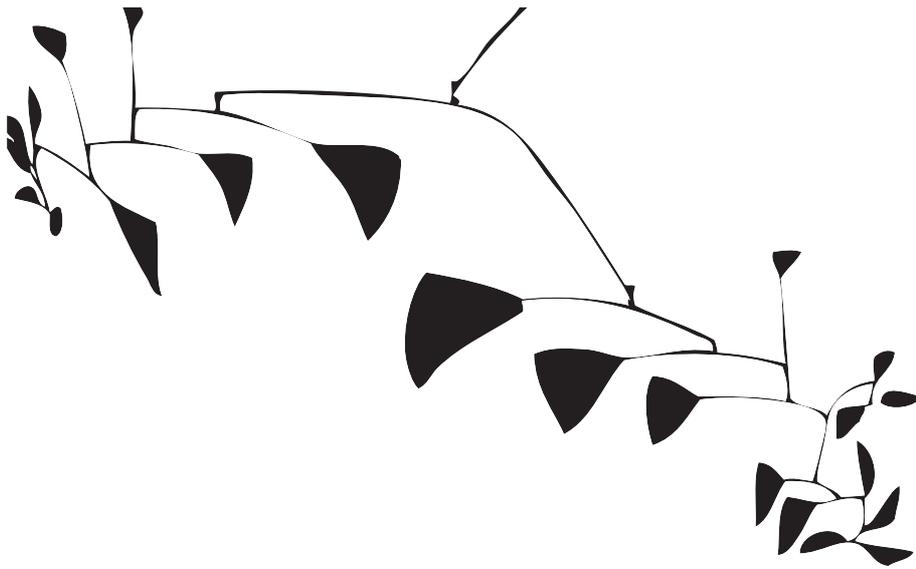


A Path Integral Approach to The Spin-Orbit Interaction

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Bachelor thesis

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*Jeg synes det trist å skulle oppgi tanken på de hardtslående oppdagelsene.
Straks man forlater den kvantitative forskning, beveger man seg inn i et minefelt.*

Erlend Loe, *L*, 1999.

Cover:
Alexander Calder (1898-1976)
American sculptor
Graphic rendition of "Mobile"

Resume in danish

Nærværende opgave har som hovedformål at give en path integral formulering af spin-bane koblingen. Spin-bane koblingen er en fysisk effekt observeret ved ladede partikler i nærvær af \mathbf{E} - og \mathbf{B} -felter, og i de senere år er denne effekt blevet fremhævet som en metode til eksperimentelt at realisere kvantecomputere, hvilket har bevirket en øget interesse for effekten. Path integral formuleringen af kvantemekanik står som et alternativ til Schrödinger og Heisenbergs formuleringer, og byder på en radikalt anderledes tilgang til, og forståelse af, kvantemekanik. Path integral formulering har klare fordele og ulemper, og spin er desværre ikke en af formuleringens stærke sider. Konceptuelt er det dog absolut nødvendigt, at denne formalisme også på tilstrækkelig vis kan behandle spin. Vigtigheden af at kunne beskrive spin fremhæves af, at Feynman, ophavsmanden til path integral formalisme, valgte ikke at undervise i path integraler, pga formalismens, på det tidspunkt, utilstrækkelighed til at beskrive spin! Det er mit ydmyge håb at denne opgave vil bidrage til en bredere forståelse af hvorledes path integraler benyttes i praksis, og i særdeleshed, hvordan spin inkorporeres i formalismen.

Fokus for opgaven er at sikre grundlaget for, og grundigt at udføre, de nødvendige beregninger, der leder frem til en sammenhængende beskrivelse af en partikel med spin-orbit kobling i path integral formalismens sprog. Opgaven er udformet således at en person med et godt fundament i Hamiltonformuleringen af kvantemekanik vil kunne læse den, uden at ty til ekstra kilder. På grund af længdebegrænsninger på bacheloropgaver ved Det Naturvidenskabelige Fakultet, er diskussionerne af spin-orbit kobling og path integral formuleringerne noget kortere end hvad man kunne ønske. De indeholder dog naturligvis den nødvendige information for at motivere de videre beregninger i opgaven. I litteraturlisten findes inspiration til videre læsning.

En tak skal lyde til min vejleder Karsten Flensberg for altid at stå klar med hjælp til drilsk algebra og for de mange oplysende og afklarende diskussioner. Desuden en til tak Emil Zeuthen for hans øje for detalje, også på tværs af atlanten. Til sidst en tak til mine forældre og min bror for deres vedvarende og uundværlige støtte, samt for deres hjælp med at opretholde et meningsfyldt næringsindtag i dette forår.

Morten Kjærgaard,
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Chapter 1

Introduction

The aim of this thesis is to provide a formulation of the spin-orbit interaction in the framework of Feynmans path integral formalism for quantum mechanics. The path integral formulation is an alternative to the Hamiltonian-based description of quantum mechanics, and it provides an interesting and radically different view and approach to the field of quantum mechanics, than the Hamiltonian formalism. The spin-orbit interaction was chosen as the physical phenomenon to which path integral formalism is applied, because spin-orbit interaction have recently proven a promising candidate as the mediator for control of the intrinsic spin of electrons. This control is integral for the emerging field of semiconductor spintronics, and as such, merits further study.

A combined interest in the foundation of quantum mechanics, and modern approaches to quantum computing, sparked the idea that would eventually lead to this thesis. The treatment of spin-orbit interaction and path integral formalism presented here, are both self-contained. However, the reader is assumed to have a fair background in basic quantum mechanics. Knowledge of neither the spin-orbit interaction nor the path integral formulation is a prerequisite, but because of time- and space limitation, the discussion of the physical consequences of spin-orbit interaction is only briefly touched upon. Likewise, the formal introduction to the path integral formalism is not exhaustive, but provides only a brief introduction to the basic concepts, and introduces the ideas relevant for the study of spin-orbit interaction in this framework.

The body of this thesis is comprised of the actual *calculations* needed to describe spin-orbit interaction with path integrals. The inclusion of spin in path integral calculations is by no means trivial, and several requisites have to be insured, before a description of spin-orbit interaction is possible. The final result is esoteric, but nonetheless, provides an interesting alternative formulation to what a Hamiltonian-based treatment yields.

Chapter 2

The spin-orbit interaction and the Hilbert space

The aim of this chapter is two-fold. First an introduction to the physical system that is of interest in this thesis, and second, to introduce the Hilbert space most suitable when dealing with the Hamiltonian for this setup. We begin with a primer on why such a system merits a study as this and briefly introduce the Hamiltonian. The Hamiltonian involves a spin-orbit interaction term, which will be explicitly derived, but, unfortunately, none of the many surprising physical consequences will be discussed in detail. The path-integral formalism is postponed for the next chapter, where we will make some general observations regarding the formalism. For now, we only use the Hamiltonian to describe the system.

2.1 The physical system

Controlling the spin of a single electron is the basis for the emerging field of semiconductor spintronics, popularized under the name quantum computing. As a consequence, several methods have been proposed as a means to control the spin [1]. Recently, a strategy that relies on the spin-orbit interaction for manipulating the spin of the electrons in a highly controlled manner have been promoted [2]. One such strategy relies on confining the electron to move in a 0D potential well, and we will in this thesis consider such a well, as inspired by Flindt *et al.* [3]. Semiconductors of type III-V such as InAs, InGaAs and InSb are very suitable for the experimental realization of such 0D devices, because of these materials asymmetric potentials in the transition layer, which are tunable by applying a gate-voltage to the setup [4]. The type of spin-orbit interaction we consider arise as a consequence of this lack of inversion symmetry in the transition layer potential, and is referred to as the Rashba spin-orbit interaction [4, 5]. Figure 2.1 illustrates such a semiconductor setup, that allows for the control of spin, through the Rashba spin-orbit interaction.

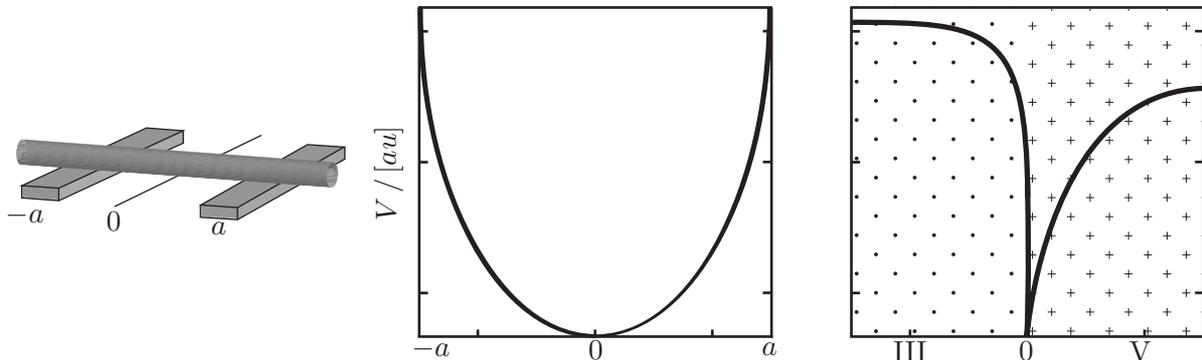


Figure 2.1: *left)* An idealized geometry allowing for control of the electron spin, through the spin-orbit interaction. The black outlined are electrodes and the tube is an III-V wire. *center)* An example of a possible potential over the wire. *right)* An example of a transition-layer potential in the III-V wire. The potential is not symmetric under inversion, and it is this potential that gives rise to the spin-orbit interaction. The lefthand side is a type III material, and the righthand side is a type V material, denoted by \cdot and $+$ respectively.

If we apply an external magnetic field \mathbf{B} to a geometry as the one in fig. 2.1, the Hamiltonian describing an electron on the wire is given by

$$\mathcal{H} = \frac{(\hat{\mathbf{p}} - q_e \mathbf{A})^2}{2m} + V(\hat{\mathbf{q}}) + \mathcal{H}_{\text{SO}}, \quad (2.1)$$

where $V(\hat{\mathbf{q}})$ is a potential such as the one in fig.2.1, q_e is the charge of the electron, \mathbf{A} satisfies $\mathbf{B} = \nabla \times \mathbf{A}$, and $\hat{\mathbf{p}}$ is the three-dimensional quantum mechanical momentum operator. The replacement $\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} - q_e \mathbf{A}$ in the kinetic term is simply a result from classical mechanics. The explicit form of the Rashba spin-orbit term, \mathcal{H}_{SO} , will be derived in section 2.1.1.

2.1.1 The spin-orbit interaction

The spin-orbit interaction is a relativistic effect. Although the electron is not in general moving with speeds that would require a relativistic treatment in a system such as this, the electric fields surrounding the atomic nuclei in the wire are large enough to yield weak relativistic effects (Section 5.4 in [6]). There are several ways to derive the explicit form of the spin-orbit interaction. However, the two most often encountered are

- *The systematically relativistic:* Solving the the Dirac equation (which is the relativistic Schrödinger equation), for a single-particle state exposed to a vector potential \mathbf{A} . This method is surprisingly cumbersome and is beyond the scope of this thesis. A detailed derivation can be found in chapter 24 of [7].
- *The ad hoc:* Assuming that an electron constitutes a magnetic dipole and finding the torque on a magnetic dipole in an electric and magnetic field. The relativistic effects are then accounted for by doing a Lorentz-transformation into the rest-frame of the electron, to find out what effective \mathbf{B} -field the electron "feels".

In this thesis, we follow the ad hoc-strategy. The two strategies are, in terms of finding the explicit form of only the spin-orbit interaction, equivalent. The ad hoc approach relegates the relativistic effects to the coordinate change, whereas the systematically relativistic uses the relativistic nature of the spin-orbit interaction as its starting point, by using the Dirac equation instead of the Schrödinger equation.

The ad hoc derivation starts with a naïve assumption: The spin of an electron is equivalent to the rotation of a classical sphere. This is a crude assumption, but the error that arises, can be corrected. It is a result from classical electrodynamics, that a spinning charged particle constitutes a magnetic dipole, meaning that an electron will also constitute a magnetic dipole [8, 9]. Thus, if the electron moves in an external \mathbf{B} -field, it will feel a torque given by

$$\boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B}, \quad (2.2)$$

where $\mathbf{B} = (B_x, B_y, B_z)$ and $\boldsymbol{\mu}$ is the magnetic dipole moment of the electron given by

$$\boldsymbol{\mu} = \left(\frac{ge}{2m_e} \right) \mathbf{S},$$

where \mathbf{S} is just the classic spin angular momentum of a rotating sphere. If we Lorentz-transform into a coordinate system moving with the electron, it turns out that the electron will feel an *effective* magnetic field given by¹

$$\mathbf{B}_{\text{eff}} = \mathbf{B} - \frac{\mathbf{v}}{c^2} \times \mathbf{E}.$$

Note here, that the \mathbf{E} -field is not an externally applied one, since this would rarely be strong enough to provoke relativistic effects, but rather, it is the \mathbf{E} -field arising from the nuclei of the atoms. Inserting this effective magnetic field into eq. (2.2) yields

$$\boldsymbol{\tau} = \left(\frac{ge}{2m_e} \right) \mathbf{S} \times \left(\mathbf{B} - \frac{\mathbf{v}}{c^2} \times \mathbf{E} \right).$$

From the torque, the energy can be calculated, and is given by²

$$U = - \left(\frac{ge}{2m_e} \right) \mathbf{S} \cdot \mathbf{B} + \left(\frac{ge}{2m_e^2 c^2} \right) \mathbf{S} \cdot (\mathbf{p} \times \mathbf{E}). \quad (2.3)$$

There is no quantum mechanics in eq. (2.3). However, boldly replacing \mathbf{S} and \mathbf{p} with their quantum mechanical counterparts, $\frac{\hbar}{2}\boldsymbol{\sigma}$ and $\hat{\mathbf{p}}$ respectively, in eq. (2.3) yields the (almost) correct form of the quantum mechanical spin-orbit coupling. Making the substitution

$$\begin{aligned} \mathbf{p} &\rightarrow \hat{\mathbf{p}} = -i\hbar\nabla \\ \mathbf{S} &\rightarrow \frac{\hbar}{2}\boldsymbol{\sigma} = \frac{\hbar}{2} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \end{aligned}$$

¹The explicit calculation can be found in section 11.10 in [10]. Note that contributions to the effective \mathbf{B} -field arising from the magnetic moment of the nuclei are not included here.

