atom interactions. In spintronics, the spin-orbit coupling is manifest as Rashba and Dresselhaus

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interactions [5]. The Rashba interaction is the signature of structure inversion asymmetry (SIA) present in essentially two-dimensional materials [6, 7]. Its Hamiltonian

$$H_R = \frac{\alpha}{\hbar} (p_y \sigma_x - p_x \sigma_y) \tag{2}$$

combines components of the spin operator **S** (related to the Pauli matrices by $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$) and the momentum operator **p**. Its overall strength, the Rashba coupling constant α , can be controlled experimentally. The Dresselhaus interaction, with coupling strength β , originates in bulk inversion asymmetry (BIA) which is inherent to zinc-blende structures [8]

$$H_D = \frac{\beta}{\hbar} (p_x \sigma_x - p_y \sigma_y). \tag{3}$$

Interesting features such as spin accumulation [9], spin-Hall effect [10], quantum spin-Hall effect [11], *Zitterbewegung* motion of the wavepacket [12] and persistent spin helix [13] have been predicted and observed for spin–orbit coupled systems. It is our goal here to derive SOC propagators in order to get a better handle on the evolution of the corresponding physical systems. To our knowledge, the propagator method has not been applied explicitly to these specific SOC systems.

The propagator method is a powerful tool to study the evolution of systems [15, 16]. The quantum propagator $K(\mathbf{r}, \mathbf{r}_0; t)$ is the conditional transition amplitude between a state $|\mathbf{r}_0\rangle$ corresponding to an initial position \mathbf{r}_0 and a state $|\mathbf{r}\rangle$ corresponding to a final position \mathbf{r} over a time interval t

$$K(\mathbf{r}, \mathbf{r}_0; t) = \langle \mathbf{r} | T(t) | \mathbf{r}_0 \rangle = \langle \mathbf{r} | e^{\frac{\pi i}{i\hbar}} | \mathbf{r}_0 \rangle,$$
(4)

where $|\mathbf{r}\rangle$ represents a position eigenvector, $\langle \mathbf{r}|$ is its conjugate and T(t) is the time-evolution operator which evolves a function from one time to another $T(t)|\psi(\mathbf{r}, 0)\rangle = |\psi(\mathbf{r}, t)\rangle$ [17]. Since we are interested in spin systems, we construct propagators for the evolution of spin distributions. By applying the propagators on a spin wavefunction $\psi(\mathbf{r}_0, 0)$ at t = 0, we gain information on the final spin wavefunction $\psi(\mathbf{r}, t)$ at any time

$$\psi(\mathbf{r},t) = \int_{-\infty}^{\infty} K(\mathbf{r},\mathbf{r}_0;t) \psi(\mathbf{r}_0,0) \, \mathbf{dr}_0.$$
(5)

There are several methods for constructing spinless propagators. In this paper, we select a classical action method [17] and an algebraic method [18] and extend them to spindependent problems. The inclusion of the spin degree of freedom introduces a new level of noncommutativity which can considerably complicate the analysis of the systems. We give specific examples from 2D electron gas spin–orbit systems with limited noncommutativity and obtain analytic expressions for the propagators. By limited we mean that we consider powers and combinations of position, momentum and spin operators that allow some factorization of exponentials so that Baker–Campbell–Hausdorff-type formulae take on simplified forms. First, we consider particles moving under the influence of the spin–orbit coupling and isotropic parabolic horizontal (xy) confinement

$$H = \frac{\mathbf{p}^2}{2m} + \gamma \boldsymbol{\sigma} \cdot \mathbf{L} + \frac{1}{2}m\eta^2 (x^2 + y^2), \tag{6}$$

where γ and η are real constants. This Hamiltonian has been shown to exhibit different chiralities for spin components [11]. We also consider specific spin–orbit-type interactions from condensed matter systems, namely specific superpositions of Rashba and Dresselhaus interactions. When both Rashba and Dresselhaus are present and balanced in strength, a simplification occurs as the degrees of freedom decouple. We consider nonrelativistic free

particles with spin under the influence of H_R and H_D and define the Equal–Strength–Rashba– Dresselhaus (ESRD) Hamiltonian for $\alpha = \beta$

$$H_{\text{ESRD}} = \frac{p_x^2 + p_y^2}{2m} + \frac{\alpha}{\hbar} (p_y \sigma_x - p_x \sigma_y + p_x \sigma_x - p_y \sigma_y), \tag{7}$$

and the Opposite–Strength–Rashba–Dresselhaus (OSRD) Hamiltonian for $\alpha = -\beta$

$$H_{\text{OSRD}} = \frac{p_x^2 + p_y^2}{2m} + \frac{\alpha}{\hbar} (p_y \sigma_x - p_x \sigma_y - p_x \sigma_x + p_y \sigma_y). \tag{8}$$

Equal–Strength–Rashba–Dresselhaus has been shown to exhibit helicoidal motion leading to a so-called persistent spin helix [13] and is relevant to the development of the nonballistic spin-field-effect transistor [14]. We also consider the case where an isotropic parabolic confinement is added to both ESRD and OSRD systems. Confinement terms can represent the finite spatial extension of realistic semiconducting samples.

The confined spin-orbit Hamiltonian corresponds to an atomic spin-orbit interaction with the Coulomb potential in equation (1) replaced by a simple harmonic oscillator (SHO) potential. Because the motion is limited to the plane, this particular coupling only brings in the *z* component of the spin. Similarly the Rashba interaction can also be obtained from equation (1) with a linear potential corresponding to a constant electric field [2]. These Hamiltonians operate on a space of spin distributions or spinorial functions $\psi(x, y)$ defined in two dimensions characterized by the coordinates *x* and *y*, and with a spin degree of freedom in 3D. These spinors obey time-dependent Pauli–Schrödinger equations.

This paper is organized as follows. We construct the quantum propagators for the atomic spin–orbit Hamiltonians (in section 2) and for specific spintronics Hamiltonians (in section 3) using both the classical action method and the algebraic method. In section 4, we illustrate the power of using these propagators to study the evolution of spin wavepackets in two particular cases of confined atomic and ESRD systems. In section 5, we weigh the relative advantages of our two methods in view of their applicability to the particular physical realizations discussed in this paper.

2. Atomic spin-orbit coupling propagator

The Hamiltonian for the confined atomic spin-orbit coupling in the xy-plane is given by

$$H_{\rm SO}^c = \frac{p_x^2 + p_y^2}{2m} + \sigma_z \gamma (xp_y - yp_x) + \frac{1}{2}m\eta^2 (x^2 + y^2).$$
(9)

Since only one Pauli operator occurs in the Hamiltonian, it corresponds to a constant of the motion. The classical action method [17] can be extended to a 2×2 spin formalism. The successive steps consist in finding the corresponding Lagrangian, solving the Euler–Lagrange equations, substituting the motion into the Lagrangian, integrating over time to find the action and exponentiating to find the quantum propagator in two dimensions

$$K(x, x_0, y, y_0; t) = C \exp\left(\frac{\mathrm{i}S}{\hbar}\right),\tag{10}$$

where S is the classical action and C is a c-number determined by the initial conditions.

