FORM-PRESERVING TRANSFORMATIONS OF THE SCHRÖDINGER EQUATION

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Abstract

Coordinate transformations of differential equations have long been studied in the context of mathematics and physics. They allow us to change a differential equation into one that is easier to solve. In nonrelativistic quantum mechanics, the time evolution of a wave function is determined by the time-dependent Schrödinger equation (TDSE). Since quantum mechanics must work in every nonrelativistic frame, there must be a TDSE for every set of coordinates one chooses to measure in. Coordinate transformations between two reference frames must then transform one Schrödinger equation into another. Called form-preserving transformations (FPTs), these transformations allow for many puzzling solutions to the TDSE and can be used for the efficient determination of symmetry groups.

In this work, we will determine the most general allowed FPT for the Schrödinger-Pauli equation of a spinless charged particle in N-dimensions. We determine that the most general allowed transformations are of the form $\vec{x}' = R(\vec{x}/\gamma + \vec{\beta})$ and $t' = \int_{t_0}^{t} d\tau\, \gamma^{-2}(\tau)$, for the real, time-dependent functions $\vec{\beta}(t)$ and $\gamma(t)$ and the rotation $R(t)$. Furthermore, we show that the FPTs form a continuous Lie group, whose algebra is discussed in detail. Well-known symmetry groups such as the Galilean and Schrödinger groups are shown to be subgroups of the form-preserving group. We conclude with an analysis of FPTs in the phase-space formulation of quantum mechanics.

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List of Abbreviations

CES coherent excited states.

DE differential equation.

FPT form-preserving transformation.

NR nonrelativistic.

PSQM phase space quantum mechanics.

QM quantum mechanics.

SHO simple harmonic oscillator.

TDSE time-dependent Schrödigner equation.

Chapter 1

Introduction

Symmetries have long been an important aspect of understanding the physical world. The most basic symmetries that we can identify in a physical system are space translation, time translation and rotation invariance. With the presence of any one of these three basic symmetries we are able to solve many problems and explain their corresponding conserved quantities: translational momentum, energy and angular momentum. More complex symmetries such as the Galilean boosts, which preserve the equations of motion for a particle of any position-independent force, or the Lorentz transformations of special relativity, which preserves the wave equation in all reference frames, provide even deeper insights to these physical systems and the nature of spacetime itself.

Symmetries are also an essential tool for solving differential equations (DEs). The methods of Sophus Lie [1] allow us to identify the symmetries of a differential equation. Knowing the symmetries of a system allows one to limit its degrees of freedom, which often simplifies its analysis. For example, rotationally invariant problems are best solved using spherical coordinates, which are suited to exploiting the symmetries of the system.

Although these stricter forms of symmetries have been an extremely useful tool throughout mathematics and physics, there exists a class of transformations that produce *quasi-symmetries*. That is, they do not preserve the DE itself, but rather the class, or form, of a DE. For this reason, they are called form-preserving transformations in [2], since they preserve the form of a DE. Like regular symmetries, the quasi-symmetries also form a differentiable group that is describable with infinitesimal generators, called a Lie group. Mathematically,

these transformations are useful for developing techniques to transform between DEs. This allows one to transform a new problem into one that is already known. This can also identify non-intuitive connections between problems that seem unrelated. Furthermore, beyond their mathematical curiosity, the form-preserving transformation (FPT) has a direct physical meaning and application.

The objective of this thesis is to derive the most general FPT of the TDSE, and generalize previously known results. In particular, we consider the group of coordinate transformations on position and time that transform one Schrödinger equation into another. This is important, since the Schrödinger equation governs the time evolution of a particle's wave function. All reference frames where the particle remains non-relativistic should have a valid Schrödinger equation for determining the time evolution of observables. Therefore, such coordinate transformations must be well-understood in the context of nonrelativistic (NR) quantum mechanics.