²The calculation is relegated to appendix A.

in eq. (2.3), we see that the quantum mechanical energy is given by

$$U_{\text{quantum}} = - \left(\frac{ge\hbar}{4m_e} \right) \boldsymbol{\sigma} \cdot \mathbf{B} + \left(\frac{ge\hbar}{4m_e^2 c^2} \right) \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \times \mathbf{E}). \quad (2.4)$$

Unfortunately, this very crude equating of classical and quantum mechanics introduces an error. The second term is *twice* the size of what a proper quantum mechanical treatment yields.³ Introducing a factor of 1/2, known as *the Thomas precession*, which arises as a consequence of relativistic effects, in eq. (2.4)

$$U_{\text{quantum}} = - \left(\frac{ge\hbar}{4m_e} \right) \boldsymbol{\sigma} \cdot \mathbf{B} + \left(\frac{ge\hbar}{8m_e^2 c^2} \right) \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \times \mathbf{E}), \quad (2.5)$$

yields the correct result. Introducing the two constants $\alpha = \frac{ge\hbar}{8m_e^2 c^2}$ and $\mu_b = -\frac{e\hbar}{4m_e}$, we arrive at the final form of the spin-dependent contribution to the potential part of the Hamiltonian

$$\boxed{\mathcal{H}_{\text{SO}} = -g\mu_b \boldsymbol{\sigma} \cdot \mathbf{B} + \alpha \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \times \mathbf{E})} \quad (2.6)$$

The first term in the above equation is the Zeeman term, which is just what we would expect from a spinful charged particle in a magnetic field. If we assume a radial electric field, such that $\mathbf{E} \sim \hat{\mathbf{r}}$, the second term can be recast as

$$\boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \times \mathbf{E}) \sim \boldsymbol{\sigma} \cdot \mathbf{L}$$

which emphasizes why we understand this term as the *spin-orbit interaction*. The name arises as a consequence of the coupling between the spin and the orbital angular momentum of the electron, through the electric field of the nuclei. As a consequence, the strength of the spin-orbit interaction is material-dependent. The factor α is a measure of the strength of the spin-orbit interaction, and numerical examples are 5.3\AA^2 in GaAs and 120\AA^2 in InAs [11].

Thus, returning to eq.(2.1), the complete Hamiltonian describing an electron in a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$, and spin-orbit interaction is given by

$$\boxed{\mathcal{H} = \frac{(\hat{\mathbf{p}} - q_e \mathbf{A})^2}{2m} + V(\hat{\mathbf{q}}) - g\mu_b \boldsymbol{\sigma} \cdot \mathbf{B} + \alpha \boldsymbol{\sigma} \cdot (\hat{\mathbf{p}} \times \mathbf{E})} \quad (2.7)$$

This is the form of the Hamiltonian that we will investigate throughout this thesis. Note, that although we considered a 0D quantum well in the beginning of this section, we will perform the rest of the calculations in this thesis in 3D, for the sake of generality.

2.2 Hilbert space and basis states

Now that we have outlined the physical system of interest, the next step is to select a proper basis, before we approach the true problem of describing a Rashba spin-orbit coupled particle

³See for example [10] section 11.8 for a full derivation.

in the path integral formalism. We will be working in $3 + 3 + 2$ dimensional Hilbert space denoted \mathcal{H} . Six of these dimensions are attributed to position and momentum (the phase-space); (x, y, z) and (p_x, p_y, p_z) . The final two dimensions arise from the spin-component of the Hamiltonian. In section 2.2.1 we review properties of the phase-space, and in section 2.2.2 we introduce the special basis of the $|z\rangle$ -states, which we will use as a basis for the spin-component of the Hamiltonian.

2.2.1 Position and momentum basis

We start out in the Schrödinger picture, and use Dirac notation. Let $|\mathbf{q}\rangle$ denote an eigenstate of the three-dimensional position-operator $\hat{\mathbf{q}} \equiv (\hat{q}_x, \hat{q}_y, \hat{q}_z)$ with eigenvalue $\mathbf{q} = (q_x, q_y, q_z)$ and $|\mathbf{p}\rangle$ denote an eigenstate of the three-dimensional momentum operator $\hat{\mathbf{p}} \equiv (\hat{p}_x, \hat{p}_y, \hat{p}_z) = \frac{\hbar}{i}\nabla$ with eigenvalue $\mathbf{p} = (p_x, p_y, p_z)$. Two different position and momentum operator eigenstates are orthogonal,

$$\langle \mathbf{q}' | \mathbf{q} \rangle = \delta^3(\mathbf{q}' - \mathbf{q}) \quad \text{and} \quad \langle \mathbf{p}' | \mathbf{p} \rangle = \delta^3(\mathbf{p}' - \mathbf{p}),$$

because $\hat{\mathbf{q}}$ and $\hat{\mathbf{p}}$ are hermitian operators. It will prove convenient to have the form of the momentum operator eigenstates represented in the basis of position operator eigenfunctions. The eigenstates are related through a fourier transform, thus

$$\langle \mathbf{q} | \mathbf{p} \rangle = (2\pi\hbar)^{-3/2} e^{i\mathbf{p}\cdot\mathbf{q}/\hbar} \quad \text{and equivalently} \quad \langle \mathbf{p} | \mathbf{q} \rangle = (2\pi\hbar)^{-3/2} e^{-i\mathbf{p}\cdot\mathbf{q}/\hbar}.$$

We need one more very important property, completeness of the eigenstates:

$$\int d^3\mathbf{q} |\mathbf{q}\rangle \langle \mathbf{q}| = \mathbf{I}_{3\times 3} \quad , \quad \int d^3\mathbf{p} |\mathbf{p}\rangle \langle \mathbf{p}| = \mathbf{I}_{3\times 3}, \quad (2.8)$$

the boldface $\mathbf{I}_{3\times 3}$ is used to signify an identity operator in the Hilbert space $\mathcal{H}_{|\mathbf{q}\rangle}$ spanned by $|\mathbf{q}\rangle$. The fact that $|\mathbf{q}\rangle$ and $|\mathbf{p}\rangle$ form complete sets, is a consequence of $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ both being hermitian operators in a finite dimensional Hilbert space, whose eigenstates are known to be complete.⁴ In table 2.1 all of the properties of the basis states are listed.

Position	Momentum
$\hat{\mathbf{q}} \mathbf{q}\rangle = \mathbf{q} \mathbf{q}\rangle, \langle \mathbf{q} \hat{\mathbf{q}} = \langle \mathbf{q} \mathbf{q}$	$\hat{\mathbf{p}} \mathbf{p}\rangle = \mathbf{p} \mathbf{p}\rangle, \langle \mathbf{p} \hat{\mathbf{p}} = \langle \mathbf{p} \mathbf{p}$
$\langle \mathbf{q}' \mathbf{q}\rangle = \delta^3(\mathbf{q}' - \mathbf{q})$	$\langle \mathbf{p}' \mathbf{p}\rangle = \delta^3(\mathbf{p}' - \mathbf{p})$
$\langle \mathbf{p} \mathbf{q}\rangle = (2\pi\hbar)^{-3/2} e^{-i\mathbf{p}\cdot\mathbf{q}/\hbar}$	$\langle \mathbf{q} \mathbf{p}\rangle = (2\pi\hbar)^{-3/2} e^{i\mathbf{p}\cdot\mathbf{q}/\hbar}$
$\int d^3\mathbf{q} \mathbf{q}\rangle \langle \mathbf{q} = \mathbf{I}_{3\times 3}$	$\int d^3\mathbf{p} \mathbf{p}\rangle \langle \mathbf{p} = \mathbf{I}_{3\times 3}$

Table 2.1: Properties of position and momentum eigenkets and -bras.

⁴Unlike the infinite-dimensional case, where completeness of eigenfunctions of hermitian operators is not insured.

2.2.2 Spin basis

Seeing as our Hamiltonian also involves spin-components we will need some appropriate set of kets (bras) to use as basis for the spin. The spin will be represented in a two-dimensional Hilbert space, called $\mathcal{H}_{|z\rangle}$ for reasons to be explained below. We equip $\mathcal{H}_{|z\rangle}$ with a basis given by the two vectors $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, which we will denote as $|\uparrow\rangle$ and $|\downarrow\rangle$ respectively. Note that these states are orthonormal. A crucial step in arriving at a path integral representation for particles involving spin is to use a suitable basis in $\mathcal{H}_{|z\rangle}$. As a consequence, the intuitive basis of $|\uparrow\rangle$ and $|\downarrow\rangle$ will not be used. Rather, in accordance with [12], we will use a basis given by

$$|z\rangle = \mathcal{N}(z) \exp(z\sigma^+) |\downarrow\rangle \quad (2.9)$$

where $z = u + iv, u, v \in \mathbb{R}^1$, $\mathcal{N}(z)$ is the normalizing factor, and σ^+ is the creation operator.⁵ We define $\mathcal{H}_{|z\rangle}$ to be the 2-dimensional Hilbert space spanned by $|z\rangle$. Creation and annihilation operators will play an important role in the next sections, so their properties in $\mathcal{H}_{|z\rangle}$, are listed in table 2.2.

Annihilation	Creation
$\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$	$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$
$(\sigma^-)^\dagger = \sigma^+$	$(\sigma^+)^\dagger = \sigma^-$
$\sigma^- \uparrow\rangle = \downarrow\rangle$	$\sigma^+ \uparrow\rangle = 0$
$\sigma^- \downarrow\rangle = 0$	$\sigma^+ \downarrow\rangle = \uparrow\rangle$.

Table 2.2: Properties of the creation and annihilation operators.

Using these properties, and that $\exp x = 1 + x + \frac{x^2}{2} + \dots$, eq. (2.9) can be recast as

$$|z\rangle = \mathcal{N}(z) \exp(z\sigma^+) |\downarrow\rangle = \mathcal{N}(z) (1 + z\sigma^+) |\downarrow\rangle = \mathcal{N}(z) (|\downarrow\rangle + z|\uparrow\rangle).$$

This expansion is exact, because only two terms are nonvanishing. In $\mathcal{H}_{|z\rangle}$, it is only possible to apply σ^+ or σ^- once without ending with the null-ket regardless of the state they are applied to, cf. table 2.2. Higher order terms in the expansion therefore vanish. Using this form of $|z\rangle$ the normalizing factor $\mathcal{N}(z)$ is easily found by taking the inner product and exploiting orthonormality of $|\downarrow\rangle$ and $|\uparrow\rangle$, which gives $\mathcal{N}(z) = 1/\sqrt{1 + |z|^2}$. Expressing a 2-dimensional spinor $|z(u, v)\rangle$ as a function of the real and imaginary parts of a complex number $z = u + iv$ is equivalent to the usual definition of a spinor $|\chi(\theta, \varphi)\rangle$ expressed in spherical coordinates. The equivalence between two points (u, v) in the complex plane and the spherical coordinates

⁵In the infinite-dimensional case, these states are eigenfunctions of the infinite dimensional annihilation operator, \hat{a} . For the proof see [13] chap. 27.

(θ, φ) is shown in appendix B.

Just as in the case of $|\mathbf{q}\rangle$ and $|\mathbf{p}\rangle$ it is necessary to have the completeness relation, i.e. the analogue of eq. (2.8) for the $|z\rangle$ states. These states are at the outset not complete. To ensure completeness we introduce a special measure⁶. In [12] it is suggested to use the measure $d\mu(z)$ given by

$$\int d\mu(z) = \int \frac{2}{\pi} \frac{1}{(1+|z|^2)^2} d^2z = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{2}{\pi} \frac{1}{(1+|z|^2)} d(\text{Re}z) d(\text{Im}z). \quad (2.10)$$

Thus, using this measure, it is necessary to show that

$$\int |z\rangle\langle z| d\mu(z) = \mathbf{I}_{2 \times 2}. \quad (2.11)$$

where $\mathbf{I}_{2 \times 2}$ is an identity operator in $\mathcal{H}_{|z\rangle}$. The calculation is straightforward, but requires a certain amount of algebra, and have therefore been relegated to appendix C. The result is, of course, that relation (2.11) holds.

Throughout this thesis, we will use a Hilbert space defined by $\mathcal{H} = \mathcal{H}_{|\mathbf{q}\rangle} \otimes \mathcal{H}_{|z\rangle}$, where $\mathcal{H}_{|\mathbf{q}\rangle, |z\rangle}$ is the Hilbert spaces spanned by the kets $|\mathbf{q}\rangle$ and $|z\rangle$ respectively. It is important to note, that the subspaces spanned by $|\mathbf{q}\rangle$ and $|z\rangle$ are linearly independent. The linear independence allows us to formally write a state $|\mathbf{q}\rangle \otimes |z\rangle$ as $|\mathbf{q}, z\rangle$. This means that a given state $|\psi\rangle$ can be represented in the basis of $|\mathbf{q}, z\rangle$ simply by $\langle \mathbf{q}, z | \psi \rangle = \psi(\mathbf{q}, z)$. For notational purposes, we will write $|\mathbf{q}, z\rangle$ as $|\mathbf{q}\rangle|z\rangle$ but still understand it as the more formal expression $|\mathbf{q}\rangle \otimes |z\rangle$, so that an operator working in $\mathcal{H}_{|\mathbf{q}\rangle}$, $\hat{\mathbf{p}}$ for example, is formally given by $\hat{\mathbf{p}} \equiv \hat{\mathbf{p}} \otimes \mathbf{I}_{2 \times 2}$, and an operator σ working in $\mathcal{H}_{|z\rangle}$ is understood as $\sigma \equiv \mathbf{I}_{3 \times 3} \otimes \sigma$ etc. In chapter 3 we will encounter terms of the form $\int d^3\mathbf{q} |\mathbf{q}\rangle\langle \mathbf{q}| \int d\mu(z) |z\rangle\langle z| = \mathbf{I}_{3 \times 3} \mathbf{I}_{2 \times 2}$. Such a term would have been meaningless, but because of the construction of our Hilbert space, we now easily recognize these identity operators as belonging to different subspaces of \mathcal{H} , and thus, the differences in dimensionality are no longer a problem. As it turns out, it is useful to represent an electron governed by the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{SO}}$ in the basis of $|\mathbf{q}, z\rangle$. This will be further explored in chapter 3.