Since only σ_z is present, the Hamiltonian in equation (9) is diagonal in the standard representation of the Pauli matrices. In what follows, we use the symbol σ_z as a place holder for (+1) and (-1) of the diagonal elements of the Pauli matrix σ_z . Therefore, our calculation proceeds in the usual way with a scalar Lagrangian.

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We find Hamilton's equations

$$= \frac{p_x}{m} + \sigma_z \gamma y, \qquad \dot{y} = \frac{p_y}{m} - \sigma_z \gamma x, \qquad (11)$$

perform a Legendre's transformation

$$L = \sum_{i} p_i \dot{q}_i - H, \tag{12}$$

and obtain the Lagrangian

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - m\gamma\sigma_z(\dot{x}y - \dot{y}x) + \frac{1}{2}m(\gamma^2 - \eta^2)(x^2 + y^2).$$
(13)

The equations of motions are obtained

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = m\ddot{x} - 2m\sigma_z\gamma\dot{y} - (\gamma^2 - \eta^2)mx = 0$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{y}} - \frac{\partial L}{\partial y} = m\ddot{y} + 2m\sigma_z\gamma\dot{x} - (\gamma^2 - \eta^2)my = 0,$$
(14)

and solved for x(t') and y(t') (which also provides $\dot{x}(t')$ and $\dot{y}(t')$) using the boundary conditions

$$x(0) = x_0,$$
 $x(t) = x,$ $y(0) = y_0,$ $y(t) = y.$ (15)

The classical action,

$$S = \int_0^t L \,\mathrm{d}t',\tag{16}$$

is found by substituting the solutions into the Lagrangian and performing a partial integration

$$S = \frac{m}{2} (x\dot{x} + y\dot{y})|_{0}^{t} - \int_{0}^{t} \left(\frac{m}{2} (x\ddot{x} + y\ddot{y}) + m\gamma\sigma_{z}(\dot{x}y - \dot{y}x) - \frac{1}{2}m(\gamma^{2} - \eta^{2})(x^{2} + y^{2}) \right) dt'$$

$$= \frac{1}{2}m(x(t)\dot{x}(t) + y(t)\dot{y}(t) - x(0)\dot{x}(0) - y(0)\dot{y}(0)).$$
(17)

Note that the integrand in equation (17) vanishes as a result of the equations of motions [19].

We distinguish three cases $\eta = 0$, $\eta = \gamma$ and arbitrary η corresponding to respectively no confinement, spin-orbit from the confinement potential and the general case. In this last, general, case, we use the algebraic method because it leads to the analytic result more elegantly than the classical action method. That result reduces to the results found in the first two cases when taking the proper limits.

2.1. Unconfined case: $\eta = 0$

For the unconfined Hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2m} + \sigma_z \gamma (x p_y - y p_x),$$
(18)

we solve the equations of motions in equation (14) with $\eta = 0$. The action in equation (17) gives

$$S = \frac{m}{2t} \left(x^2 + x_0^2 + y^2 + y_0^2 - 2(xx_0 + yy_0) \cos \gamma t + 2\sigma_z (-xy_0 + x_0y) \sin \gamma t \right)$$
(19)

and, as a result, the unconfined spin-orbit propagator is

$$K_{\rm SO}^{(\eta=0)}(x, x_0, y, y_0; t) = \frac{m}{2\pi i\hbar t} \exp\left(\frac{\mathrm{i}m}{2\hbar t} \left(x^2 + x_0^2 + y^2 + y_0^2 - 2(xx_0 + yy_0)\cos\gamma t + 2\sigma_z(-xy_0 + x_0y)\sin\gamma t\right)\right),$$
(20)

where the front coefficient is determined by the initial condition on the propagator

$$\lim_{t \to 0} K(x, x_0, y, y_0; t) = \delta(x - x_0)\delta(y - y_0).$$
⁽²¹⁾

This result can be checked against the free-particle propagator [17] by taking the limit $\gamma \rightarrow 0$

$$K^{\text{Free}}(x, x_0, y, y_0; t) = \frac{m}{2\pi i \hbar t} \exp\left(-\frac{m(x - x_0)^2 + m(y - y_0)^2}{2i \hbar t}\right).$$
 (22)

2.2. Larmor case (confined and balanced): $\eta \neq 0, \eta = \gamma$

When the confinement strength η matches the SOC strength γ such that $\eta = \gamma$, the Hamiltonian

$$H = \frac{p_x^2 + p_y^2}{2m} + \sigma_z \gamma (xp_y - yp_x) + \frac{1}{2}m\gamma^2 (x^2 + y^2)$$
(23)

can be recognized as describing a charged particle in a homogeneous magnetic field, where γ plays the role of the Larmor frequency but exhibits an additional factor σ_z ($\sigma_z^2 = 1$). The propagator (without the σ_z factor) has been obtained for this Larmor case [20]

$$K(x, x_0, y, y_0; t) = \frac{m}{2\pi i\hbar t} \frac{\gamma t}{\sin \gamma t} \exp\left(\frac{im\gamma}{2\hbar} \left(\frac{(x - x_0)^2 + (y - y_0)^2}{\tan \gamma t} + 2(x_0y - xy_0)\right)\right),$$
(24)

where the front coefficient is found using the Feynman trick [21].

The propagator including the σ_z factor is now obtained by replacing γ by $\gamma \sigma_z$, $\gamma \cot \gamma t$ by $\gamma \sigma_z \cot \gamma \sigma_z t = \gamma \cot \gamma t$, and $\sin \gamma t$ by $\sin \gamma \sigma_z t = \sigma_z \sin \gamma t$. As a result

$$K_{\rm SO}^{(\eta=\gamma)}(x, x_0, y, y_0; t) = \frac{m}{2\pi i\hbar t} \frac{\gamma t}{\sin \gamma t} \exp\left(\frac{\mathrm{i}m\gamma}{2\hbar} \left(\frac{(x-x_0)^2 + (y-y_0)^2}{\tan \gamma t} + 2\sigma_z(x_0y - xy_0)\right)\right).$$
(25)

In the limit $\gamma \to 0$, equation (25) reduces also to the free-particle propagator. Note that the propagators in the section can also be obtained following the same steps as in section 2.1.