In the literature, there are several examples of wave functions produced by FPTs. Such examples include the well-known coherent excited states (CES) [3], which have many applications in optics [4], and the Airy beam [5, 6], which seems, paradoxically, to represent an accelerating free particle; however, these accelerating states have been observed experimentally with an optical analog system [7]. Form preservation of the Schrödinger equation appears to have been first discussed in [8] and subsequently in [2, 9–11]. However, in the literature, specific FPTs, such as the symmetry group of the free TDSE, known as the Schrödinger symmetry [12–16] as well as the symmetry group of the harmonic oscillator TDSE [17], have been well-explained. Another well-known example is the equivalence of the free particle and the simple harmonic oscillator [17–19]. Lastly, in addition to the Airy beam, more works relate free-space solutions to that of a linear potential [20, 21]. These have been confirmed experimentally with gravitationally induced phase shifts on neutron beams in the famous COW (Colella-Overhauser-Werner) experiment [22] and more recently confirmed experimentally [23] for cold atoms. Other examples include the Sagnac

effect [24, 25] and work relating the simple harmonic oscillator (SHO) to a time-dependent SHO frequency [26].

We will begin in Chapter 2 by introducing the FPT in the position basis for the one-dimensional TDSE, and then for the Schrödinger-Pauli equation of a spinless particle with scalar and vector potentials in N-dimensions. We will show how the scalar and vector potentials transform for the most general allowed FPT. We then go on to show the specific properties of the FPT in three-dimensions, and demonstrate its use in rotating reference frames. We will then discuss the physical interpretation of the FPT without the position basis. Elementary probabilistic arguments lead one to the conclusion that the coordinate transformation must be linear, regardless of the Hamiltonian's exact form. Furthermore, we are able to derive the FPT while avoiding the position basis entirely by considering the time evolution of expectation values of the position and kinetic momentum operators. We conclude by considering a non-trivial example of the FPT, which features a time-dependent scaling transformation.

Next, we open Chapter 3 with a brief description of unitary transformations and symmetries in quantum mechanics. This is followed by a derivation of the Galilean and Schödinger groups in §3.2.2 and §3.2.3, respectively. We show these to be subgroups of the form-preserving group. We then detail the Lie algebra and the generators for the form-preserving group and show that the operators can reproduce the FPT identically. We conclude this chapter by discussing the group of time transformations and extending our work to the of a spin-1/2 particle in $3+1$ dimensions.

In Chapter 4 we extend the FPT to the phase-space formalism of quantum mechanics. We show that linear canonical transformations preserve the Moyal star product, and therefore, they also preserve the Moyal bracket. We are then able to derive the FPT for the Wigner function and the transformation of its corresponding scalar potential. Lastly, we conclude by demonstrating the free-harmonic equivalence, CES, and the Airy beam in phase space quantum mechanics.

Chapter 2

The Form-Preserving Transformation

In this chapter, we will introduce the form-preserving transformation of the Schrödinger equation in one spatial dimension, followed by the generalization to higher dimensions with vector and scalar potentials. We will follow this with a discussion about the special case of three spatial dimensions and provide two examples of its applications: understanding rotating reference frames and a non-trivial example of a time-dependent scale factor. We then introduce a physical interpretation of the FPT in §2.3, and introduce a method for determining the FPT without the position basis using the Ehrenfest theorem. We conclude with a non-trivial example of the FPT by discussing the free–harmonic equivalence. We determine the free dispersion of wave functions that are the SHO stationary states at $t = 0$.

2.1 One-Dimensional Form Preservation

The form-preserving transformations are the set of all coordinate transformations that preserve the form of the TDSE. That is, these are all of the real coordinate transformations $(x,t) \to (x',t')$ that transform the TDSE

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x,t) = i\hbar\frac{\partial\psi}{\partial t} \tag{2.1}$$

to the TDSE in the new coordinates

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi'}{\partial x'^2} + V'(x',t') = i\hbar\frac{\partial\psi'}{\partial t'}, \tag{2.2}$$

where $\psi'(x',t')$ is the wave function in the new coordinates. Physically, this restriction represents a kind of transformation to a "quasi-inertial" reference frame in quantum mechanics that preserves the form of the equations of motion. And since the transformed equation is also a Schrödinger equation, we may interpret ψ' as being the wave function for the particle in the new coordinates.