In the present chapter we briefly touched on a possible device for quantum computing, which relied on the use of the Rashba spin-orbit interaction. An interest in this device motivated a derivation of the explicit form of the Rashba spin-orbit interaction term, \mathcal{H}_{SO} , in section 2.1.1. After this derivation, the complete Hamiltonian was found in eq. (2.7). In sections 2.2.1 and 2.2.2, the basis in which we will represent our system was introduced. The special measure $d\mu(z)$ was introduced to ensure completeness of the $|z\rangle$ states and a short discussion of the construction of the Hilbert space \mathcal{H} ensued. The next chapter will introduce Feynmans Lagrangian-based formulation of quantum mechanics, the path integral formalism, and some general observations on how to qualitatively approach such a formulation, from the Schrödinger picture.

⁶The explicit form of the measure can be *derived* explicitly by SU(2) group theory. Here, we will merely just show that it *works* in the sense that it gives completeness of the $|z\rangle$ states. For details on the SU(2) group and $|z\rangle$ -states, see [14, 15].

Chapter 3

The path integral formalism

After a presentation of the physical system, and the basis which we will use to represent our system, we are ready to attack the true problem: The path integral formalism of quantum mechanics, and how to represent a spin-orbit coupled electron in this formalism. In section 3.1 a brief introduction to the fundamentals of the path integral formalism is discussed. However, this is a vast field, and it is beyond the scope of this thesis to go into many of the interesting consequences of this formalism. Feynman's book [16] is a comprehensive introduction, and discusses in great detail the physical interpretation of path integrals. The path integrals have some mathematical difficulties, especially in terms of convergence, which will not be touched upon here. The mathematically inclined reader may benefit from the discussions in [17].

The strategy we will use to approach the path integral formalism will not follow Feynman's. His elegant approach relies on the double-slit experiment, and physical arguments. Here we will instead use an, at the outset, conceptually simple approach. The idea is to cut the time-evolution operator, $U(t', t)$, which is the generator of time-translation from the state $|\mathbf{q}, z\rangle$ at $t_i = t$ to the state $|\mathbf{q}', z'\rangle$ at $t_f = t'$, into a large number of pieces, and investigate how *one* such small piece changes in time. This method is conceptually and mathematically clear, and it accomodates neatly for spin, which is not treated in Feynman's book [16]. For the sake of clarity, we start in section 3.2.1 with just cutting $U(t', t)$ into two smaller pieces. Section 3.2.2 will then show how to cut $U(t', t)$ into an arbitrary number of pieces. But first, a short introduction to the formalism.

3.1 The third formulation of quantum mechanics

The path integral, a formulation of quantum mechanics, was introduced by the late physicist R.P. Feynman in his now-classic paper from *Reviews of Modern Physics*, 1948. It stands as a third formulation of quantum mechanics, besides Schrödinger's wave mechanics, and Heisenberg's matrix mechanics, both of which the groundwork was laid for in the 1920s. It has been shown that all three formulations are equivalent. The idea that lead Feynman to formulate the theory of path integrals, came from a comment Dirac had made about the possibility of an alternative formulation of quantum mechanics, based on the lagrangian, \mathcal{L} , instead of the hamiltonian, \mathcal{H} , of Schrödinger's wave mechanics. Dirac argued that the propagator from

Schrödinger and Heisenberg could be equated with $\exp(i\mathcal{S}/\hbar)$, where \mathcal{S} is the action of the classical path (which is dependent on the lagrangian), such that¹

$${}_{t_f=t'}\langle \mathbf{q}', z' | U(t', t) | \mathbf{q}, z \rangle_{t_i=t} \sim \exp\left(\frac{i}{\hbar} \int_t^{t'} \mathcal{L}(\mathbf{q}_{cl}, \dot{\mathbf{q}}_{cl}, z_{cl}, \dot{z}_{cl}) dt\right),$$

where $U(t', t)$ is the time-evolution operator, which, in the case of a time-independent hamiltonian, is given by

$$U(t', t) = \exp\left(-\frac{i}{\hbar} \mathcal{H}(t' - t)\right).$$

Feynman showed that a formulation of quantum mechanics is possible, if we sum *all* such paths connecting endstates, and not just the classical [16]. If we imagine cutting the propagator from the state $|\mathbf{q}, z\rangle_{t_i=t}$ to $|\mathbf{q}', z'\rangle_{t_f=t'}$ into N infinitely small pieces (and denoting $|\mathbf{q}, z\rangle_{t_i=t} = |\mathbf{q}_0, z_0\rangle$ and $|\mathbf{q}', z'\rangle_{t_f=t'} = |\mathbf{q}_N, z_N\rangle$), we may understand the equivalence of Feynmans formulation by

$${}_{t_f=t'}\langle \mathbf{q}_N, z_N | U(t', t) | \mathbf{q}_0, z_0 \rangle_{t_i=t} \sim \sum_{\text{all paths}} \exp\left(\frac{i}{\hbar} \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \mathcal{L}(\mathbf{q}_{j-1}, \dot{\mathbf{q}}_{j-1}, z_{j-1}, \dot{z}_{j-1}) dt\right), \quad (3.1)$$

The summation is over *all possible paths* connecting the endstates, i.e. an innumerable large amount of paths! This means that the particle, in going from state $|\mathbf{q}_0, z_0\rangle$ to state $|\mathbf{q}_N, z_N\rangle$ takes *all the paths that connect them*, but with varying probability. This summing over paths may seem odd and problematic, and is one of the consequences that the path integral formulation of quantum mechanics have both great advantages and several shortcomings. One more point should be made when discussing the path integral formalism; it neatly accomodates for classical mechanics. Simply by taking the classical limit $\hbar \rightarrow 0$, all of classical mechanics is recovered – a comforting thought. A more thorough discussion of this point, and a proof of the equivalence of the path integral formalism and Schrödingers and Heisenbergs mechanics can be found in [18] section 2.5.

3.2 General observations

Considering a particle in the basis $|\mathbf{q}, z\rangle$, we will, in accordance with Feynmans conjecture eq.(3.1), be looking for an alternative formulation of what in Dirac-notation is given by

$$A = \langle \mathbf{q}', z' | U(T, 0) | \mathbf{q}, z \rangle = \langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H}T} | \mathbf{q}, z \rangle \equiv K(\mathbf{q}', z', T; \mathbf{q}, z, 0), \quad (3.2)$$

where we have dropped the time-referring subscript. These equations are physically equivalent to asking the question; "if a particle starts out in state $|\mathbf{q}, z\rangle$ at $t_i = 0$, what is then the probability of finding the particle in the state $|\mathbf{q}', z'\rangle$ at time $t_f = T$?". In equation (3.2) we introduced the notation, $K(\mathbf{q}', z', T; \mathbf{q}, z, 0)$, henceforth called *the kernel*, which is to be

¹According to [18]

understood as the amplitude for going from the state $|\mathbf{q}, z\rangle$ at $t_i = 0$ to state $|\mathbf{q}', z'\rangle$ at $t_f = T$. At this point we remind ourselves, that there are *no* path integrals so far. We are still in the Schrödinger picture, and formally, we are just looking to find the matrix elements of the time evolution operator, in the basis of $|\mathbf{q}, z\rangle$.

3.2.1 A first approach to division of the time evolution operator

In order to evaluate the matrix elements, it will prove useful to investigate what happens if we cut the time evolution operator into two smaller pieces. If $T > 0$ there must exist some t_1 such that $0 < t_1 < T$. Thus, we can split the time-evolution operator into two smaller pieces, one going from 0 to t_1 , and one going from t_1 to T . This can be written as

$$\begin{aligned}\langle \mathbf{q}', z' | U(T, 0) | \mathbf{q}, z \rangle &= \langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H} T} | \mathbf{q}, z \rangle \\ &= \langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H} (T-t_1)} e^{-\frac{i}{\hbar} \mathcal{H} (t_1)} | \mathbf{q}, z \rangle,\end{aligned}$$

we proceed by inserting a complete set of position-operator eigenstates and a complete set of spin states

$$\begin{aligned}\langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H} (T-t_1)} e^{-\frac{i}{\hbar} \mathcal{H} (t_1)} | \mathbf{q}, z \rangle &= \\ \langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H} (T-t_1)} \underbrace{\int d^3 \mathbf{q}_1 | \mathbf{q}_1 \rangle \langle \mathbf{q}_1 |}_{= \mathbf{I}_{3 \times 3}} \underbrace{\int d\mu(z_1) | z_1 \rangle \langle z_1 |}_{= \mathbf{I}_{2 \times 2}} e^{-\frac{i}{\hbar} \mathcal{H} (t_1)} | \mathbf{q}, z \rangle &= \\ \int d^3 \mathbf{q}_1 \int d\mu(z_1) \langle \mathbf{q}', z' | e^{-\frac{i}{\hbar} \mathcal{H} (T-t_1)} | \mathbf{q}_1 \rangle | z_1 \rangle \langle z_1 | \langle \mathbf{q}_1 | e^{-\frac{i}{\hbar} \mathcal{H} (t_1)} | \mathbf{q}, z \rangle &= \\ \int d^3 \mathbf{q}_1 \int d\mu(z_1) K(\mathbf{q}', z', T; \mathbf{q}_1, z_1, t_1) K(\mathbf{q}_1, z_1, t_1; \mathbf{q}, z, 0). &\end{aligned}\tag{3.3}$$

If we disregard the integrations, we may interpret this last equation as the amplitude, and hence probability, for the particle to go from state $|\mathbf{q}, z\rangle$ at $t_0 = 0$ to state $|\mathbf{q}', z'\rangle$ at time $t_f = T$ *via* the state $|\mathbf{q}_1, z_1\rangle$ at time $0 < t_1 < T$. If we include the integration in our interpretation, we may understand $|\mathbf{q}_1, z_1\rangle$ as being *any* state, somewhere in between the start and end states. This seems reasonable – that the particle is in *some* state with *some* spin in between the end states. Figure 3.1 illustrates how we might interpret equation (3.3). Considering only the kernels, we see that equation (3.3) can be identified as simply the quantum mechanical probability of two events occurring in succession. In this case, the two events are, that the particle will at first propagate from state $|\mathbf{q}, z\rangle$ to state $|\mathbf{q}_1, z_1\rangle$, and then propagate to the state $|\mathbf{q}', z'\rangle$.

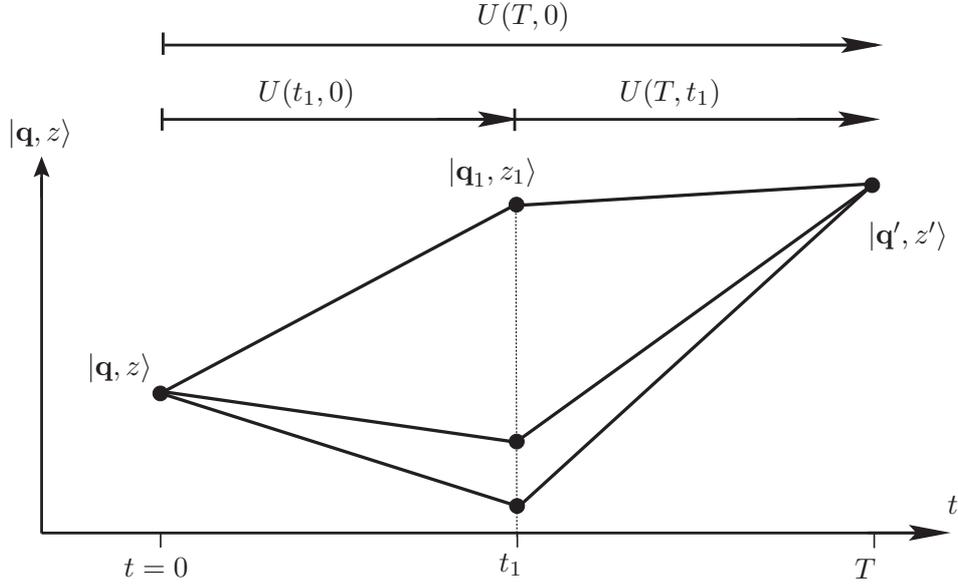


Figure 3.1: Splitting the time evolution operator $U(T,0)$ into two pieces, $U(t_1,0)$ and $U(T,t_1)$. The dots symbolizes states in \mathcal{H} . The black lines connecting the states can be thought of as the kernels in eq. (3.3), and the thin dotted line is equivalent to the two integrations over $d^3\mathbf{q}_1$ and $d\mu(z_1)$ in (3.3), meaning that $|\mathbf{q}_1, z_1\rangle$ is *any* state between the endpoints.