2.3. General case: $\eta \neq \gamma$

For arbitrary η solving the equations of motions is cumbersome. Instead we use an algebraic method introduced by Wang [18] to calculate the propagator. In the Hamiltonian in equation (9), the spin–orbit term, which is linear in *x*, commutes with the sum of the confining term, which is quadratic in *x*, and the kinetic term. Because of this limited noncommutativity, the time-evolution operator *T* can be expressed as

$$T = \exp\left(-\frac{\mathrm{i}Ht}{\hbar}\right)$$

= $\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\mathbf{p}^{2}}{2m} + \sigma_{z}\gamma(xp_{y} - yp_{x}) + \frac{1}{2}m\eta^{2}(x^{2} + y^{2})\right)\right)$
= $\exp\left(-\frac{\mathrm{i}t}{\hbar}\sigma_{z}\gamma(xp_{y} - yp_{x})\right)\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\mathbf{p}^{2}}{2m} + \frac{1}{2}m\eta^{2}(x^{2} + y^{2})\right)\right).$ (26)

Note that we have isolated to the right of this expression the complete simple harmonic oscillator evolution.

By applying equation (26) to a wavefunction, we obtain

$$\psi(x, y, t) = T(t, 0)\psi(x, y, 0)$$

$$= \exp\left(-\frac{\mathrm{i}t}{\hbar}\sigma_z\gamma(xp_y - yp_x)\right)\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\eta^2(x^2 + y^2)\right)\right)\psi(x, y; 0),$$
(27)

where $\exp\left(-\frac{it}{\hbar}\left(\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\eta^2(x^2 + y^2)\right)\right)\psi(x, y; 0)$ is known since it represents the result of SHO evolution,

$$\psi(x, y, t) = T^{\text{SHO}}(t, 0)\psi(x, y, 0)$$

= $\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\eta^2(x^2 + y^2)\right)\right)\psi(x, y, 0)$
= $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}K^{\text{SHO}}(x, x_0, y, y_0; t)\psi(x_0, y_0, 0)\,\mathrm{d}x_0\,\mathrm{d}y_0,$ (28)

where $K^{\text{SHO}}(x, x_0, y, y_0; t)$ is the propagator for the simple harmonic oscillator [17]

$$K^{\text{SHO}}(x, x_0, y, y_0; t) = \frac{m\eta}{2\pi i\hbar \sin \eta t} \exp\left(\frac{\mathrm{i}m\eta}{2\hbar \sin \eta t} \left(\left(x^2 + x_0^2 + y^2 + y_0^2\right) \cos \eta t - 2xx_0 - 2yy_0 \right) \right).$$
(29)

By substituting equation (29) into equation (28) and by comparing to equation (27) we obtain

$$\psi(x, y, t) = \exp\left(-\frac{\mathrm{i}t}{\hbar}\sigma_z\gamma(xp_y - yp_x)\right)\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\mathbf{p}^2}{2m} + \frac{1}{2}m\eta^2(x^2 + y^2)\right)\right)\psi(x, y, 0)$$
$$= \exp\left(-\frac{\mathrm{i}t}{\hbar}\sigma_z\gamma(xp_y - yp_x)\right)\frac{m\eta}{2\pi\mathrm{i}\hbar\sin\eta t}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left(\frac{\mathrm{i}m\eta}{2\hbar\sin\eta t}\left(\left(x^2 + x_0^2 + y^2 + y_0^2\right)\cos\eta t - 2xx_0 - 2yy_0\right)\right)\psi(x_0, y_0, 0)\,\mathrm{d}x_0\,\mathrm{d}y_0.$$
(30)

The first factor $\exp\left(-\frac{it}{\hbar}\sigma_z\gamma(xp_y - yp_x)\right)$ corresponds to a spin-dependent rotation operator around the *z*-axis. Comparing with the usual rotation operator $R_z(\phi) = \exp\left(-\frac{i\phi L_z}{\hbar}\right)$, we extract the rotation angle $\phi = \sigma_z\gamma t$. The effect of the rotation operator on a wavefunction is given by

$$R_{z}(\phi)f(x, y) = \exp\left(-\frac{\mathrm{i}\phi L_{z}}{\hbar}\right)f(x, y) = f(x\cos\phi + y\sin\phi, -x\sin\phi + y\cos\phi).$$
(31)

Therefore by applying equation (31) to equation (30)

$$\psi(x, y, t) = \exp\left(-\frac{it}{\hbar}\sigma_z \gamma (xp_y - yp_x)\right) \frac{m\eta}{2\pi i\hbar \sin \eta t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta}{2\hbar \sin \eta t} \left(\left(x^2 + x_0^2 + y^2 + y_0^2\right)\cos \eta t - 2xx_0 - 2yy_0\right)\right) \psi(x_0, y_0, 0) \, dx_0 \, dy_0$$

$$= \frac{m\eta}{2\pi i\hbar \sin \eta t} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(\frac{im\eta}{2\hbar \sin \eta t} \left(\left((x\cos\phi + y\sin\phi)^2 + x_0^2 + (-x\sin\phi + y\cos\phi)^2 + y_0^2\right)\cos(\eta t) - 2(x\cos\phi + y\sin\phi)x_0 - 2(-x\sin\phi + y\cos\phi)y_0\right)\right) \psi(x_0, y_0, 0) \, dx_0 \, dy_0.$$
(32)

By comparing with the propagator integral formula in equation (5), it is straightforward to extract the propagator for the generalized case

$$K(x, x_0, y, y_0; t) = \frac{m\eta}{2\pi i\hbar \sin \eta t} \exp\left(\frac{m\eta}{2\hbar \sin \eta t} \left(\left((x\cos\phi + y\sin\phi)^2 + x_0^2 + (-x\sin\phi + y\cos\phi)^2 + y_0^2 \right)\cos\eta t - 2(x\cos\phi + y\sin\phi)x_0 - 2(-x\sin\phi + y\cos\phi)y_0 \right) \right).$$
(33)

Substituting the rotation angle $\phi = \sigma_z \gamma t$ back into equation (33) and using $\cos \sigma_z \gamma t = \cos \gamma t$, and $\sin \sigma_z \gamma t = \sigma_z \sin \gamma t$, we obtain the propagator for arbitrary η and γ

$$K_{\rm SO}^{(\eta\neq\gamma)}(x, x_0, y, y_0; t) = \frac{m\eta}{2\pi i\hbar \sin \eta t} \exp\left(\frac{im\eta}{2\hbar \sin \eta t} \left(\left(x^2 + y^2 + x_0^2 + y_0^2\right)\cos \eta t - 2(xx_0 + yy_0)\cos\gamma t - 2\sigma_z(x_0y - xy_0)\sin\gamma t\right)\right).$$
(34)

This result for the general confined atomic spin–orbit propagator reduces to the expression of the propagator for the unconfined (equation (20)), Larmor (equation (25)), simple harmonic oscillator (equation (29)), and the free particle (equation (22)). Applications to equation (34) are discussed in section 5. Note that it is also straightforward to apply the algebraic method to the unconfined case directly since the kinetic energy itself commutes with the spin–orbit term.