Following a similar method to Senitzky and Nauenberg [3, 21], we introduce the polar ansatz

$$\psi(x,t) = \sqrt{J(t)}\psi'(x',t')e^{iS(x,t)/\hbar}, \tag{2.3}$$

where S and J are real functions and ψ' is a complex function in general. The inclusion of the scale factor $\sqrt{J}$ is not necessary if S is allowed to be complex. It is, however, a cleaner derivation to include this scale factor, which we will see later in §2.3 preserves the probability density of finding a particle at a particular location in space.

Our goal is to perform the coordinate transformation $(x,t) \to (x',t')$ along with our polar ansatz to arrive at the Schrödinger equation in the transformed coordinates (2.2). Substituting the modified polar ansatz (2.3) into the Schrödinger equation (and dividing out $\sqrt{J}e^{iS/\hbar}$), we get the equation

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi'}{\partial x^2} + \frac{2i}{\hbar}\frac{\partial S}{\partial x}\frac{\partial\psi'}{\partial x} + \frac{i}{\hbar}\frac{\partial^2 S}{\partial x^2}\psi' - \left(\frac{1}{\hbar}\frac{\partial S}{\partial x}\right)^2\psi'\right] + V\psi' = i\hbar\left(\frac{\dot{J}}{2J}\psi' + \frac{i}{\hbar}\frac{\partial S}{\partial t}\psi' + \frac{\partial\psi'}{\partial t}\right), \tag{2.4}$$

where $\dot{J}$ is the total time derivative of J. The phase function S is a function of the original position coordinate x, so its derivatives can remain unchanged. The rest of the derivatives on ψ' will be changed to the primed coordinates by the chain rule. This results in the

differential equation

$$-\frac{\hbar^2}{2m}\Bigg\{\left[\left(\frac{\partial x'}{\partial x}\right)^2\frac{\partial^2}{\partial x'^2}+\frac{\partial^2 x'}{\partial x^2}\frac{\partial}{\partial x'}+2\frac{\partial x'}{\partial x}\frac{\partial t'}{\partial x}\frac{\partial^2}{\partial x'\partial t'}+\left(\frac{\partial t'}{\partial x}\right)^2\frac{\partial^2}{\partial t'^2}+\frac{\partial^2 t'}{\partial x^2}\frac{\partial}{\partial t'}\right]$$
$$+\frac{2i}{\hbar}\frac{\partial S}{\partial x}\left(\frac{\partial x'}{\partial x}\frac{\partial}{\partial x'}+\frac{\partial t'}{\partial x}\frac{\partial}{\partial t'}\right)+\frac{i}{\hbar}\frac{\partial^2 S}{\partial x^2}-\left(\frac{1}{\hbar}\frac{\partial S}{\partial x}\right)^2\Bigg\}\psi'+V\psi'$$
$$=i\hbar\left(\frac{\dot{J}}{2J}+\frac{i}{\hbar}\frac{\partial S}{\partial t}+\frac{\partial t'}{\partial t}\frac{\partial}{\partial t'}+\frac{\partial x'}{\partial t}\frac{\partial}{\partial x'}\right)\psi'. \quad (2.5)$$