3.2.2 The time evolution operator in N divisions

Instead of just cutting $U(T,0)$ into two smaller pieces, we divide $U(T,0)$ into some large number, N , pieces. If we denote $\epsilon = \frac{T}{N}$, where $N \in \mathbb{N}$, then N successive applications of $U(\epsilon)$ should equal $U(T,0)$. Formally

$$\begin{aligned}
 A &= \langle \mathbf{q}', z' | U(T,0) | \mathbf{q}, z \rangle = \langle \mathbf{q}', z' | (U(\epsilon))^N | \mathbf{q}, z \rangle = \\
 &\langle \mathbf{q}', z' | \left(e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} \right)^N | \mathbf{q}, z \rangle = \langle \mathbf{q}', z' | \underbrace{e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} \dots e^{-\frac{i}{\hbar} \mathcal{H} \epsilon}}_{N \text{ times}} | \mathbf{q}, z \rangle
 \end{aligned}$$

Just as in the previous section, we insert complete states between each successive application of $U(\epsilon)$. For notational convenience call $q' = q_n$, $z' = z_n$, $q = q_0$ and $z = z_0$. Thus,

$$\begin{aligned}
 A &= \langle \mathbf{q}_N, z_N | (U(\epsilon))^N | \mathbf{q}_0, z_0 \rangle \\
 &= \langle \mathbf{q}_N, z_N | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} \int d^3 \mathbf{q}_{N-1} | \mathbf{q}_{N-1} \rangle \langle \mathbf{q}_{N-1} | \int d\mu(z_{N-1}) | z_{N-1} \rangle \langle z_{N-1} | \\
 &\quad e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} \int d^3 \mathbf{q}_{N-2} | \mathbf{q}_{N-2} \rangle \langle \mathbf{q}_{N-2} | \int d\mu(z_{N-2}) | z_{N-2} \rangle \langle z_{N-2} | \cdots \\
 &\quad e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} \int d^3 \mathbf{q}_1 | \mathbf{q}_1 \rangle \langle \mathbf{q}_1 | \int d\mu(z_1) | z_1 \rangle \langle z_1 | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_0, z_0 \rangle \\
 &= \iiint \cdots \iiint d^3 \mathbf{q}_{N-1} d\mu(z_{N-1}) d^3 \mathbf{q}_{N-2} d\mu(z_{N-2}) \cdots d^3 \mathbf{q}_1 d\mu(z_1) \cdot \\
 &\quad \langle \mathbf{q}_N, z_N | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_{N-1} \rangle | z_{N-1} \rangle \langle z_{N-1} | \langle \mathbf{q}_{N-1} | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_{N-2} \rangle | z_{N-2} \rangle \cdots \langle z_1 | \langle \mathbf{q}_1 | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_0, z_0 \rangle \\
 &= \iiint \cdots \iiint d^3 \mathbf{q}_{N-1} d\mu(z_{N-1}) d^3 \mathbf{q}_{N-2} d\mu(z_{N-2}) \cdots d^3 \mathbf{q}_1 d\mu(z_1) \cdot \\
 &\quad K(\mathbf{q}_N, z_N, T; \mathbf{q}_{N-1}, z_{N-1}, (N-1)\epsilon) K(\mathbf{q}_{N-1}, z_{N-1}, (N-1)\epsilon; \mathbf{q}_{N-2}, z_{N-2}, (N-2)\epsilon) \cdots \\
 &\quad K(\mathbf{q}_1, z_1, 1\epsilon; \mathbf{q}_0, z_0, 0). \tag{3.4}
 \end{aligned}$$

The last equations are large and unwieldy, but they have an interpretation analogue to eq. (3.3). Introduce the following notation

$$\sum_{\text{all paths}} = \prod_{j=1}^{N-1} \int d^3 \mathbf{q}_j \prod_{j=1}^{N-1} \int d\mu(z_j) \tag{3.5}$$

$$A_{\text{path}} = K(\mathbf{q}_N, z_N, T; \mathbf{q}_{N-1}, z_{N-1}, (N-1)\epsilon) \cdots K(\mathbf{q}_1, z_1, 1\epsilon; \mathbf{q}_0, z_0, 0). \tag{3.6}$$

so that eq. (3.4) can be written as²

$$\boxed{A = \sum_{\text{all paths}} A_{\text{path}}} \tag{3.7}$$

This form clearly emphasizes what is happening: We are summing *all* the possible paths in the composite Hilbert space $\mathcal{H}_{|\mathbf{q}} \otimes \mathcal{H}_{|z}$ connecting the end states $|\mathbf{q}_0, z_0\rangle$ and $|\mathbf{q}_N, z_N\rangle$ with *all* possible states between, and at each interval we evaluate the kernel for that small time segment. Figure 3.2 illustrates a possible interpretation of (3.7). Equation (3.7) can be seen as our analogy to Feynmans original conjecture, in the form of eq. (3.1).

²The idea to recast eq.(3.4) in this manner, is inspired from [19].

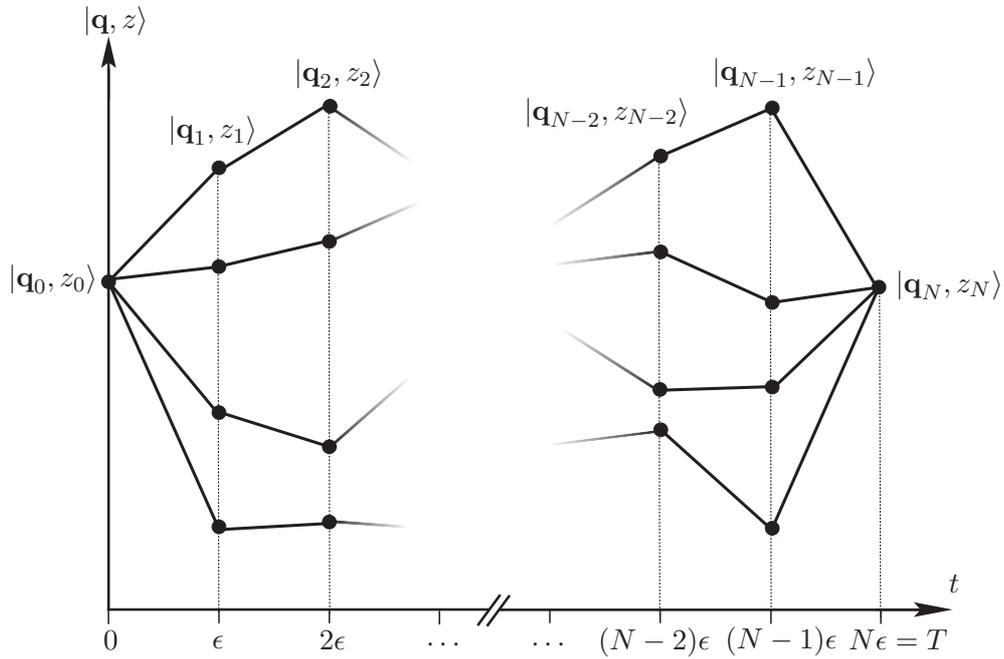


Figure 3.2: Some of the paths that go from $|\mathbf{q}_0, z_0\rangle$ to $|\mathbf{q}_N, z_N\rangle$, via the states $|\mathbf{q}_j, z_j\rangle$, $0 < j < N$. As in the case of fig. 3.1, the integration in eq. (3.5) can be interpreted as the thin dotted lines, symbolizing that $|\mathbf{q}_1, z_1\rangle, |\mathbf{q}_2, z_2\rangle \dots$ can be any state between the end states.

This chapter started with a very short introduction to the path integral formalism. It is by no means a thorough discussion, such discussions is given in Feynmans book [16] and Schulmans application oriented book [13]. The introduction, however, motivated us to investigate how we could cut the time-evolution operator into a large number of small pieces, without choosing a specific path along which the time-evolution operator translates. The result is given in eq.(3.7), and figure 3.2 gives an illustration of how we might interpret eq. (3.7). The next logical question to ask ourselves is; how *does* a kernel as the ones in eq. (3.6) look for a spin-orbit coupled electron in a magnetic field? This is not a trivial problem to solve, and is the theme of the next chapter.

Chapter 4

Evaluating kernels

Calculating a kernel is mathematically equivalent to finding the matrix element of the time-evolution operator in the basis of $|\mathbf{q}, z\rangle$. Physically, it means finding an explicit form of how some state $|\mathbf{q}_{j-1}, z_{j-1}\rangle$ has changed into a new state $|\mathbf{q}_j, z_j\rangle$ in a timespan ϵ , according to the time-evolution operator $U(\epsilon)$. Finding one such kernel is by no means trivial, and requires a lot of algebra. Thus, for the sake of clarity, this chapter is split into five sections. The first section introduce the problem mathematically, the next two deal with evaluating the part of the kernel independent of the spin operator $\boldsymbol{\sigma}$, the fourth deal with the spin-dependent elements and finally all these terms will be combined in the last section.

4.1 General remarks on the evaluation of kernels

Recalling the definition of the kernels eq.(3.6) the goal for this chapter is to evaluate terms of the form

$$K(\mathbf{q}_j, z_j, j\epsilon; \mathbf{q}_{j-1}, z_{j-1}, (j-1)\epsilon) = \langle \mathbf{q}_j | \langle z_j | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle. \quad (4.1)$$

where the Hamiltonian is given by eq.(2.7) in chapter 2, and can be written as

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{SO}} \quad (4.2)$$

where

$$\mathcal{H}_0 = \frac{(\hat{\mathbf{p}} - q_e \mathbf{A})^2}{2m} + V(\hat{\mathbf{p}}) \quad , \quad \mathcal{H}_{\text{SO}} = \alpha(\hat{\mathbf{p}} \times \mathbf{E}) \cdot \boldsymbol{\sigma} - g\mu_b \mathbf{B} \cdot \boldsymbol{\sigma}.$$

Thus, eq. (4.1) can be written as

$$K(\mathbf{q}_j, z_j, j\epsilon; \mathbf{q}_{j-1}, z_{j-1}, (j-1)\epsilon) = \langle \mathbf{q}_j | \langle z_j | e^{-\frac{i}{\hbar} (\mathcal{H}_0 + \mathcal{H}_{\text{SO}}) \epsilon} | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle. \quad (4.3)$$

We wish to expand the exponential function in (4.3), using that $\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$. Using this expansion to first order in ϵ yields

$$\begin{aligned} \langle \mathbf{q}_j | \langle z_j | e^{-\frac{i}{\hbar} \mathcal{H} \epsilon} | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle &\approx \langle \mathbf{q}_j | \langle z_j | 1 - \frac{i}{\hbar} \mathcal{H}_0 \epsilon - \frac{i}{\hbar} \mathcal{H}_{\text{SO}} \epsilon + \mathcal{O}(\epsilon^2) | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle \\ &= \langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle \langle z_j | z_{j-1} \rangle - \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle - \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_{\text{SO}} \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle + \mathcal{O}(\epsilon^2). \end{aligned} \quad (4.4)$$

In equating $\langle \mathbf{q}_j | \langle z_j | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle$ with $\langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle \langle z_j | z_{j-1} \rangle$ the previously discussed linear independence of the subspaces of \mathcal{H} was used. This subtle, but very important property, will be used several times throughout this chapter.

The rest of this chapter will be devoted to calculating an explicit form of three terms in eq. (4.4). They will be calculated individually in sections 4.1.1, 4.1.2 and 4.1.3 respectively. Finally, in section 4.2, the result of our labors will be combined into the final explicit form of one kernel.

4.1.1 Evaluating the inner products

In eq.(4.4) consider first $\langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle$. We know that these states are orthonormal, so that $\langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle = \delta^3(\mathbf{q}_j - \mathbf{q}_{j-1})$. However, it will prove useful to use another representation of the δ -function, which can be found by inserting an identity operator of momentum eigenstates and recalling the momentum representation of position eigenfunctions (table 2.1),

$$\begin{aligned} \langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle &= \langle \mathbf{q}_j | \int_{-\infty}^{\infty} d^3 \mathbf{p}_j | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle \\ &= \int_{-\infty}^{\infty} \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp(i\mathbf{q}_j \cdot \mathbf{p}_j / \hbar) \exp(-i\mathbf{q}_{j-1} \cdot \mathbf{p}_j / \hbar) \\ &= \int_{-\infty}^{\infty} \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar) = \delta^3(\mathbf{q}_j - \mathbf{q}_{j-1}). \end{aligned} \quad (4.5)$$

This is the form of the δ -function which will prove most useful.

The next step is to evaluate $\langle z_j | z_{j-1} \rangle$. We start out by using the expansion of $|z_j\rangle$,

$$|z_j\rangle = \mathcal{N}(z_j) \exp(z_j \sigma^+) |\downarrow\rangle = \mathcal{N}(z_j) (1 + z_j \sigma^+) |\downarrow\rangle = \mathcal{N}(z_j) (|\downarrow\rangle + z_j |\uparrow\rangle),$$

and equivalently

$$\langle z_{j-1}| = \mathcal{N}(z_{j-1})^* \langle \downarrow| (1 + z_{j-1}^* \sigma^-) = \mathcal{N}(z_{j-1}) (\langle \downarrow| + z_{j-1}^* \langle \uparrow|).$$

The complex conjugate on the normalizing factor have been dropped, since $\mathcal{N}(z) \rightarrow \mathcal{N}(|z|^2)$. The overlap $\langle z_j | z_{j-1} \rangle$ can be found, exploiting that $|\downarrow\rangle$ and $|\uparrow\rangle$ are orthonormal

$$\begin{aligned} \langle z_j | z_{j-1} \rangle &= \mathcal{N}(z_{j-1}) (\langle \downarrow| + z_{j-1}^* \langle \uparrow|) \mathcal{N}(z_j) (|\downarrow\rangle + z_j |\uparrow\rangle) \\ &= \frac{1}{\sqrt{1 + |z_{j-1}|^2}} \frac{1}{\sqrt{1 + |z_j|^2}} (1 + z_{j-1}^* z_j). \end{aligned} \quad (4.6)$$

This next part of the derivation requires a lot of expansions, and have therefore been relegated to appendix D. The result is, that the inner product $\langle z_j | z_{j-1} \rangle$ can be expressed as

$$\langle z_j | z_{j-1} \rangle = 1 + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} i\epsilon, \quad (4.7)$$

where $\dot{u}_j = \frac{u_j - u_{j-1}}{\epsilon}$ and terms of higher-than first order in ϵ have been dropped.

Combining eq.(4.5) and eq.(4.7) allows us to write

$$\langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle \langle z_j | z_{j-1} \rangle = \int_{-\infty}^{\infty} \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}/\hbar)) \left(1 + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} i\epsilon \right) \quad (4.8)$$

This is the form of the inner products that will be used, when all the terms in eq.(4.4) are combined.