3. ESRD and OSRD spintronics propagators

The confined ESRD and OSRD Hamiltonians are given by

$$H_{\rm ESRD}^{c} = \frac{\mathbf{p}^{2}}{2m} + \frac{\alpha}{\hbar} (p_{x} + p_{y})(\sigma_{x} - \sigma_{y}) + \frac{1}{2}m\eta^{2}(x^{2} + y^{2})$$
(35)

$$H_{\text{OSRD}}^{c} = \frac{\mathbf{p}^{2}}{2m} + \frac{\alpha}{\hbar} (p_{x} - p_{y})(\sigma_{x} + \sigma_{y}) + \frac{1}{2}m\eta^{2}(x^{2} + y^{2}).$$
(36)

We start by considering the unconfined case ($\eta = 0$) and later proceed to arbitrary confinement.

3.1. Unconfined case $\eta = 0$

In the ESRD case, we see from equation (35) that the two dimensions are decoupled unlike in the Rashba-only (equation (2)) and Dresselhaus-only (equation (3)) cases. Decoupling means that the total Hamiltonian can be written as a sum of two commuting Hamiltonians corresponding to the motion in two independent dimensions

$$H_{\text{ESRD}} = H_{(x)} + H_{(y)}, \qquad H_{(x)} = \frac{p_x^2}{2m} + \frac{\alpha}{\hbar} p_x (\sigma_x - \sigma_y), \qquad H_{(y)} = \frac{p_y^2}{2m} + \frac{\alpha}{\hbar} p_y (\sigma_x - \sigma_y).$$

We apply the classical action method to the Hamiltonian in the x dimension

$$H = \frac{p_x^2}{2m} + v p_x,\tag{37}$$

where ν stands for the factor $\frac{\alpha}{\hbar}(\sigma_x - \sigma_y)$. Applying Hamilton's equation

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m} + \nu \tag{38}$$

and using a Legendre transformation, we find

$$L = p_x \dot{x} - H = \frac{m \dot{x}^2}{2} - m v \dot{x} + \frac{m v^2}{2}.$$
(39)

The corresponding equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = \ddot{x} = 0 \tag{40}$$

describe a free particle. The classical action can now be evaluated

$$S = \int_0^t L \, \mathrm{d}t' = \frac{mx\dot{x}}{2} \Big|_0^t - \int_0^t \left(\frac{mx\ddot{x}}{2} + mv\dot{x} - \frac{mv^2}{2}\right) \mathrm{d}t'. \tag{41}$$

As opposed to the examples in section 2, the integrand does not equate zero but it can be integrated directly

$$S = \int_0^t L \, \mathrm{d}t' = \frac{mx\dot{x}}{2} \Big|_0^t - mvx|_0^t + \frac{mv^2t}{2},\tag{42}$$

where the first term corresponds to the usual free-particle component. It is shifted by a second term which is time independent and position dependent. The third term is just a time-dependent phase. Therefore, the propagator for the Hamiltonian in equation (37) is obtained from equation (10)

$$K(x, x_0; t) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(-\frac{m}{2i\hbar t}(x - x_0)^2 + \frac{m\nu(x - x_0)}{i\hbar} - \frac{m\nu^2 t}{2i\hbar}\right)$$
$$= \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(-\frac{m}{2i\hbar t}(x - x_0 - \nu t)^2\right)$$
(43)

or, replacing ν by its value,

$$K(x, x_0; t) = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(-\frac{m}{2i\hbar t}(x - x_0 - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)t)^2\right).$$
 (44)

The propagator in the other dimension $K(y, y_0; t)$ can be obtained in a similar manner. As a result of the decoupling in the Hamiltonian, we find immediately the 2D propagator as a product of two 1D propagators

$$K_{\text{ESRD}}^{(\eta=0)}(x, y, x_0, y_0; t) = \frac{m}{2\pi i \hbar t} \exp\left(-\frac{m}{2i\hbar t} \left(\left(x - x_0 - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)t\right)^2 + \left(y - y_0 - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)t\right)^2\right)\right).$$
(45)

In the OSRD case, the two dimensions are again decoupled but ν takes on a different value. The OSRD propagator is thus obtained similarly

$$K_{\text{OSRD}}^{(\eta=0)}(x, y, x_0, y_0; t) = \frac{m}{2\pi i\hbar t} \exp\left(-\frac{m}{2i\hbar t} \left(\left(x - x_0 - \frac{\alpha}{\hbar}(\sigma_x + \sigma_y)t\right)^2 + \left(y - y_0 + \frac{\alpha}{\hbar}(\sigma_x + \sigma_y)t\right)^2\right)\right).$$
(46)

For completeness we now derive the K_{ESRD} and K_{OSRD} propagators using the algebraic method. Regarding the ESRD propagator, we first consider each dimension separately and find the effect on the spinorial function $\psi(x)$. Since the kinetic term in $H_{(x)}$ commutes with the potential ψ

term, we use the coordinate representation for the momentum operator $p_x = \frac{\hbar}{i} \partial_x$ to rewrite the ESRD time-evolution operator

$$T(t, 0)_{\text{ESRD}}^{\eta=0} = \exp\left(\frac{\left(\frac{-\hbar^2 \partial_{xx}}{2m} + \frac{\alpha}{i} \partial_x (\sigma_x - \sigma_y)\right)t}{i\hbar}\right)$$
$$= \exp\left(-\frac{\alpha \partial_x (\sigma_x - \sigma_y)t}{\hbar}\right) \exp\left(\frac{\left(\frac{-\hbar^2 \partial_{xx}}{2m}\right)t}{i\hbar}\right).$$
(47)

The expression $\exp\left(\frac{(-\frac{\hbar^2 \partial_{XX}}{2m})t}{i\hbar}\right)\psi(x,0)$ is known since

$$\psi(x,t) = T^{\text{Free}}(t,0)\psi(x,0) = \exp\left(-\frac{t}{i\hbar}\left(\frac{\hbar^2\partial_{xx}}{2m}\right)\right)\psi(x,0)$$
$$= \int_{-\infty}^{\infty} K^{\text{Free}}(x,x_0;t)\psi(x_0,0)\,\mathrm{d}x_0,$$
(48)

where $K^{\text{Free}}(x, x_0; t)$ is the propagator for the free particle provided in equation (22) in one dimension. After substitution, we obtain

$$\psi(x,t) = T(t,0)\psi(x,0)$$

= $\exp\left(-\frac{\alpha\partial_x(\sigma_x - \sigma_y)t}{\hbar}\right)\sqrt{\frac{m}{2\pi i\hbar t}}\int_{-\infty}^{\infty}\exp\left(-\frac{m(x-x_0)^2}{2i\hbar t}\right)\psi(x_0,0)\,\mathrm{d}x_0.$ (49)