Comparing (2.5) with the transformed TDSE (2.2), we see that there are second-order derivatives in t' as well as mixed derivatives in x' and t' that should be zero. This restricts the time transformation so that $\partial_x t' = 0$. This removes a lot of the complexity from the second-order spatial derivative

$$-\frac{\hbar^2}{2m}\Bigg\{\left(\frac{\partial x'}{\partial x}\right)^2\frac{\partial^2}{\partial x'^2}+\frac{\partial^2 x'}{\partial x^2}\frac{\partial}{\partial x'}+\frac{2i}{\hbar}\frac{\partial S}{\partial x}\frac{\partial x'}{\partial x}\frac{\partial}{\partial x'}+\frac{i}{\hbar}\frac{\partial^2 S}{\partial x^2}-\left(\frac{1}{\hbar}\frac{\partial S}{\partial x}\right)^2\Bigg\}\psi'+V\psi'$$
$$=i\hbar\left(\frac{\dot{J}}{2J}+\frac{i}{\hbar}\frac{\partial S}{\partial t}+\frac{\partial t'}{\partial t}\frac{\partial}{\partial t'}+\frac{\partial x'}{\partial t}\frac{\partial}{\partial x'}\right)\psi'. \quad (2.6)$$

Comparing this to the TDSE in the new coordinates, we necessitate that the coefficient of the second-order spatial derivative $(\partial_x x')^2$ be the same as the coefficient of the first-order time derivative, $\partial_t t'$. Since t' must be a function of time only, this requires that $\partial_x x'$ also be independent of x. We then define the relationship between the spatial and temporal derivatives to be

$$\frac{\partial t'}{\partial t}=\left(\frac{\partial x'}{\partial x}\right)^2\equiv\left(\frac{1}{\gamma(t)}\right)^2, \quad (2.7)$$

where $\gamma(t)$ is a real function of time only. Therefore, the most general form of coordinate transformations allowed is the 1D transformation

$$x'=\frac{1}{\gamma(t)}x+\beta(t); \quad (2.8)$$
$$t'=\int_{t_0}^{t}\frac{d\tau}{\gamma^2(\tau)}, \quad (2.9)$$

where $\beta(t)$ is a real time-dependent translation.

Furthermore, since $x'(x,t)$ is linear in x, its second-order spatial derivative $\partial_x^2 x'$ is zero. Collecting coefficients, we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi'}{\partial x'^2}-\frac{i\gamma\hbar}{m}\frac{\partial\psi'}{\partial x'}\left(\frac{\partial S}{\partial x}+m\gamma\frac{\partial x'}{\partial t}\right)+\gamma^2\left(V+\frac{\partial S}{\partial t}-\frac{i\hbar\dot{J}}{2J}-\frac{i\hbar}{2m}\frac{\partial^2 S}{\partial x^2}+\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2\right)\psi' = i\hbar\frac{\partial\psi'}{\partial t'}. \quad (2.10)$$

The coefficient of the first-order spatial derivative of the transformed wave function must add to zero if the overall form of the TDSE is preserved. This gives the derivative of the phase function as

$$\frac{\partial S}{\partial x}=-m\gamma\frac{\mathrm{d}x'}{\mathrm{d}t}=m\left(\frac{\dot{\gamma}}{\gamma}x-\gamma\dot{\beta}\right). \quad (2.11)$$

Integrating results in the phase

$$S(x,t)=\frac{m}{2}\left(\frac{\dot{\gamma}}{\gamma}x^2-2\gamma\dot{\beta}x\right)+\alpha(t), \quad (2.12)$$

where $\alpha(t)$ is an arbitrary function of time.

The linear term in ψ' can be identified with the transformed potential $V'(x',t')$ in (2.10). This function must be real, so the imaginary part must add to zero. With $\partial_x^2 S=m\dot{\gamma}/\gamma$,

$$\frac{i\hbar\dot{J}}{2J}+\frac{i\hbar\dot{\gamma}}{2\gamma}=0 \implies J=\frac{1}{\gamma}, \quad (2.13)$$

meaning that J is the same as the Jacobian of the transformation from $x'\to x$ (which we will show is true in general later).