4.1.2 Evaluating terms independent of spin

Now that the inner products have been calculated, we move on to find the evolution of terms involving operators in eq.(4.4). This section will deal with the terms in the Hamiltonian independent of spin, namely

$$\mathcal{H}_0 = \frac{(\hat{\mathbf{p}} - q_e \mathbf{A})^2}{2m} + V(\hat{\mathbf{q}}).$$

Before calculating the elements $\langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle$ in eq.(4.4), some notation will be introduced. Set

$$\hat{\boldsymbol{\rho}} = \begin{pmatrix} \hat{\rho}_x \\ \hat{\rho}_y \\ \hat{\rho}_z \end{pmatrix} = \begin{pmatrix} \hat{p}_x + q_e A_x \\ \hat{p}_y + q_e A_y \\ \hat{p}_z + q_e A_z \end{pmatrix}, \quad (4.9)$$

so that the Hamiltonian can be written as

$$\mathcal{H}_0 = \frac{\hat{\boldsymbol{\rho}}^2}{2m} + V(\hat{\mathbf{q}}).$$

It can quickly be shown that the $|\mathbf{p}\rangle$ -states are also eigenfunctions of $\hat{\boldsymbol{\rho}}$, and thus also $\hat{\boldsymbol{\rho}}^2$,

$$\begin{aligned} \hat{\boldsymbol{\rho}} |\mathbf{p}\rangle &= \begin{pmatrix} \hat{p}_x + q_e A_x \\ \hat{p}_y + q_e A_y \\ \hat{p}_z + q_e A_z \end{pmatrix} |\mathbf{p}\rangle = \begin{pmatrix} \hat{p}_x |\mathbf{p}\rangle + q_e A_x |\mathbf{p}\rangle \\ \hat{p}_y |\mathbf{p}\rangle + q_e A_y |\mathbf{p}\rangle \\ \hat{p}_z |\mathbf{p}\rangle + q_e A_z |\mathbf{p}\rangle \end{pmatrix} = \begin{pmatrix} p_x |\mathbf{p}\rangle + q_e A_x |\mathbf{p}\rangle \\ p_y |\mathbf{p}\rangle + q_e A_y |\mathbf{p}\rangle \\ p_z |\mathbf{p}\rangle + q_e A_z |\mathbf{p}\rangle \end{pmatrix} \\ &= \begin{pmatrix} p_x + q_e A_x \\ p_y + q_e A_y \\ p_z + q_e A_z \end{pmatrix} |\mathbf{p}\rangle = \boldsymbol{\rho} |\mathbf{p}\rangle, \end{aligned} \quad (4.10)$$

where $\boldsymbol{\rho}$ is a vector with scalar entries. In this notation,

$$\begin{aligned} \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle &= \frac{i}{\hbar} \epsilon \langle \mathbf{q}_j | \langle z_j | \left(\frac{\hat{\boldsymbol{\rho}}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle \\ &= \frac{i}{\hbar} \epsilon \langle z_j | z_{j-1} \rangle \langle \mathbf{q}_j | \left(\frac{\hat{\boldsymbol{\rho}}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{q}_{j-1} \rangle. \end{aligned} \quad (4.11)$$

From eq. (4.7) we know what the term $\langle z_j | z_{j-1} \rangle$ will contribute with. The second term can be evaluated by inserting a complete set of momentum eigenstates, and exploiting the result of (4.10), that $|\mathbf{p}\rangle$ is also an eigenstate of $\hat{\rho}$, and hence also an eigenstate of $\hat{\rho}^2$

$$\langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{q}_{j-1} \rangle = \langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) \int d^3 \mathbf{p}_j | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle \quad (4.12)$$

$$= \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}_j \cdot \mathbf{q}_{j-1}/\hbar) \langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{p}_j \rangle \quad (4.13)$$

The term involving the operators $\hat{\rho}$ and $V(\hat{\mathbf{q}})$ can be evaluated by noting that $\hat{\rho}|\mathbf{p}_j\rangle = \boldsymbol{\rho}_j|\mathbf{p}_j\rangle$ and $\langle \mathbf{q}_j | V(\hat{\mathbf{q}}) = (V(\hat{\mathbf{q}})|\mathbf{q}_j)\dagger$, an equality that is justified because $V(\hat{\mathbf{q}})$ is a hermitian operator. Exploiting that $|\mathbf{q}_j\rangle$ is an eigenstate of $\hat{\mathbf{q}}$ with eigenvalue \mathbf{q}_j gives

$$\langle \mathbf{q}_j | V(\hat{\mathbf{q}}) = (V(\hat{\mathbf{q}})|\mathbf{q}_j)\dagger = (V(\mathbf{q}_j)|\mathbf{q}_j)\dagger = \langle \mathbf{q}_j | V(\mathbf{q}_j), \quad \text{where } \mathbf{q}_j = (q_{j,x}, q_{j,y}, q_{j,z}).$$

Equation (4.13) can thus be rewritten as

$$\begin{aligned} & \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}_j \cdot \mathbf{q}_{j-1}/\hbar) \langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{p}_j \rangle = \\ & \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3/2} \exp(-i\mathbf{p}_j \cdot \mathbf{q}_{j-1}/\hbar) \langle \mathbf{q}_j | \mathbf{p}_j \rangle \left(\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}_j) \right) = \\ & \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar) \left(\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}_j) \right). \end{aligned} \quad (4.14)$$

At this point, we could be tempted to say that this is the correct form of the spin-independent term (sans the inner product $\langle z_j | z_{j-1} \rangle$). But in eq. (4.12) we introduced an ambiguity – the complete set of momentum eigenstates were inserted to the *right* of \mathcal{H}_0 . Had we instead inserted the complete set to the *left* of the \mathcal{H}_0 , it would have yielded $\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}_{j-1})$ instead of $\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}_j)$. This ambiguity can be resolved by introducing the variable $\mathbf{q}'_j = \frac{1}{2}(\mathbf{q}_j + \mathbf{q}_{j-1})$, so that eq. (4.14) can be written as

$$\langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{q}_{j-1} \rangle = \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar) \left(\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}'_j) \right). \quad (4.15)$$

Plugging equations (4.7) and (4.15) into (4.11) yields

$$\begin{aligned} & \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle = \frac{i}{\hbar} \epsilon \langle z_j | z_{j-1} \rangle \langle \mathbf{q}_j | \left(\frac{\hat{\rho}^2}{2m} + V(\hat{\mathbf{q}}) \right) | \mathbf{q}_{j-1} \rangle = \\ & \frac{i}{\hbar} \epsilon \left(1 + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} i \epsilon \right) \int d^3 \mathbf{p}_j (2\pi\hbar)^{-3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar) \left(\frac{\boldsymbol{\rho}_j^2}{2m} + V(\mathbf{q}'_j) \right). \end{aligned}$$

But, the expansion is only to first order in ϵ , so higher order terms should be dropped. Doing so, and recalling the definition of $\boldsymbol{\rho}$ (eq. (4.9)) yields the final result of this section

$$\boxed{\langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle = \frac{i}{\hbar} \epsilon \int d^3 \mathbf{p}_j \frac{1}{(2\pi\hbar)^3} e^{(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar)} \left(\frac{(\mathbf{p}_j - q_e \mathbf{A})^2}{2m} + V(\mathbf{q}'_j) \right)} \quad (4.16)$$

4.1.3 Evaluating terms dependent of spin

The goal is now to find the terms dependent of spin. Recall that the spin-orbit part of the Hamiltonian, \mathcal{H}_{SO} , is given by

$$\mathcal{H}_{\text{SO}} = \alpha(\hat{\mathbf{p}} \times \mathbf{E}) \cdot \boldsymbol{\sigma} - g\mu_b \mathbf{B} \cdot \boldsymbol{\sigma}. \quad (4.17)$$

Note here, that the electric and magnetic field are both independent of position, momentum and spin polarization. We will combine the two terms such that in the following, we look for matrix elements of the time-evolution operator with a Hamiltonian of the form

$$\mathcal{H}_{\text{SO}} = (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b \mathbf{B}) \cdot \boldsymbol{\sigma}.$$

Thus, according to eq.(4.4), we are looking for the elements

$$\begin{aligned} \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \epsilon \mathcal{H}_{\text{SO}} | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle &= \frac{i}{\hbar} \epsilon \langle \mathbf{q}_j | \langle z_j | (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b \mathbf{B}) \cdot \boldsymbol{\sigma} | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle \\ &= \frac{i}{\hbar} \epsilon \langle \mathbf{q}_j | (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b \mathbf{B}) | \mathbf{q}_{j-1} \rangle \cdot \langle z_j | \boldsymbol{\sigma} | z_{j-1} \rangle \end{aligned} \quad (4.18)$$

In the last step we once again exploited the linear independence of the $|\mathbf{q}\rangle$ and $|z\rangle$ -subspaces of \mathcal{H} . The evaluation of the term involving momentum eigenstates requires no other techniques than those applied in the previous section. The algebra is lengthy, and as a consequence, is relegated to appendix E. The result is, that

$$\langle \mathbf{q}_j | (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b \mathbf{B}) | \mathbf{q}_{j-1} \rangle = \boldsymbol{\Gamma}_j \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar), \quad (4.19)$$

where

$$\boldsymbol{\Gamma}_j = \begin{pmatrix} \alpha [p_{j,y} E_z - p_{j,z} E_y] - g\mu_b B_x \\ \alpha [p_{j,z} E_x - p_{j,x} E_z] - g\mu_b B_y \\ \alpha [p_{j,x} E_y - p_{j,y} E_x] - g\mu_b B_z \end{pmatrix}. \quad (4.20)$$

Returning to eq. (4.18) there is now only one term left, the one involving Pauli spin matrices,

$$\langle z_j | \boldsymbol{\sigma} | z_{j-1} \rangle. \quad (4.21)$$

The explicit form of the Pauli spin matrices is

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z) = \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right],$$

So calculating eq. (4.21) is just matrix and vector multiplication *en masse*. The x -part is

$$\begin{aligned}
 \langle z_j | \sigma_x | z_{j-1} \rangle &= \mathcal{N}(z_j)^* \mathcal{N}(z_{j-1}) (\langle \downarrow | + z_j^* \langle \uparrow |) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (\langle \downarrow | + z_{j-1} \langle \uparrow |) \\
 &= \mathcal{N}(z_j, z_{j-1}) [(0 \quad 1) + z_j^* (1 \quad 0)] \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \left[\begin{pmatrix} 0 \\ 1 \end{pmatrix} + z_{j-1} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right] \\
 &= \mathcal{N}(z_j, z_{j-1}) (z_j^* + z_{j-1}).
 \end{aligned}$$

Once again, the complex conjugation on the normalization factor have been dropped, and the two normalization factors have been combined into the composite factor $\mathcal{N}(z_j, z_{j-1})$. Analogous calculations for the y and z -parts yield

$$\begin{aligned}
 \langle z_j | \sigma_y | z_{j-1} \rangle &= \mathcal{N}(z_j, z_{j-1}) (-iz_j^* + iz_{j-1}) \\
 \langle z_j | \sigma_z | z_{j-1} \rangle &= \mathcal{N}(z_j, z_{j-1}) (-1 + z_j^* z_{j-1}).
 \end{aligned}$$

And thus

$$\langle z_j | \boldsymbol{\sigma} | z_{j-1} \rangle = \mathcal{N}(z_j, z_{j-1}) \begin{pmatrix} z_j^* + z_{j-1} \\ -iz_j^* + iz_{j-1} \\ -1 + z_j^* z_{j-1} \end{pmatrix} = \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}), \quad (4.22)$$

where the vector \mathbf{Z} have been introduced. Combining (4.19) and (4.22) with eq. (4.18), we arrive at

$$\boxed{\begin{aligned} & \frac{i}{\hbar} \epsilon \langle \mathbf{q}_j | (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b \mathbf{B}) | \mathbf{q}_{j-1} \rangle \cdot \langle z_j | \boldsymbol{\sigma} | z_{j-1} \rangle = \\ & \frac{i}{\hbar} \epsilon \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar} \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) \cdot \boldsymbol{\Gamma}_j \end{aligned}} \quad (4.23)$$

4.2 Combination of terms

In sections 4.1.1, 4.1.2 and 4.1.3 the three terms in eq. (4.4) were calculated. Plugging equations (4.8), (4.16) and (4.23) into (4.4) gives

$$\begin{aligned}
 & \langle \mathbf{q}_j | \mathbf{q}_{j-1} \rangle \langle z_j | z_{j-1} \rangle - \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_0 \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle - \langle \mathbf{q}_j | \langle z_j | \frac{i}{\hbar} \mathcal{H}_{\text{SO}} \epsilon | \mathbf{q}_{j-1} \rangle | z_{j-1} \rangle + \mathcal{O}(\epsilon^2) \\
 &= \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar} \left(1 + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} i\epsilon \right) - \frac{i}{\hbar} \epsilon \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar} \cdot \\
 & \left(\frac{(\mathbf{p}_j - q_e \mathbf{A})^2}{2m} + V(\mathbf{q}'_j) \right) - \frac{i}{\hbar} \epsilon \int \frac{d^3 \mathbf{p}_j}{2\pi\hbar} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar} \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) \cdot \boldsymbol{\Gamma}_j + \mathcal{O}(\epsilon^2) \\
 &= \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1}) / \hbar)} \left[1 + \left(\frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \frac{(\mathbf{p}_j - q_e \mathbf{A})^2}{2m} - V(\mathbf{q}'_j) \right. \right. \\
 & \quad \left. \left. - \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) \cdot \boldsymbol{\Gamma}_j \right) \frac{i}{\hbar} \epsilon + \mathcal{O}(\epsilon^2) \right]. \quad (4.24)
 \end{aligned}$$

For the sake of clarity, we re-introduce the notation of the Hamiltonian, but now its a number, and not an operator, such that

$$\mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) = \frac{(\mathbf{p}_j - q_e \mathbf{A})^2}{2m} + V(\mathbf{q}'_j) + \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) \cdot \mathbf{\Gamma}_j.$$

Introducing this notation into eq. (4.24) and recasting the term in brackets back into exponential form yields

$$\begin{aligned} & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar)} \left[1 + \left(\frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon + \mathcal{O}(\epsilon^2) \right] \approx \\ & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} e^{(i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar)} \exp \left[\left(\frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2)) = \\ & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp \left[\left(\frac{\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})}{\epsilon} + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2)) = \\ & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp \left[\left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2)), \end{aligned} \quad (4.25)$$

where $\dot{\mathbf{q}}_j = \frac{\mathbf{q}_j - \mathbf{q}_{j-1}}{\epsilon}$.

We have reached the goal for this chapter, which is the evaluation of a kernel in the "sum over paths"-equation (3.7). This chapter started by expanding the exponential function that appears in one kernel, and calculating the three resulting terms in sections 4.1.1, 4.1.2 and 4.1.3. In section 4.2 the three terms were combined, and it was shown that one kernel in eq. (3.7) is given as

$$\boxed{K(\mathbf{q}_j, z_j, j\epsilon; \mathbf{q}_{j-1}, z_{j-1}, (j-1)\epsilon) = \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp \left[\left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2))} \quad (4.26)$$

Now the we have found an explicit form of *one* kernel for our spin-orbit coupled electron, the theme for the next chapter will be, in accordance with eq. (3.7) to combine N such terms, and finally taking the contiuum limit $N \rightarrow \infty$. This will finally give the path integral for a spin-orbit coupled particle.