The term $\exp\left(-\frac{\alpha \partial_x (\sigma_x - \sigma_y)t}{\hbar}\right)$ acts as a spin-dependent displacement in the *x* coordinate. By applying the usual displacement formula

$$\exp(-\xi\partial_x)\psi(x) = \psi(x-\xi) \tag{50}$$

with ξ replaced by a diagonalizable matrix $\alpha(\sigma_x - \sigma_y)t/\hbar$, we immediately obtain

$$(x,t) = T(t,0)\psi(x,0)$$

= $\sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} \exp\left(-\frac{m\left(x-x_0-\frac{\alpha(\sigma_x-\sigma_y)t}{\hbar}\right)^2}{2i\hbar t}\right)\psi(x_0) dx_0.$ (51)

We then extract the quantum propagator from equations (5) and (51)

$$K(x, x_0, t) = \sqrt{\frac{m}{2\pi i\hbar t}} \int_{-\infty}^{\infty} \exp\left(-\frac{m\left(x - x_0 - \frac{\alpha(\sigma_x - \sigma_y)t}{\hbar}\right)^2}{2i\hbar t}\right).$$
 (52)

Note that we have only obtained the propagator for the motion in x. $K(y, y_0; t)$ is obtained in analogy with $K(x, x_0; t)$. The 2D ESRD propagator is simply the product of $K(x, x_0; t)$ and $K(y, y_0; t)$

$$K_{\text{ESRD}}^{(\eta=0)}(x, y, x_0, y_0; t) = \frac{m}{2\pi i\hbar t} \exp\left(-\frac{m}{2i\hbar t} \left(\left(x - x_0 - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)t\right)^2 + \left(y - y_0 - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)t\right)^2\right)\right).$$
(53)

The construction of the OSRD propagator is similar

$$K_{\text{OSRD}}^{(\eta=0)}(x, y, x_0, y_0; t) = \frac{m}{2\pi i\hbar t} \exp\left(-\frac{m}{2i\hbar t} \left(\left(x - x_0 - \frac{\alpha}{\hbar}(\sigma_x + \sigma_y)t\right)^2 + \left(y - y_0 + \frac{\alpha}{\hbar}(\sigma_x + \sigma_y)t\right)^2\right)\right).$$
(54)

We thus recover the results from equations (45) and (46). By comparing with the usual free-particle propagator in equation (22), it is interesting to note that a shift in the position appears in both dimensions in the exponential. The shift reflects two different inertial frames in relative motion. This effect is caused by the term linear in p in the Hamiltonian.

3.2. Confined case: $\eta \neq 0$

We first consider the classical action method. The two dimensions are again decoupled and it is straightforward to work out the one-dimensional propagator. The Hamiltonian

$$H = \frac{p_x^2}{2m} + \nu p_x + \frac{1}{2}m\eta^2 x^2$$
(55)

corresponds to the Lagrangian

$$L = \frac{m\dot{x}^2}{2} - m\nu\dot{x} + \frac{m\nu^2}{2} - \frac{1}{2}m\eta^2 x^2$$
(56)

after applying a Legendre transformation with $\nu = \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)$ in the constrained ESRD case or $\nu = \frac{\alpha}{\hbar}(\sigma_x + \sigma_y)$ in the constrained OSRD case. It is interesting to note that the Euler–Lagrange equations are identical to those of the usual simple harmonic oscillator potential. The action, however, is different

$$S = \int_0^t L \, \mathrm{d}t' = \int_0^t \left(\frac{m\dot{x}^2}{2} - m\nu\dot{x} + \frac{m\nu^2}{2} - \frac{1}{2}m\eta^2 x^2\right) \mathrm{d}t'$$

= $\frac{1}{2}mx\dot{x}\Big|_0^t - \int_0^t \left(\frac{1}{2}mx\ddot{x} + \frac{1}{2}m\eta^2 x^2 + m\nu\dot{x} - \frac{1}{2}m\nu^2\right) \mathrm{d}t',$ (57)

where the first two terms inside the integral add up to zero from the equations of motion for the simple harmonic oscillator. Therefore

$$S = \frac{1}{2}mx\dot{x}\Big|_{0}^{t} - \int_{0}^{t} \left(mv\dot{x} - \frac{1}{2}mv^{2}\right)dt'$$

= $\frac{1}{2}m(x(t)\dot{x}(t) - x(0)\dot{x}(0)) - mv(x(t) - x(0)) + \frac{1}{2}mv^{2}t,$ (58)

where the first term $\frac{1}{2}m(x(t)\dot{x}(t) - x(0)\dot{x}(0))$ corresponds to the classical action for the usual harmonic oscillator potential. By substituting the harmonic oscillator solution

$$x(t') = \csc \eta t (x \sin \eta t' - x_0 \sin \eta (t' - t))$$
(59)

into the action S, we obtain

2

$$S(x, x_0; t) = \frac{m}{2} \left(\left(x_0^2 + x^2 \right) \eta \cot \eta t - 2x_0 x \eta \csc \eta t \right) + \frac{m\nu}{2} (2x_0 - 2x + t\nu).$$

Therefore the propagator has the form

$$K(x, x_0; t) = C \exp\left(\frac{\mathrm{i}S}{\hbar}\right)$$

= $C \exp\left(\frac{\mathrm{i}m}{2\hbar}\left(\left(x_0^2 + x^2\right)\eta \cot\eta t - 2x_0x\eta \csc\eta t + \nu(2x_0 - 2x + t\nu)\right)\right),$ (60)

where C is again obtained using Feynman's trick

$$K(x, x_0; t) = \sqrt{\frac{m\eta}{2\pi i\hbar \sin \eta t}} \exp\left(\frac{\mathrm{i}m}{2\hbar} \left(\left(x_0^2 + x^2\right)\eta \cot \eta t - 2x_0 x\eta \csc \eta t + \nu(2x_0 - 2x + t\nu) \right) \right).$$
(61)