Finally we arrive at the transformed Schrödinger equation as reported in [2]

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi'}{\partial x'^2}+V'\psi'=i\hbar\frac{\partial\psi'}{\partial t'}, \quad (2.14)$$

where the transformed potential is

$$\begin{aligned}\frac{V'(x',t')}{\gamma^2} &= V(x,t)+\frac{\partial S}{\partial t}+\frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 \\ &= V(x,t)+\dot{\alpha}+\frac{m\ddot{\gamma}}{2\gamma}x^2-mx(2\dot{\gamma}\dot{\beta}+\gamma\dot{\beta})+\frac{m}{2}\gamma^2\dot{\beta}^2,\end{aligned} \tag{2.15}$$

and the wave function is

$$\psi(x,t)=\frac{1}{\sqrt{\gamma}}\psi'(x',t')\exp\left[\frac{im}{2\hbar}\left(\frac{\dot{\gamma}}{\gamma}x^2-2\gamma\dot{\beta}x\right)+i\frac{\alpha}{\hbar}\right]. \tag{2.16}$$

The arbitrary time-dependent function $\alpha(t)$ then corresponds to the gauge freedom of the Schrödinger equation (without introducing a 1D "vector" potential $\vec{A}\propto\nabla\alpha$).

The ability to use strategic coordinate transformations to change the potential of a solution has utility when trying to solve the Schrödinger equation. With an appropriate choice of α,β,γ, we can sometimes transform a Schrödinger equation into one we already know how to solve. This was demonstrated in [2] for the anharmonic potential $V=x^6+2\alpha x^4+(\alpha^2-4n-3)x^2$ where $\alpha\in\mathbb{R}$ and $n\in\mathbb{N}$. Another example is the solution to the time-dependent oscillator $V=\frac{1}{2}\omega(t)x^2$ written in terms of the stationary oscillator found by Yan [26].

2.2 Form Preservation in Higher Dimensions

Form preservation of the TDSE under coordinate transformations works much the same in N spatial dimensions as it does in one dimension. If we exclude the special case of time-dependent rotations, then even with the inclusion of a fixed rotation, the N-dimensional case is much the same as the one-dimensional case. Since the potential and the phase are scalar valued, the simplest generalization to N-dimensions is to replace the scalar products of two real numbers with the vector scalar product, which is indeed what happens. For the most part, time-independent rotations are a trivial extension of the one-dimensional case, so we will not treat them directly. Instead, we move straight to the most general case, as was

mostly covered in [9, 10], though our treatment will include the use of vector potentials to describe a spinless-charged particle in a magnetic field.

The Hamiltonian in N-dimensions for a charged, spinless particle [27, 28] is identical to the classical Hamiltonian of a charged particle with nonzero electric and magnetic fields. As usual, we take the regular Hamiltonian of kinetic plus potential energy and replace the kinetic momentum with $\vec{p} - q\vec{A}/c$, where $\vec{p}$ is the conjugate momentum, which is $\vec{p} \to -i\hbar\nabla$ in the position representation. This results in the Schrödinger-Pauli equation for a spinless charged particle

$$\left[\frac{1}{2m}\left(-i\hbar\nabla - \frac{q}{c}\vec{A}\right)^2 + q\Phi\right]\psi = i\hbar\frac{\partial\psi}{\partial t}, \tag{2.17}$$

where $\Phi(\vec{x},t)$ is the electric scalar potential and $\vec{A}(\vec{x},t)$ is the magnetic vector potential, whose curl determines the magnetic field. For our purposes, we will drop the q/c coefficient in front of the vector potential, and replace $q\Phi$ with $V(\vec{x},t)$.