Chapter 5

A complete path integral for the spin-orbit interaction

We are now in a position to calculate what we set out to, back in chapter 3 – finding the sum over all paths in eq. (3.7). Chapter 4 showed what *one* kernel contributes with in eq. (4.25), and thus, according to eq. (3.7) this chapter will deal with combining N such terms. Since we are physically interested in being able to describe *any* path from state $|\mathbf{q}_0, z_0\rangle$ to state $|\mathbf{q}_N, z_N\rangle$, and not just a discrete, the continuum limit $N \rightarrow \infty$ will be calculated. Finally, some facets of the semi-classical approach to solving path integrals for spin-dependent systems will be discussed.

5.1 The amplitude

Recall the definition of the amplitude eq. (3.7)

$$A = \sum_{\text{all paths}} A_{\text{path}}.$$

For the sake of clarity, we start by calculating just two terms in $A_{\text{all paths}}$, eq. (3.6),

$$\begin{aligned} & K(\mathbf{q}_j, z_j, j\epsilon; \mathbf{q}_{j-1}, z_{j-1}, (j-1)\epsilon) \cdot K(\mathbf{q}_{j-1}, z_{j-1}, (j-1)\epsilon; \mathbf{q}_{j-2}, z_{j-2}, (j-2)\epsilon) \\ = & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp \left[\left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2)) \cdot \int \frac{d^3 \mathbf{p}_{j-1}}{(2\pi\hbar)^3} \\ & \exp \left[\left(\mathbf{p}_{j-1} \dot{\mathbf{q}}_{j-1} + \frac{v_{j-1} \dot{u}_{j-1} - \dot{v}_{j-1} u_{j-1}}{1 + |z_{j-1}|^2} \hbar - \mathcal{H}(\mathbf{q}_{j-1}, \mathbf{p}_{j-1}, z_{j-1}) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2)) \\ = & \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \int \frac{d^3 \mathbf{p}_{j-1}}{(2\pi\hbar)^3} \exp \left[\left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) + \right. \right. \\ & \left. \left. \mathbf{p}_{j-1} \dot{\mathbf{q}}_{j-1} + \frac{v_{j-1} \dot{u}_{j-1} - \dot{v}_{j-1} u_{j-1}}{1 + |z_{j-1}|^2} \hbar - \mathcal{H}(\mathbf{q}_{j-1}, \mathbf{p}_{j-1}, z_{j-1}) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2))^2 \end{aligned}$$

$$= \prod_{k=j-1}^j \int \frac{d^3 \mathbf{p}_k}{(2\pi\hbar)^3} \exp \left[\sum_{k=j-1}^j \left(\mathbf{p}_k \dot{\mathbf{q}}_k + \frac{v_k \dot{u}_k - \dot{v}_k u_k}{1 + |z_k|^2} \hbar - \mathcal{H}(\mathbf{q}_k, \mathbf{p}_k, z_k) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2))^2.$$

Generalizing this result to all the N terms in A_{path} thus gives

$$\prod_{j=0}^{N-1} \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \exp \left[\sum_{j=0}^{N-1} \left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2))^N. \quad (5.1)$$

We introduce the product of integrals in the above equation into $\sum_{\text{all paths}}$ such that

$$\begin{aligned} \sum_{\text{all paths}} &= \prod_{j=1}^{N-1} \int d^3 \mathbf{q}_j \prod_{j=1}^{N-1} \int d\mu(z_j) \prod_{j=0}^{N-1} \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \\ A_{\text{path}} &= \exp \left[\sum_{j=0}^{N-1} \left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right]. \end{aligned}$$

Note in this equation that there are only position- and spinintegrals for intermediate position ($N - 1$ total), whereas there are momentum integrals for each interval (N total). We have thus arrived at the final form of the amplitude for a particle to go in *discrete* steps from state $|\mathbf{q}_0, z_0\rangle$ to state $|\mathbf{q}_N, z_N\rangle$ via *any* position and spin state in between, namely

$$\begin{aligned} A &= \sum_{\text{all paths}} A_{\text{path}} = \prod_{j=1}^{N-1} \int d^3 \mathbf{q}_j \prod_{j=1}^{N-1} \int d\mu(z_j) \prod_{j=0}^{N-1} \int \frac{d^3 \mathbf{p}_j}{(2\pi\hbar)^3} \\ &\exp \left[\sum_{j=0}^{N-1} \left(\mathbf{p}_j \dot{\mathbf{q}}_j + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} \hbar - \mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j) \right) \frac{i}{\hbar} \epsilon \right] (1 + \mathcal{O}(\epsilon^2))^N. \quad (5.2) \end{aligned}$$

5.1.1 Continuum limit

Real physical particles do not change in discrete steps from one state to another, they change continuously. As a consequence, we investigate the continuum limit. This limit can be approached by cutting $U(T, 0)$ into infinitely many small segments and mathematically, this is equivalent to taking the limit as $N \rightarrow \infty$ in (5.2).

In this limit the summation in (5.2) turns, despite a few mathematical details, into a Riemann integral over the continuous parameter t with the limiting values $0 < t < T$, and the discrete points $\mathbf{q}_j, \mathbf{p}_j$ are replaced by functions over t , in the sense that $\mathbf{q}_j \rightarrow \mathbf{q}(t)$, $\mathbf{p}_j \rightarrow \mathbf{p}(t)$, i.e.

$$\lim_{N \rightarrow \infty} \sum_{j=0}^{N-1} \mathbf{p}_j \dot{\mathbf{q}}_j \sim \int_0^T \mathbf{p}(t) \dot{\mathbf{q}}(t) dt.$$

If we once again (recall the discussion in appendix D) make the assumption that as $N \rightarrow \infty$ then $z_{j-1} \rightarrow z_j$, and replace the discrete indices with functions of t , the vector $\mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1})$

in $\mathcal{H}(\mathbf{q}_j, \mathbf{p}_j, z_j)$ reduces to

$$\lim_{N \rightarrow \infty} \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) = \lim_{z_{j-1} \rightarrow z_j} \mathcal{N}(z_j, z_{j-1}) \mathbf{Z}(z_j, z_{j-1}) = \frac{1}{1 + |z(t)|^2} \begin{pmatrix} 2u(t) \\ -2v(t) \\ -1 + |z(t)|^2 \end{pmatrix}.$$

The error term $(1 + \mathcal{O}(\epsilon^2))^N$ will tend to unity, since $\epsilon \rightarrow 0$ as $N \rightarrow \infty$. Thus, the continuous form of eq. (5.2) is

$$\begin{aligned} \lim_{N \rightarrow \infty} A &= \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} \int d^3 \mathbf{q}(t_j) \prod_{j=1}^{N-1} \int d\mu(z(t_j)) \prod_{j=0}^{N-1} \int \frac{d^3 \mathbf{p}(t_j)}{(2\pi\hbar)^3} \\ &\exp \left[\frac{i}{\hbar} \int_0^T dt \left(\mathbf{p}(t) \dot{\mathbf{q}}(t) + \frac{v(t)\dot{u}(t) - \dot{v}(t)u(t)}{1 + |z(t)|^2} \hbar - \mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), z(t)) \right) \right] \end{aligned} \quad (5.3)$$

where

$$\mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), z(t)) = \frac{(\mathbf{p}(t) - q_e \mathbf{A})^2}{2m} + V(\mathbf{q}'(t)) + \frac{1}{1 + |z(t)|^2} \begin{pmatrix} 2u(t) \\ -2v(t) \\ -1 + |z(t)|^2 \end{pmatrix} \cdot \mathbf{\Gamma}(t), \quad (5.4)$$

and the vector $\mathbf{\Gamma}(t)$ is given by

$$\mathbf{\Gamma}(t) = \begin{pmatrix} \alpha [p_y(t) E_z - p_z(t) E_y] - g\mu_b B_x \\ \alpha [p_z(t) E_x - p_x(t) E_z] - g\mu_b B_y \\ \alpha [p_x(t) E_y - p_y(t) E_x] - g\mu_b B_z \end{pmatrix}.$$

It is customary to introduce a special notation in this context. Let

$$\mathcal{D}[\mathbf{q}] \mathcal{D}[\mathbf{p}] \mathcal{D}\mu[z] = \lim_{N \rightarrow \infty} \prod_{j=1}^{N-1} d^3 \mathbf{q}(t_j) \prod_{j=1}^{N-1} d\mu(z(t_j)) \prod_{j=0}^{N-1} \frac{d^3 \mathbf{p}(t_j)}{(2\pi\hbar)^3}, \quad (5.5)$$

so that eq. (5.3) can be written as

$$\boxed{\lim_{N \rightarrow \infty} A = \int \mathcal{D}[\mathbf{q}] \int \mathcal{D}[\mathbf{p}] \int \mathcal{D}\mu[z] \exp \left(\frac{i}{\hbar} \mathcal{S}(\mathbf{p}, \mathbf{q}, z, t) \right)} \quad (5.6)$$

where

$$\mathcal{S}(\mathbf{p}, \mathbf{q}, z, t) = \int_0^T dt \left(\mathbf{p}(t) \dot{\mathbf{q}}(t) + \frac{v(t)\dot{u}(t) - \dot{v}(t)u(t)}{1 + |z(t)|^2} \hbar - \mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), z(t)) \right),$$

and $\mathcal{H}(\mathbf{q}(t), \mathbf{p}(t), z(t))$ is given by eq. (5.4). Equations (5.6), (5.5) and (5.4) is *the path integral for a Rashba spin-orbit coupled particle*. It is a summation (integration) over all the possible states connecting $|\mathbf{q}_0, z_0\rangle$ and $|\mathbf{q}_N, z_N\rangle$ in the 6 + 2-dimensional extended phasespace \mathcal{H} . It is important to emphasize that eq. (5.6) is just a shorthand notation for the more

ominous eq. (5.3), in all practical manners, we are forced to use eq. (5.3). We have so far not dealt with normalizability of these functionals, and at the outset eq. (5.6) does not look nearly normalizable - each of the N integrals are not even convergent. Some methods exist for ensuring an *ad hoc* convergence of the \mathbf{q} and \mathbf{p} integrals, but for hamiltonians of our type, this method is not sufficient¹. Despite this grave difficulty, there exists a course of action, that allows us to approach eq. (5.6), the semi-classical approximation.

5.2 The semi-classical approximation

For the sake of argument, we only investigate the semi-classical approximation for the spin-dependent part of eq. (5.6), so that the integral in eq. (5.6) reduces to

$$\lim_{N \rightarrow \infty} \int \mathcal{D}\mu[z] \exp\left(\frac{i}{\hbar} \mathcal{S}(u(t), v(t))\right), \quad (5.7)$$

where

$$\mathcal{S}(u(t), v(t)) = \int_0^T dt \left(\frac{v(t)\dot{u}(t) - \dot{v}(t)u(t)}{1 + |z(t)|^2} \hbar - \mathcal{H}(z(t)) \right).$$

The explicit time-dependence is for notational convenience dropped, and we note that $\mathcal{S}(u, v)$ can be recast in terms of z and z^* ,

$$z^* \dot{z} - z \dot{z}^* = 2i(\dot{v}u - v\dot{u}) \Leftrightarrow v\dot{u} - \dot{v}u = \frac{i}{2}(z^* \dot{z} - z \dot{z}^*),$$

so that eq. (5.7) can be written as

$$\lim_{N \rightarrow \infty} \int \mathcal{D}\mu[z] \exp\left(\frac{i}{\hbar} \int_0^T dt \left[\frac{i}{2} \frac{(z^* \dot{z} - z \dot{z}^*)}{1 + |z|^2} \hbar - \mathcal{H}(z, z^*) \right]\right) = \lim_{N \rightarrow \infty} \int \mathcal{D}\mu[z] \exp\left(\frac{i}{\hbar} \mathcal{S}(z, z^*)\right). \quad (5.8)$$

Paths that make $\exp(\frac{i}{\hbar} \mathcal{S}(z, z^*))$ oscillate quickly will tend to cancel, and therefore the dominant contribution to the path integral in eq. (5.8) will come from paths that do not make the exponential function fluctuate too quickly. Mathematically, this path is the one that makes the action functional $\mathcal{S}(z, z^*)$ stationary, and physically, it is the classical path, that obeys Hamilton's principle $\delta\mathcal{S} = 0$. This gives us the two equations of motion

$$\frac{\partial \mathcal{S}}{\partial z^*} = 0 \quad \text{and} \quad \frac{\partial \mathcal{S}}{\partial z} = 0. \quad (5.9)$$

Before calculating these equations of motion, we assume periodic boundary conditions,

$$z(T+t) = z(t), \quad z^*(T+t) = z^*(t) \quad \text{and} \quad \dot{z}(T+t) = \dot{z}(t), \quad \dot{z}^*(T+t) = \dot{z}^*(t)$$

¹The *ad hoc* convergence can be achieved by inserting an exponentially damping factor $e^{-i\gamma\mathbf{q}(t)^2}$ or $e^{-i\gamma\mathbf{p}(t)^2}$, which turns our integrals into gaussians. Gaussian integrals can be solved analytically, and finally the limit $\gamma \rightarrow 0$ can be taken.

which allows us to move the derivative from \dot{z}^* to z in eq. (5.8), if we switch the sign, so that the action in (5.8) can be written as

$$\mathcal{S}(z, z^*) = \oint_0^T dt \left[i\hbar \frac{\dot{z}z^*}{1+|z|^2} - \mathcal{H}(z, z^*) \right]$$

Using this form of the action, the first equation of motion in eq. (5.9) can be calculated as

$$\begin{aligned} \frac{\partial \mathcal{S}}{\partial z^*} &= \frac{\partial}{\partial z} \left(\frac{i}{2} \frac{(z^* \dot{z} - z \dot{z}^*)}{1+|z|^2} \hbar - \mathcal{H}(z, z^*) \right) = \frac{\partial}{\partial z^*} \left(i \frac{\dot{z}z^*}{1+|z|^2} \hbar - \mathcal{H}(z, z^*) \right) = 0 \Leftrightarrow \\ i\hbar \left(\frac{\dot{z}}{1+|z|^2} - \frac{\dot{z}z^*}{(1+|z|^2)^2} z \right) + \frac{\partial \mathcal{H}(z, z^*)}{\partial z^*} &= i\hbar \left(\frac{(1+|z|^2) - |z|^2}{(1+|z|^2)^2} \right) \dot{z} - \frac{\partial \mathcal{H}(z, z^*)}{\partial z^*} = 0 \Leftrightarrow \\ \dot{z} &= \frac{(1+|z|^2)^2}{i\hbar} \frac{\partial \mathcal{H}(z, z^*)}{\partial z^*}. \end{aligned} \quad (5.10)$$

Parallel calculations for z yields

$$\dot{z}^* = - \frac{(1+|z|^2)^2}{i\hbar} \frac{\partial \mathcal{H}(z, z^*)}{\partial z} \quad (5.11)$$

These are the equations of motion for z and z^* , which define the classical orbits. If we solve these in terms of z and z^* we find the classical paths, denoted by z_{cl} and z_{cl}^* respectively. So far, we have just treated this as a classical rotating sphere, where z and z^* can be recast into spherical coordinates using appendix B. However, if we introduce a new path, as the variation from the classical path

$$(\xi, \zeta) = (z - z_{cl}, z^* - z_{cl}^*),$$

we can rewrite the action as

$$\mathcal{S}(\zeta, \xi) = \mathcal{S}_{cl}(z_{cl}, z_{cl}^*) + \mathcal{S}^{(2)}(\xi, \zeta).$$

The second variation of the action $\mathcal{S}^{(2)}(\xi, \zeta)$ can be interpreted as the quantum fluctuations around the classical orbit. The second variation is thus the quantum mechanical contribution to the propability, since in a purely classical system all higher-order than zeroth order variations vanish. The explicit calculation of $\mathcal{S}^{(2)}(\xi, \zeta)$ is not trivial, but it is quadratic, and hence analytically solvable, see [20, 21]. Numerical calculations can be found in [12].