Note that in the constrained ESRD case, the *x* and *y* dimensions have the same sign multiplying ν due to the presence of the term $\nu(p_x + p_y)$, whereas in the constrained OSRD the *x* and *y* dimensions have opposite signs multiplying ν due to $\nu(p_x - p_y)$. As a result, the twodimensional propagators K_{ESRD}^c and K_{OSRD}^c are simply the products of two 1D propagators, and the only difference between the two appears in the terms linear in ν

$$K_{\text{ESRD}}^{c}(x, y, x_{0}, y_{0}; t) = \frac{m\eta}{2\pi i\hbar \sin \eta t} \exp\left(\frac{\mathrm{i}m}{2\hbar} \left(\left(x_{0}^{2} + x^{2} + y_{0}^{2} + y^{2}\right)\eta \cot \eta t\right)\right)$$

$$-2(x_{0}x + y_{0}y)\eta \csc \eta t + \nu(2x_{0} - 2x + 2y_{0} - 2y + 2t\nu)\right)$$

$$K_{\text{OSRD}}^{c}(x, y, x_{0}, y_{0}; t) = \frac{m\eta}{2\pi i\hbar \sin \eta t} \exp\left(\frac{\mathrm{i}m}{2\hbar} \left(\left(x_{0}^{2} + x^{2} + y_{0}^{2} + y^{2}\right)\eta \cot \eta t\right)\right)$$
(62)

$$-2(x_0x + y_0y)\eta \csc \eta t + \nu(2x_0 - 2x - 2y_0 + 2y + 2t\nu))\Big).$$
(63)

In equations (62) and (63), ν takes on the values $\nu = \alpha(\sigma_x - \sigma_y)/\hbar$ (ESRD) and $\nu = \alpha(\sigma_x + \sigma_y)/\hbar$ (OSRD). It can be verified that the limits $\eta \to 0$ (unconfined) and $\nu \to 0$ (simple harmonic oscillator) reduce to the corresponding propagators.

We now proceed with the algebraic method for the confined case. When including a harmonic oscillator potential, the algebraic method becomes challenging due to the noncommutativity $[p_x, p_x^2 + (1/2)m\omega^2 x^2] \neq 0$. As a consequence, the kinetic and potential terms cannot be simply factorized. The usual simple harmonic oscillator propagator has been derived using the algebraic method [18] with the operators

$$L_{-} = -\frac{1}{2}\partial_{xx}, \qquad L_{+} = \frac{1}{2}x^{2}, \qquad L_{3} = \frac{1}{2}x\partial_{x} + \frac{1}{4},$$
 (64)

which satisfy the commutation relation of the Lie algebra su(2), namely

$$[L_+, L_-] = 2L_3, \qquad [L_3, L_\pm] = \pm L_\pm. \tag{65}$$

We first consider the Hamiltonian in equation (55) with a shift in the momentum. Therefore we set out to modify the operators to

$$L_{-} = -\frac{1}{2}\partial_{xx} + \frac{m\nu}{i\hbar}\partial_{x} + \frac{m^{2}\nu^{2}}{2\hbar^{2}}, \qquad L_{+} = \frac{1}{2}x^{2}, \qquad L_{3} = \frac{1}{2}x\partial_{x} + \frac{1}{4} - \frac{xm\nu}{2i\hbar}, \tag{66}$$

which still satisfy equation (65).

By applying a Baker–Campbell–Hausdorff-like relation [23, 24]

$$\exp(\tau L_{+} - \overline{\tau}L_{-}) = \exp\left(\frac{\tau}{|\tau|}\tan(|\tau|)L_{+}\right)\exp(-2\ln\cos(|\tau|)L_{3})\exp\left(-\frac{\overline{\tau}}{|\tau|}\tan(|\tau|)L_{-}\right)$$
(67)

and substituting $\tau = \frac{-itm\eta^2}{\hbar}$, $\overline{\tau} = \frac{it\hbar}{m}$ and $|\tau| = \eta t$, we rewrite the time-evolution operator as

$$T = \exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\hbar^2}{m}\left(-\frac{\partial_{xx}}{2} + \frac{m\nu}{\mathrm{i}\hbar}\partial_x + \frac{m^2\nu^2}{2\hbar^2} + \frac{1}{2}m\eta^2x^2 - \frac{m^2\nu^2}{2\hbar^2}\right)\right)$$
$$= \exp\left(\frac{\mathrm{i}tm\nu^2}{2\hbar}\right)\exp\left(-\frac{\mathrm{i}t}{\hbar}\left(\frac{\hbar^2}{m}\left(-\frac{\partial_{xx}}{2} + \frac{m\nu}{\mathrm{i}\hbar}\partial_x + \frac{m^2\nu^2}{2\hbar^2} + \frac{1}{2}m\eta^2x^2\right)\right)\right)$$
$$= \exp\left(\frac{\mathrm{i}tm\nu^2}{2\hbar}\right)\exp\left(-\frac{\mathrm{i}m\eta}{\hbar}\frac{x^2}{2}\tan\eta t\right)\exp\left(-2\left(\frac{1}{2}x\partial_x + \frac{1}{4} - \frac{xm\nu}{2\mathrm{i}\hbar}\right)\ln\cos\eta t\right)$$
$$\times \exp\left(-\frac{\mathrm{i}\hbar}{m\eta}\left(-\frac{1}{2}\partial_{xx} + \frac{m\nu}{\mathrm{i}\hbar}\partial_x + \frac{m^2\nu^2}{2\hbar^2}\right)\tan\eta t\right). \tag{68}$$

By applying the product of exponentials to a wavefunction, the last line in equation (68) corresponds to two commuting operators ∂_{xx} and ∂_x , and it is straightforward to apply them to a wavefunction using equation (48) and the usual displacement formula [17]

$$\exp(a\partial_x)f(x) = f(x+a),\tag{69}$$

which gives

$$\psi(x,t) = T(t,0)\psi(x,0)$$

$$= \exp\left(\frac{\mathrm{i}tmv^{2}}{2\hbar}\right)\exp\left(\frac{-\mathrm{i}m\eta}{\hbar}\frac{x^{2}}{2}\tan\eta t\right)\exp\left(-\left(x\partial_{x}+\frac{1}{2}-\frac{xmv}{\mathrm{i}\hbar}\right)\ln\cos\eta t\right)$$

$$\times \sqrt{\frac{m\eta}{2\pi\mathrm{i}\hbar}\tan\eta t}\int_{-\infty}^{\infty}\exp\left(-\frac{m\eta}{2\mathrm{i}\hbar}\tan\eta t}\left((x-x_{0})^{2}-2\frac{v(x-x_{0})}{\eta}\tan\eta t\right)\right)$$

$$\times \psi(x_{0},0)\,\mathrm{d}x_{0}.$$
(70)