Since the magnetic field is determined by the curl of the vector potential $\vec{B} = \nabla \times \vec{A}$, we can add the gradient of any scalar field $\nabla\Lambda$ to the vector potential without altering the resulting magnetic field. In higher dimensions, we can still add the 4-gradient of a scalar field to the vector four-potential $A_\mu \to A_\mu + \partial_\mu\Lambda$. The electromagnetic tensor $F_{\mu\nu}$ is invariant to this transformation, and therefore so is the force on a charged particle. This is the *gauge symmetry* of the electromagnetic field, and the outcome of an experiment should not depend on our particular choice of gauge. For example, computing the time derivative of the expectation value of position by the Ehrenfest theorem [28], we get the quantization of the Lorentz force law [29]

$$m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\langle\vec{X}\rangle = \left\langle -\nabla V - \frac{\partial\vec{A}}{\partial t} + \frac{1}{2}(\vec{V}\times\vec{B} - \vec{B}\times\vec{V})\right\rangle, \tag{2.18}$$

where $m\vec{V} = \vec{P} - \vec{A}$ is the "velocity" operator of the kinetic momentum (see Appendix A.2 for higher dimensions).

Examination of the Schrödinger equation (2.17) shows that this is not invariant under the

sole gauge transformation $\vec{A} \to \vec{A} + \nabla\Lambda$. In classical electromagnetism, the potential transforms as $V - \partial_t\Lambda$, so we might expect this helps, but it is not enough. For the Schrödinger equation to be invariant, the wave function itself must be transformed accordingly. Since the only way to transform a wave function without changing the probability density in the position representation is to introduce a phase factor, we might correctly guess that a gauge transformation changes the phase of the wave function. Indeed, if we set $\vec{A}$, V and ψ to transform simultaneously as

$$\vec{A} \to \vec{A} + \nabla\Lambda \qquad V \to V - \frac{\partial\Lambda}{\partial t} \qquad \psi \to \psi e^{i\Lambda/\hbar}, \tag{2.19}$$

the Schrödinger equation remains invariant. The potential fields are normally said to be nonphysical, and only the electric and magnetic fields are said to have any direct physical consequences. However, since the gauge transformation can affect the phase of the wave function, this may not be the case, as evidenced by the Aharonov-Bohm effect [27]. Though the Aharanov-Bohm effect seems to detect the presence of a magnetic vector potential in a region of zero magnetic field, the result of experiments will always be gauge-independent.

We can now expand the square of (2.17) to obtain the differential equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{i\hbar}{m}\vec{A}\cdot\nabla\psi + \left(\frac{i\hbar\nabla\cdot\vec{A} + \vec{A}^2}{2m} + V\right)\psi = i\hbar\frac{\partial\psi}{\partial t}. \tag{2.20}$$

It is often customary in the treatment of electromagnetism to choose the Coulomb gauge in which a gauge transformation (2.19) is applied to fix the divergence to be zero, or $\nabla\cdot\vec{A} = 0$. Thus, it is natural for the sake of completeness to ask whether or not we are guaranteed to find a gauge parameter Λ so that we can always transform into the Coulomb gauge. Taking an initial nonzero divergence and requiring that the divergence vanishes, yields the equation $\nabla\cdot\vec{A} + \nabla^2\Lambda = 0$. This is the Poisson equation for the gauge parameter Λ and can always be solved using the appropriate Green's function. Furthermore, Λ is not even unique since we can add the homogeneous solution Φ of the Laplace equation $\nabla^2\Phi = 0$ to the gauge

parameter and it will still solve the Poisson equation. Thus, we are always guaranteed to be able to fix a gauge so that $\nabla \cdot \vec{A} = 0$ without loss of generality. It would therefore be safe to assume that we can use the Coulomb gauge in both Schrödinger equations without loss of generality. We choose not to do this for the sake of clarity.