It should be noted however, that there are several severe difficulties with this approximation. If we only consider the classical action, equations (5.10) and (5.11) do not yield a correct description, in the sense that it does not agree with a full Hamiltonian treatment [22]. A further discussion of this discrepancy and a technique for circumventing it (Klauder's ϵ -prescription) can be found in [22]. However, if we include the second variation, these calculations provide satisfactory agreement with a Hamiltonian treatment [15].

Chapter 6

Conclusion

This thesis introduced the spin-orbit interaction, which arises as a relativistic consequence of the electric fields exerted by the nuclei on electrons. We moved on to a discussion of the basis states used to describe a Hamiltonian with spin-dependent elements, $|\mathbf{q}\rangle$ and $|z\rangle$, and the Hilbert-space \mathcal{H} spanned by the composition of $\mathcal{H}_{|\mathbf{q}\rangle}$ and $\mathcal{H}_{|z\rangle}$, followed. Once these prerequisites had been covered, we formally introduced the path integral formulation of quantum mechanics. The treatment of the path integral formalism urged us to investigate what happens, if the time-evolution operator from Hamiltonian-based quantum mechanics, is "cut" into a large number N smaller parts. It turned out, that we could interpret the result of such a time-cutting as a sum over all the paths, in the Hilbert space of position and spin states $|\mathbf{q}, z\rangle$, connecting the initial and final state, denoted by $|\mathbf{q}_0, z_0\rangle$ and $|\mathbf{q}_N, z_N\rangle$. Instead of trying to compute the full propagation, the problem could thus be reduced to finding *one* of the N propagators. The detailed calculation proved labourous, and the inclusion of spin in the problem, had several important consequences for these calculations. However, a closed form of one kernel was found, and according to the introduction to path integral formalism, N such terms were combined to obtain a discrete description of propagation from the initial to the final state. The result of taking the continuum limit $N \rightarrow \infty$ was found, which finally gave the *path integral formulation of a Rashba spin-orbit coupled particle*. The final formula is not easy to interpret, but the semi-classical approximation was introduced as a means to approach it.

6.1 Perspectives

After arriving at a path integral formulation of the spin-orbit interaction, and seeing eq. (5.6) one might be left with a feeling of "What now?". Returning to the notion of quantum computing introduced in chapter 2, we are in principle looking to control the spin of an electron. An example of such "control" could be the calculation of the time necessary to force a complete spin flip for an electron confined to a 0D well for a given magnetic field (the strength of which we control). Equation (5.6) does not look too inviting in treating this problem, and it is by no means the most approachable formula. As it turned out, (5.6) failed already at analytical solutions in the classical limit of a semiclassical approximation. A technique

known as Klauders ϵ -prescription exists, that in certain special cases, can provide satisfactory results, that work in the semiclassical limit. An interesting account of this technique with special applications to discrete and continuous forms of the path integral (equations (5.2) and (5.6)) can be found in [22]. However, the bottom line is, that in almost all practical manners application of eq. (5.6) requires numerical treatments. Such a numerical treatment can be found in [12], and these calculations, could prove to be superior to a numerical treatment of a full Hamiltonian description.

6.2 Omissions

Although this thesis have tried to provide an introduction to the spin-orbit interaction, the path integral formalism and a comprehensive examination of the steps needed to describe the spin-orbit interaction in this formalism, several facets of all three subjects have been left out. The spin-orbit interaction is very important when describing atomic spectra, and have several suprising physical consequences. A discussion of these can be found in [18, 23]. We only mentioned that the states $|z\rangle$ are somehow related to the SU(2)-group. It turns out, that $|z\rangle$ are SU(2) coherent states, which can be utilised in many ways, see [14]. One example, is that the measure $d\mu(z)$ arises naturally as a consequence of the link between $|z\rangle$ and SU(2)! Our discussion of the path integral only touched upon two of the many philosophical and physical consequences of the formalism. One fundamental question was not discussed "How are we to inerpret that a particle *takes all the paths, even the most unlikely, between the endpoints?*". It is a very relevant question, and the standard reference on these discussions is still Feynman's book [16]. Schulman's more modern approach [13], uses the formalism in some very interesting cases. Likewise, we only introduced the the semi-classical theory, and presented how one might continue with eq. (5.6), [24, 22, 15] and [21] discusses the semi-classical approximation in greater detail.

Appendix A

Calculation of energy from torque

From classical mechanics, it is known that the energy of a rotating rigid body can be found from its torque by

$$U = - \int_{\theta_0}^{\theta} d\theta \tau(\theta) \quad (\text{A.1})$$

where θ_0 is the angle at which we set the zero-point for the energy. Orienting our coordinate system such that $\mathbf{B} = (0, 0, B)$ and $\boldsymbol{\mu} = (0, \mu, 0)$, and changing to polar coordinates, gives a torque given by

$$\boldsymbol{\mu} \times \mathbf{B} = -\hat{\mathbf{x}}\mu B \sin \theta \cos \varphi$$

Without loss of generality, we set $\varphi = 0$. Plugging into eq. (A.1)

$$\begin{aligned} U &= - \int_{\theta_0}^{\theta} d\theta (-\mu B \sin \theta) \\ &= -(\cos \theta - \cos \theta_0) \mu B \\ &= \cos \theta \mu B = -\boldsymbol{\mu} \cdot \mathbf{B}. \end{aligned}$$

In the last equation it was exploited that θ_0 was defined as the zero-point energy, and therefore dropped. Finally re-introducing the effective magnetic field that the electron feels, gives the final result

$$\begin{aligned} U &= -\boldsymbol{\mu} \cdot \mathbf{B}_{\text{eff}} \\ &= -\left(\frac{ge}{2m_e}\right) \mathbf{S} \cdot \mathbf{B} + \left(\frac{ge}{2m_e^2 c^2}\right) \mathbf{S} \cdot (\mathbf{p} \times \mathbf{E}) \end{aligned}$$

Appendix B

Spin states in spherical coordinates

The $|z\rangle$ -states can also be represented in spherical coordinates. This has been avoided in the main body of the thesis, since it would only clutter notation. This appendix will show the relationship between the complex number $z = u + iv$ appearing in $|z\rangle$ and the polar coordinates φ, θ . First recall the definition of $|z\rangle$

$$|z\rangle = \mathcal{N}(z) (|\downarrow\rangle + z|\uparrow\rangle) = \frac{1}{\sqrt{1+|z|^2}} \begin{pmatrix} u + iv \\ 1 \end{pmatrix}. \quad (\text{B.1})$$

A generic 2-dimensional spin-state, can in spherical coordinates be written as

$$\chi(\theta, \varphi) = \begin{pmatrix} \cos \frac{\theta}{2} e^{i\varphi/2} \\ \sin \frac{\theta}{2} e^{-i\varphi/2} \end{pmatrix}. \quad (\text{B.2})$$

Two examples suffice to show that this equation gives the correct spinors in the x, y, z -directions. In accordance with the definition of spherical coordinates, the values $\theta = 0$ and $\varphi = 0$ should yield spin up in the z -direction, and the values $\theta = \frac{\pi}{2}$ and $\varphi = \pi$ should yield spin down in the x -direction

$$\chi(\theta = 0, \varphi = 0) = \begin{pmatrix} \cos \frac{0}{2} e^{i \cdot 0} \\ \sin \frac{0}{2} e^{-i \cdot 0} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi(\theta = \pi/2, \varphi = \pi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

which agrees with the literature [9]. Equating (B.1) and (B.2) and plugging in a physically irrelevant phase-factor yields

$$\frac{1}{\sqrt{1+|z|^2}} \begin{pmatrix} u + iv \\ 1 \end{pmatrix} = \begin{pmatrix} \cos \frac{\theta}{2} e^{i\varphi/2} \\ \sin \frac{\theta}{2} e^{-i\varphi/2} \end{pmatrix} \cdot e^{i\varphi/2} = \sin \theta/2 \begin{pmatrix} \frac{\cos \theta/2}{\sin \theta/2} e^{i\varphi} \\ 1 \end{pmatrix}.$$

This gives the two equations

$$u + iv = \cot \frac{\theta}{2} e^{i\varphi}. \quad (\text{B.3})$$

$$\frac{1}{\sqrt{1+|z|^2}} = \sin \frac{\theta}{2} \quad (\text{B.4})$$

With the aid of elementary trigonometry, equation (B.3) yields the two equations

$$\cot \frac{\theta}{2} = |z| \Leftrightarrow \theta = 2 \cdot \cot^{-1} \left(\sqrt{u^2 + v^2} \right), \quad (\text{B.5})$$

$$e^{i\varphi} = e^{i\text{Arg}(z)} \Leftrightarrow \varphi = \tan^{-1} \left(\frac{u}{v} \right). \quad (\text{B.6})$$

For consistency, we check that these two equations agree with eq. (B.4). Using the trigonometric identity

$$\sin \theta/2 = \frac{1}{\sqrt{1 + \cot \theta/2}}$$

and inserting eq. (B.5)

$$\sin \theta/2 = \frac{1}{\sqrt{1 + \cot \theta/2}} = \frac{1}{\sqrt{1 + |z|}}$$

we see the consistency with eq. (B.4). From these calculations, it is clear why the states $|z\rangle$ have been expressed in terms of (u, v) instead of (θ, φ)

Appendix C

Completeness of spin states

In this appendix we are interested in showing that

$$\int |z\rangle\langle z|d\mu(z) = \mathbf{I}_{2\times 2} \quad (\text{C.1})$$

using

$$\int d\mu(z) = \int \frac{2}{\pi} \frac{1}{(1+|z|^2)^2} d^2z = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{2}{\pi} \frac{1}{(1+|z|^2)^2} d(\text{Re}z)d(\text{Im}z).$$

The proof only requires algebra. Simply writing out what eq. (C.1) means, yields

$$\begin{aligned} \int |z\rangle\langle z|d\mu(z) &= \int |\mathcal{N}(z)|^2 (|\downarrow\rangle + z|\uparrow\rangle) (\langle\downarrow| + z^*\langle\uparrow|) d\mu(z) \\ &= \int \frac{1}{1+|z|^2} \begin{pmatrix} z & \\ & 1 \end{pmatrix} \begin{pmatrix} z^* & \\ & 1 \end{pmatrix} d\mu(z) \\ &= \int \frac{1}{1+|z|^2} \begin{pmatrix} |z|^2 & z \\ z^* & 1 \end{pmatrix} d\mu(z) \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{2}{\pi} \frac{1}{(1+|z|^2)^3} \begin{pmatrix} |z|^2 & z \\ z^* & 1 \end{pmatrix} d(\text{Re}z)d(\text{Im}z). \end{aligned}$$

The off-diagonal elements in the matrix are zero as a consequence of parity, since

$$\frac{2}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \underbrace{\frac{1}{(1+|z|^2)^3}}_{\text{even}} \underbrace{z}_{\text{odd}} d(\text{Re}z)d(\text{Im}z) = 0. \quad (\text{C.2})$$

Because z depends linearly on $\text{Re}z$ and $\text{Im}z$, an even-ness or odd-ness in z will result in an even-ness or odd-ness in $\text{Re}z$ and $\text{Im}z$, and hence the integrals will evaluate to zero. Naturally, this result also holds for z^* . The diagonal elements can be found by using polar coordinates,

$$\begin{aligned} \frac{2}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(1+|z|^2)^3} |z|^2 d(\text{Re}z)d(\text{Im}z) &= \frac{2}{\pi} \int_0^{2\pi} d\phi \int_0^{\infty} \frac{R^2}{(1+R^2)^3} \cdot R dR \\ \frac{2}{\pi} \cdot 2\pi \cdot \frac{1}{4} &= 1. \end{aligned} \quad (\text{C.3})$$

Where it has been used that $\int_0^\infty x^3/(1+x^2)^3 dx = 1/4$. Analogous calculations for the lower right term gives

$$\begin{aligned} \frac{2}{\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{(1+|z|^2)^3} d(\operatorname{Re}z)d(\operatorname{Im}z) &= \frac{2}{\pi} \int_0^{2\pi} d\phi \int_0^\infty \frac{1}{(1+R^2)^3} \cdot R dR \\ \frac{2}{\pi} \cdot 2\pi \cdot \frac{1}{4} &= 1. \end{aligned} \tag{C.4}$$

and the integral $\int_0^\infty 1/(1+x^2)^3 dx = 1/4$ was used. Combining the results of equations (C.2), (C.3) and (C.4) gives

$$\int |z\rangle\langle z| d\mu(z) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and thus, the completeness

$$\int |z\rangle\langle z| d\mu(z) = \mathbf{I}_{2 \times 2},$$

has been shown.