The term $\exp\left(-\left(x\partial_x + \frac{1}{2} - \frac{xm\nu}{i\hbar}\right)\ln\cos\eta t\right)$ cannot be factorized immediately due to the commutator $[x\partial_x, x] = x$. Instead the Zassenhaus formula which relates noncommuting operators in exponentials [25]

$$e^{t(X+Y)} = e^{tX} e^{tY} e^{-\frac{t^2}{2!}[X,Y]} e^{\frac{t^3}{3!}(2[Y,[X,Y]] + [X,[X,Y]])} \times e^{-\frac{t^4}{4!}(3[Y,[Y,[X,Y]]] + 3[X,[Y,[X,Y]]] + [X,[X,[X,Y,]]])} \dots$$
(71)

is needed. It is interesting to note that $exp(ax\partial_x + abx)$ can be factorized even in the presence of a non-terminating series in the Zassenhaus formula, namely

$$\exp(ax\partial_x + abx) = \exp(ax\partial_x)\exp(abx)\exp\left(-\frac{a^2bx}{2!}\right)\exp\left(\frac{a^3bx}{3!}\right)\dots$$
$$= \exp(ax\partial_x)\exp\left(\sum_{n=1}^{\infty}\frac{a^n(-1)^{n-1}}{n!}bx\right)$$
$$= \exp(ax\partial_x)\exp((1 - \exp(-a))bx).$$
(72)

By comparing $\exp\left(-\left(x\partial_x - \frac{xm\nu}{i\hbar}\right)\ln\cos\eta t\right)$ with equation (72) we extract $a = -\ln\cos\eta t$, $b = -\frac{m\nu}{i\hbar}$. As a result we obtain that

$$\exp\left(-\left(x\partial_x + \frac{1}{2} - \frac{xm\nu}{i\hbar}\right)\ln\cos\eta t\right)$$

$$= \frac{1}{\sqrt{\cos\eta t}}\exp\left(-\left(x\partial_x - \frac{xm\nu}{i\hbar}\right)\ln\cos\eta t\right)$$

$$= \frac{1}{\sqrt{\cos\eta t}}\exp(-x\partial_x\ln\cos\eta t)\exp\left(-(1 - \exp(\ln\cos\eta t))\frac{m\nu x}{i\hbar}\right)$$

$$= \frac{1}{\sqrt{\cos\eta t}}\exp(-x\partial_x\ln\cos\eta t)\exp\left(-(1 - \cos\eta t)\frac{m\nu x}{i\hbar}\right).$$
(73)

Now the term $\exp(-x\partial_x \ln \cos \eta t)$ corresponds to a dilatation operator. The effect of a dilatation operator on a function is given by [18, 22]

$$\exp(ax\partial_x)f(x) = f(e^a x).$$
(74)

Therefore the operator $\exp(-x\partial_x \ln \cos \eta t)$ changes every x to $x/\cos \eta t$.

Combining these results we obtain

$$\begin{aligned} \psi(x,t) &= T(t,0)\psi(x,0) \\ &= \exp\left(\frac{\mathrm{i}tm\,\nu^2}{2\hbar}\right)\exp\left(\frac{-\mathrm{i}m\eta}{\hbar}\frac{x^2}{2}\tan\eta t\right)\exp\left(-(1-\cos\eta t)\frac{m\nu x}{\mathrm{i}\hbar\cos\eta t}\right)\sqrt{\frac{m\eta}{2\pi\mathrm{i}\hbar\sin\eta t}} \\ &\times \int_{-\infty}^{\infty}\exp\left(-\frac{m\eta}{2\mathrm{i}\hbar\tan\eta t}\left(\left(\frac{x}{\cos\eta t}-x_0\right)^2-2\frac{\nu\left(\frac{x}{\cos\eta t}-x_0\right)}{\eta}\tan\eta t\right)\right)\right) \\ &\times \psi(x_0,0)\,\mathrm{d}x_0 \\ &= \sqrt{\frac{m\eta}{2\pi\mathrm{i}\hbar\sin\eta t}}\int_{-\infty}^{\infty}\exp\left(\frac{\mathrm{i}m}{2\hbar}((x^2+x_0^2)\eta\cot\eta t-2xx_0\eta\csc\eta t)\right) \\ &+ 2\nu(x_0-x)+\nu^2t\right)\psi(x_0,0)\,\mathrm{d}x_0. \end{aligned}$$
(75)

The propagator for the confined ESRD (OSRD) in one dimension can be extracted

$$K(x, x_0; t) = \sqrt{\frac{m\eta}{2\pi i\hbar \sin \eta t}} \exp\left(\frac{\mathrm{i}m}{2\hbar} \left(\left(x^2 + x_0^2\right)\eta \cot \eta t - 2xx_0\eta \csc \eta t + 2\nu(x_0 - x) + \nu^2 t \right) \right),$$
(76)

which matches equation (61). Again in 2D we obtain the results from equations (62) and (63) as the product of two 1D propagators.

4. Applying the propagator to spin wavepacket evolution

We now apply the propagators for the confined atomic spin-orbit coupled system and for the confined ESRD system to a localized spin wavepacket. The spin wavepacket we consider $\psi(x_0, y_0; t)$ is a Gaussian distribution in space centered at (x', y') with widths w_x and w_y and with spin polarizations determined by constants χ and λ such that $|\chi|^2 + |\lambda|^2 = 1$ and

$$\psi(x_0, y_0; t) = \frac{1}{\pi w_x w_y} \exp\left(-\frac{(x_0 - x')^2}{2w_x^2} - \frac{(y_0 - y')^2}{2w_y^2}\right) \begin{pmatrix} \chi \\ \lambda \end{pmatrix}.$$
 (77)

By applying $K_{SO}^{\eta\neq\gamma}$ (equation (34)) to $\psi(x_0, y_0; t)$ as in equation (5) we obtain

$$\psi(x, y; t) = \frac{1}{\pi w_x w_y} \sqrt{\frac{1}{\left(\cos \eta t - \frac{\hbar \sin \eta t}{im\eta w_x^2}\right)\left(\cos \eta t - \frac{\hbar \sin \eta t}{im\eta w_y^2}\right)}}{exp\left(\frac{im\eta (x^2 + y^2)\cos \eta t}{2\hbar \sin \eta t}\right)} - \frac{x'^2}{2w_x^2} - \frac{y'^2}{2w_y^2} + \frac{m\left(x\cos\gamma t + y\sigma_z\sin\gamma t + \frac{x'\hbar\sin\eta t}{im\eta w_x^2}\right)^2}{2i\hbar \sin\eta t\left(\cos\eta t - \frac{\hbar \sin\eta t}{im\eta w_x^2}\right)} + \frac{m\left(y\cos\gamma t - x\sigma_z\sin\gamma t + \frac{y'\hbar\sin\eta t}{im\eta w_y^2}\right)^2}{2i\hbar \sin\eta t\left(\cos\eta t - \frac{\hbar \sin\eta t}{im\eta w_y^2}\right)^2}\right) \binom{\chi}{\lambda}.$$
(78)

Note that we use natural units in generating the plots. We provide an initial spin state with spin-up (\uparrow) ($\chi = 1, \lambda = 0$), center the initial wavepacket at (x', y') = (1, 1) for simplicity



Figure 1. Spin probability density ρ_{\uparrow} contour plot for a spin state initially up for six successive times from 0 to 0.5 from (*a*)–(*f*) with an increment of 0.1 between plots. The parameters are chosen as follows: $m = 1, \hbar = 1, w_x = w_y = 1, \eta = 1, \gamma = 10$.

and display the spin probability density $\rho_{\uparrow} = |\psi_{\uparrow}|^2$ at six different times in figures 1(*a*)–(*f*). We see that the spin wavepacket performs a counterclockwise rotation.

Next, by applying the propagator for the confined ESRD system (equation (62)) to $\psi(x_0, y_0; t)$ (equation (77)) in equation (5) we obtain

$$\psi(x, y; t) = \frac{1}{\pi w_x w_y} \sqrt{\frac{1}{\left(\cos \eta t - \frac{\hbar \sin \eta t}{im \eta w_x^2}\right)\left(\cos \eta t - \frac{\hbar \sin \eta t}{im \eta w_y^2}\right)}} \exp\left(\frac{\mathrm{i}m}{2\hbar} \left((x^2 + y^2)\eta \cot \eta t\right) + \frac{\alpha}{\hbar}(\sigma_x - \sigma_y)\left(-2x - 2y + \frac{2\alpha}{\hbar}(\sigma_x - \sigma_y)t\right)\right)}$$



Figure 2. Spin probability density ρ_{κ} contour plot for a spin state initially $\chi = (-1-i)/2$, $\lambda = 1$ for six successive times from 0 to 5 from (a)-(f) with an increment of 1 between plots. The parameters are chosen as follows: m = 1, $\hbar = 1$, $w_x = w_y = 1$, $\eta = 1$, $\alpha = 1$.

$$-\frac{x^{\prime 2}}{2w_x^2} - \frac{y^{\prime 2}}{2w_y^2} + \frac{m\left(x\eta\csc\eta t - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y) + \frac{i\hbar x^{\prime}}{mw_x^2}\right)^2}{2i\hbar(\eta\cot\eta t + \frac{i\hbar}{mw_y^2})} + \frac{m\left(y\eta\csc\eta t - \frac{\alpha}{\hbar}(\sigma_x - \sigma_y) + \frac{i\hbar y^{\prime}}{mw_y^2}\right)^2}{2i\hbar(\eta\cot\eta t + \frac{i\hbar}{mw_y^2})}\right) \begin{pmatrix}\chi\\\lambda\end{pmatrix}.$$
(79)

For simplicity, we choose the initial spin state to be one of the eigenspinors of $\sigma_x - \sigma_y$ such that $\chi = (-1 - i)/2$, $\lambda = 1$ and we denote this spin state as κ . This choice guarantees that spin-flipping does not occur. The initial Gaussian is again chosen to be centered at (x', y') = (1, 1). We plot the spin probability density $\rho_{\kappa} = |\psi_{\kappa}|^2$ at six different times in figures 2(a)-(f). We see that the spin wavepacket performs oscillations on the diagonal axis. In these and other cases the propagator clearly determines the wavepacket evolution. More complex behavior can be observed when the initial wavepacket consists of superpositions of eigenspinors.

5. Discussion

We have obtained propagators for atomic spin-orbit coupled systems and for ESRD and OSRD spintronics systems by using two different methods. The first method is based on the classical action and is familiar from spinless systems [20]. It relies on direct integration, substitution, Legendre transformation and the application of the initial conditions. In reality, the actual integration can often be avoided [19]. However, as the Hamiltonians get more complex, the differential equations to be solved contain more terms and an alternate method becomes preferable. In particular for the most general confined atomic spin-orbit case (section 2.3) we choose to obtain the propagator with the algebraic method. In the algebraic method, we permute noncommutative operators in the exponentials in order to extract factors corresponding to recognizable propagators. This method is not algorithmic but involves the identification of mutually commuting parts. These parts either correspond to systems whose propagators are known or whose action on the wavefunction can be evaluated directly. In the atomic spin-orbit case, the algebraic method involves the propagator of the simple harmonic oscillator and a spin-dependent rotation operator. Both operations can be applied directly to the wavefunctions. The two methods illustrate different approaches and we have used them both to derive the ESRD and ORSRD propagators. Both methods yield the same result with comparable levels of complexity. In the ESRD/OSRD confined case, the confining harmonic oscillator does complicate the algebraic method significantly. This shows that each method has its merits and that the choice of method should be determined carefully by taking into consideration the complexity of the Hamiltonian. This does not exclude the possibility of looking into extending still other methods such as the path-integral method [20] or Schwinger's method [26, 27] to the spin degree of freedom when dealing with spin-orbit coupled Hamiltonians.

The physical systems that we have considered all display the spin-orbit coupling. We have limited our attention to a dependence that is at most quadratic in x and p. Because of the properties of the spin, $\sigma^2 = 1$, quadratic or higher orders of spin do not appear. In general, a linear term in the momentum p can be absorbed in the kinetic energy by shifting the momentum and by adding a constant energy. The equations of motion will be unaffected. This is the momentum equivalent of shifting the equilibrium of an oscillator in the presence of a constant force. However, the action and the propagator of such systems will contain extra terms. This can be compared to the description of motion in inertial frames that are in relative motion. Our systems are also effectively two dimensional only, as momentum in z is frozen out. These effective 2D Hamiltonians find application in real systems. Bernevig *et al* [11] have recently found that the Hamiltonian for strained materials with quantum well parabolic confinement is of the form

$$H = \frac{\mathbf{p}^2}{2m} + \frac{C_3 g}{2\hbar} (y p_x - x p_y) \sigma_z + D(x^2 + y^2), \tag{80}$$

where C_3 is a material-dependent constant and D corresponds to the confinement strength. Landau levels result from such a Hamiltonian without the presence of a magnetic field. Bernevig *et al* [13] also found that ESRD Hamiltonian leads to interesting persistent spin helix phenomena in condensed matter systems. Both Rashba and Dresselhaus interactions can also be replicated in ultracold atoms [4]. ESRD and OSRD apply to systems that have equal amounts of Rashba and Dresselhaus interactions only. Because of the noncommutativities of the Rashba and Dresselhaus parts, the propagator of the combined interactions differs from the product of the individual propagator.

The construction of propagators in spin–orbit coupled systems remains challenging. Nevertheless for those specific cases treated in this paper, the propagators can be found in closed form and can be applied to predict and display spin evolution.

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