Appendix D

Expansion of spin states

In this appendix we are interested in calculating what the term $\langle z_j | z_{j-1} \rangle$ will contribute with, to the expansion of the Hamiltonian. We know from eq. (4.6) that the overlap between two states is

$$\langle z_j | z_{j-1} \rangle = \frac{1}{\sqrt{1 + |z_{j-1}|^2}} \frac{1}{\sqrt{1 + |z_j|^2}} (1 + z_{j-1}^* z_j). \quad (\text{D.1})$$

Now note, that the difference between to successive z 's can be expressed as

$$z_j - z_{j-1} \propto \Delta.$$

Using this, eq. (D.1) can be rewritten as

$$\frac{1}{\sqrt{1 + |z_j - \Delta|^2}} \frac{1}{\sqrt{1 + |z_j|^2}} (1 + (z_j - \Delta)^* z_j) = \frac{1 + (z_j - \Delta)^* z_j}{\sqrt{1 + |z_j - \Delta|^2} \sqrt{1 + |z_j|^2}}.$$

Using the approximation $(1 + x)^n \approx 1 + nx + \mathcal{O}(x^2)$, the above equation will, setting $\Delta = 0$ in denominator, to first order in Δ in the nominator give

$$\frac{1 + (z_j - \Delta)^* z_j}{\sqrt{1 + |z_j - \Delta|^2} \sqrt{1 + |z_j|^2}} \approx \frac{\Delta^* z_j}{1 + |z_j|^2}$$

Recasting the denominator, dropping higher-than first order terms, and setting $\Delta = 0$ in the nominator, yields to first order in Δ in the denominator

$$\begin{aligned} & \frac{1 + (z_j - \Delta)^* z_j}{\sqrt{1 + |z_j - \Delta|^2} \sqrt{1 + |z_j|^2}} = \frac{1 + |z_j|^2}{\sqrt{1 + |z_j|^2 + |\Delta|^2 + z_j \Delta^* + z_j^* \Delta} \sqrt{1 + |z_j|^2}} \\ &= \frac{1 + |z_j|^2}{\sqrt{\left(1 + \frac{z_j \Delta^* + z_j^* \Delta}{1 + |z_j|^2}\right) (1 + |z_j|^2)} \sqrt{1 + |z_j|^2}} = \frac{1}{\sqrt{\left(1 + \frac{z_j \Delta^* + z_j^* \Delta}{1 + |z_j|^2}\right)}} \\ &\approx \left(1 + \frac{z_j \Delta^* + z_j^* \Delta}{2(1 + |z_j|^2)}\right)^{-1} \approx 1 - \frac{z_j \Delta^* + z_j^* \Delta}{2(1 + |z_j|^2)}. \end{aligned}$$

Thus, the complete expansion is

$$\begin{aligned}
\frac{(1 + (z_j - \Delta)^* z_j)}{\sqrt{1 + |z_j - \Delta|^2} \sqrt{1 + |z_j|^2}} &\approx 1 - \frac{1}{2} \frac{z_j \Delta^* + z_j^* \Delta}{1 + |z_j|^2} + \frac{z_j \Delta^*}{1 + |z_j|^2} + \mathcal{O}(\Delta^2) \\
&= 1 + \frac{z_j \Delta^* - z_j^* \Delta}{2(1 + |z_j|^2)} + \mathcal{O}(\Delta^2).
\end{aligned} \tag{D.2}$$

Note here, that Δ , by assumption, is a very small number, because, physically, the size of Δ can be controlled by cutting the time-evolution operator into an appropriate amount of pieces by increasing or decreasing N . In the limit $N \rightarrow \infty$, our physical intuition would expect Δ to be an infinitesimal small number, since it represents a *very* small change of state, and thus allowing us to drop terms of order $\mathcal{O}(\Delta^2)$. However, mathematically this is not obvious - the $|z\rangle$ states are not orthogonal, so we have no mathematical justification, for saying that Δ goes continuously to zero as $N \rightarrow \infty$. This is a serious problem, and the only justification is, that in the end, this method gives the correct result, i.e. tangent with what Schrödingers formulation yields. This has been thoroughly discussed in the litterature, see [15]. With this complication *in mente*, we drop $\mathcal{O}(\Delta^2)$ and introduce the variable $\dot{z}_j = \frac{\Delta}{\epsilon} = \frac{z_j - z_{j-1}}{\epsilon}$, so that eq. (D.2) can be recast as

$$1 + \frac{z_j \epsilon \dot{z}_j^* - z_j^* \epsilon \dot{z}_j}{2(1 + |z_j|^2)}.$$

Recalling the definition of $z_j = u_j + iv_j$ the nominator can be rewritten as

$$1 + \frac{(2v_j \dot{u}_j - 2\dot{v}_j u_j) i \epsilon}{2(1 + |z_j|^2)} = 1 + \frac{v_j \dot{u}_j - \dot{v}_j u_j}{1 + |z_j|^2} i \epsilon, \tag{D.3}$$

which is the form used in the calculation of a single kernel in section 4.1.1.

Appendix E

Evaluation of terms involving momentum operators in spin-dependent Hamiltonian

The goal of this appendix is to evaluate the terms involving momentum eigenstates in eq. (4.18). First, some new notation will need introducing. Recall that $\mathcal{H}_{\text{SO}} = (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b\mathbf{B}) \cdot \boldsymbol{\sigma}$. Writing out the cross-product yields

$$\begin{aligned} (\alpha(\hat{\mathbf{p}} \times \mathbf{E}) - g\mu_b\mathbf{B}) &= (\alpha[\hat{p}_y E_z - \hat{p}_z E_y] - g\mu_b B_x) \hat{\mathbf{x}} + \\ &\quad (\alpha[\hat{p}_z E_x - \hat{p}_x E_z] - g\mu_b B_y) \hat{\mathbf{y}} + \\ &\quad (\alpha[\hat{p}_x E_y - \hat{p}_y E_x] - g\mu_b B_z) \hat{\mathbf{z}} \\ &\equiv (\hat{\Gamma}_x, \hat{\Gamma}_y, \hat{\Gamma}_z) = \hat{\mathbf{\Gamma}}. \end{aligned} \tag{E.1}$$

The vector $\hat{\mathbf{\Gamma}}$ has the three operator $\hat{\Gamma}_x, \hat{\Gamma}_y$ and $\hat{\Gamma}_z$ as its entries. Thus, the spin-dependent part of the hamiltonian can be written as

$$\mathcal{H}_{\text{SO}} = \hat{\mathbf{\Gamma}} \cdot \boldsymbol{\sigma}.$$

In this notation, this appendix aims at calculating

$$\langle \mathbf{q}_j | \hat{\mathbf{\Gamma}} | \mathbf{q}_{j-1} \rangle = \langle \mathbf{q}_j | (\hat{\Gamma}_x, \hat{\Gamma}_y, \hat{\Gamma}_z) | \mathbf{q}_{j-1} \rangle,$$

Only one term, $\hat{\Gamma}_x$, will be calculated in detail. The other two will follow from permutations of the indices. Recalling the explicit form of the $\hat{\Gamma}_x$ -operator, eq.(E.1), the problem has thus been reduced to finding

$$\langle \mathbf{q}_j | \hat{\Gamma}_x | \mathbf{q}_{j-1} \rangle = \langle \mathbf{q}_j | (\alpha[\hat{p}_y E_z - \hat{p}_z E_y] - g\mu_b B_x) | \mathbf{q}_{j-1} \rangle.$$

This is exactly, apart from some scalars, what we've already calculated in section 4.1.1, when the matrix elements of the time evolution operator for the spin-independent part of the hamiltonian were found. For this reason, it is natural to use the same recipe here, as in section

4.1.1. Insert complete momentum representation eigenstates and exploit that these are eigenfunctions of \hat{p}_y and \hat{p}_z respectively. Since E_y , E_z and B_x are just scalar numbers, they will have no effect on the bra's and ket's, so

$$\begin{aligned}
& \langle \mathbf{q}_j | (\alpha [\hat{p}_y E_z - \hat{p}_z E_y] - g\mu_b B_x) | \mathbf{q}_{j-1} \rangle \\
&= \langle \mathbf{q}_j | \int d^3 \mathbf{p}_j (\alpha [\hat{p}_y E_z - \hat{p}_z E_y] - g\mu_b B_x) | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle \\
&= \int d^3 \mathbf{p}_j \langle \mathbf{q}_j | \mathbf{p}_j \rangle (\alpha [p_{j,y} E_z - p_{j,z} E_y] - g\mu_b B_x) \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle \quad (\text{E.2})
\end{aligned}$$

$$= \int d^3 \mathbf{p}_j \langle \mathbf{q}_j | \mathbf{p}_j \rangle \Gamma_{j,x}(p_{j,z}, p_{j,y}, E_z, E_y, B_x) \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle. \quad (\text{E.3})$$

In eq. (E.2) the momentum operator operated on its eigenfunctions, and produced its eigenvalues, $p_{j,y}$ and $p_{j,z}$. Thus, all the terms were reduced to simple scalars, and have been recombined into the new constant $\Gamma_{j,x}(p_{j,z}, p_{j,y}, E_z, E_y, B_x) \equiv \Gamma_{j,x}$ in eq. (E.3), where the hat have been dropped, to signify that $\Gamma_{j,x}$ is now just a number, and not an operator.

It is reasonable to assume that analogue calculations on $\hat{\Gamma}_y$ and $\hat{\Gamma}_z$ will yield the same results, except for a cyclic permutation of the indices. Thus

$$\begin{aligned}
\langle \mathbf{q}_j | \hat{\Gamma} | \mathbf{q}_{j-1} \rangle &= \langle \mathbf{q}_j | (\hat{\Gamma}_x, \hat{\Gamma}_y, \hat{\Gamma}_z) | \mathbf{q}_{j-1} \rangle = \int dp_j \langle \mathbf{q}_j | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle (\Gamma_{j,x}, \Gamma_{j,y}, \Gamma_{j,z}) \\
&\equiv \mathbf{\Gamma}_j \int dp_j \langle \mathbf{q}_j | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle, \quad (\text{E.4})
\end{aligned}$$

where the vector $\mathbf{\Gamma}_j$ with the scalar entries $(\Gamma_{j,x}, \Gamma_{j,y}, \Gamma_{j,z})$ have been introduced. Recalling from eq.(4.5) that $\langle \mathbf{q}_j | \mathbf{p}_j \rangle \langle \mathbf{p}_j | \mathbf{q}_{j-1} \rangle = (2\pi\hbar)^{-3} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar}$, (E.4) can be recast as

$$\langle \mathbf{q}_j | \hat{\Gamma} | \mathbf{q}_{j-1} \rangle = \mathbf{\Gamma}_j \int \frac{dp_j}{(2\pi\hbar)^3} e^{i\mathbf{p}_j \cdot (\mathbf{q}_j - \mathbf{q}_{j-1})/\hbar}, \quad (\text{E.5})$$

where

$$\mathbf{\Gamma}_j = \begin{pmatrix} \alpha [p_{j,y} E_z - p_{j,z} E_y] - g\mu_b B_x \\ \alpha [p_{j,z} E_x - p_{j,x} E_z] - g\mu_b B_y \\ \alpha [p_{j,x} E_y - p_{j,y} E_x] - g\mu_b B_z \end{pmatrix}$$

This is the final form of the momentum eigenstate dependent term in eq. (4.18).

Appendix F

List of symbols

Everywhere, a hat " ^ " denotes an operator, and the same symbol, without a hat denotes the corresponding eigenvalue. Boldface is a 3-dimensional vector.

$$\begin{aligned}
 \hat{p}_{x_i} &= -i\hbar \frac{\partial}{\partial x_i} \quad , \quad x_i = (x, y, z) \\
 \hat{\mathbf{p}} &= -i\hbar \nabla = -i\hbar \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \\
 \boldsymbol{\sigma} &= \frac{\hbar}{2} \left[\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right] \\
 \mathcal{N}(z) &= \frac{1}{\sqrt{1+|z|^2}} \\
 \dot{z}_j &= \frac{z_j - z_{j-1}}{\epsilon} \\
 \hat{\boldsymbol{\rho}} &= (\hat{\rho}_x, \hat{\rho}_y, \hat{\rho}_z) = (\hat{p}_x + qA_x, \hat{p}_y + qA_y, \hat{p}_z + qA_z) \\
 \rho_j &= (p_{j,x} + qA_x, p_{j,y} + qA_y, p_{j,z} + qA_z) \\
 \mathbf{q}'_j &= \frac{1}{2}(\mathbf{q}_j - \mathbf{q}_{j-1}) \\
 \hat{\boldsymbol{\Gamma}} &= (\hat{\Gamma}_x, \hat{\Gamma}_y, \hat{\Gamma}_z) = \begin{pmatrix} \alpha [\hat{p}_y E_z - \hat{p}_z E_y] + g\mu_b B_x \\ \alpha [\hat{p}_z E_x - \hat{p}_x E_z] + g\mu_b B_y \\ \alpha [\hat{p}_x E_y - \hat{p}_y E_x] + g\mu_b B_z \end{pmatrix} \\
 \boldsymbol{\Gamma} &= (\Gamma_x, \Gamma_y, \Gamma_z) = \begin{pmatrix} \alpha [p_y E_z - p_z E_y] + g\mu_b B_x \\ \alpha [p_z E_x - p_x E_z] + g\mu_b B_y \\ \alpha [p_x E_y - p_y E_x] + g\mu_b B_z \end{pmatrix} \\
 \mathcal{N}(z_j, z_{j-1}) &= \frac{1}{\sqrt{1+|z_j|^2} \sqrt{1+|z_{j-1}|^2}} \\
 \mathbf{Z}(z_j, z_{j-1}) &= \begin{pmatrix} z_j^* + z_{j-1} \\ -iz_j^* + iz_{j-1} \\ -1 + z_j^* z_{j-1} \end{pmatrix}
 \end{aligned}$$

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