We begin with the same ansatz as the one-dimensional case, generalized to higher dimensions:

$$\psi(\vec{x},t) = \sqrt{J(t)}e^{iS(\vec{x},t)}\psi'(\vec{x}',t'), \tag{2.21}$$

where ψ' is assumed to satisfy the TDSE (2.20) in the primed coordinates with vector potential $\vec{A}'$ and scalar potential V'. For the higher-dimensional case, we are expecting an equation for the transformed potential analogous to (2.15), which should be invariant to gauge transformations. Since it is possible to fix the divergence of the vector potential, it would be reasonable to expect the divergence to be absent from the resulting transformed potential. Applying the gauge transformation (2.19) to the ansatz (2.21) leaves ψ' unaffected, and the phase shift can be absorbed by S. Our transformation should then be independent of the particular gauge we chose for the wave function in either coordinate system.

We now insert our ansatz (2.21) into the Schrödinger equation (2.20) to obtain

$$-\frac{\hbar^2}{2m}\left[\nabla^2\psi' + \frac{2i}{\hbar}\nabla\psi'\cdot\nabla S + \frac{i}{\hbar}\psi'\nabla^2 S - \psi'(\nabla S/\hbar)^2\right] + \frac{i\hbar}{m}\vec{A}\cdot(\nabla\psi' + \frac{i}{\hbar}\psi'\nabla S) + \left(\frac{i\hbar\nabla\cdot\vec{A} + \vec{A}^2}{2m} + V\right)\psi' = i\hbar\left(\frac{\dot{J}}{2J}\psi' + \psi'\frac{i}{\hbar}\frac{\partial S}{\partial t} + \frac{\partial\psi'}{\partial t}\right). \tag{2.22}$$

As before, we must turn the derivatives of ψ' into the primed derivatives. For the same reason as the 1D case, we will take t' to be independent of position, as the mixed derivatives of time and space are not present in the Schrödinger equation. Using Einstein's summation convention with $\partial_i = \partial_{x_i}$ and $\partial'_i = \partial_{x'_i}$, the components of the gradient are

$$\partial_i = \frac{\partial x'_j}{\partial x_i}\partial'_j = J_{ji}\partial'_j, \tag{2.23}$$

where $J_{ji}(\vec{x},t) = \partial_i x'_j$ is the Jacobian matrix of the transformation $\vec{x} \to \vec{x}'$. The Laplacian can then be written as

$$\begin{aligned} \partial_i \partial_i &= J_{ki} J_{ji} \partial'_k \partial'_j + (\partial_i J_{ji}) \partial'_j \\ &= (\mathbf{J}\mathbf{J}^T)_{jk} \partial'_j \partial'_k + (\nabla^2 x'_i) \partial'_i, \end{aligned} \tag{2.24}$$

since $\partial_i J_{ij} = \nabla^2 x'_j$.

The Schrödinger equation in the primed frame must contain a Laplacian in the primed coordinates, ∇'^2. Therefore, since this is the only source of second-order derivatives in x'_i, the diagonal terms of $\mathbf{J}\mathbf{J}^T$ must be equal. Furthermore, since the non-diagonal terms of this product introduce mixed derivatives of the form $\partial'_i \partial'_j$ for $i \neq j$ which are not present in the Schrödinger equation, we require that the non-diagonal coefficients are zero also. Therefore, the only allowed Jacobian matrices of this transformation must satisfy

$$\mathbf{J}\mathbf{J}^T = \frac{1}{\gamma^2} I \implies (\pm\gamma\mathbf{J})(\pm\gamma\mathbf{J})^T = I, \tag{2.25}$$

for the arbitrary real function[1] $\gamma(\vec{x},t)$.

According to (2.25), the matrix $\pm\gamma\mathbf{J} = R$ is orthogonal, so that its transpose is also its inverse, $RR^T = I$, in N dimensions. Furthermore, since $\det(\pm\gamma\mathbf{J}) = \det R = \pm 1$, we obtain that the Jacobian $J = \det \mathbf{J}$ is γ^{-N}. We will drop the $\pm$ in front since it can be taken up by the orthogonal matrix. The significance of this being an orthogonal matrix is that it represents general rotations and reflections. The definition of an orthogonal matrix allows it to have two different determinants, $\det R = \pm 1$. When the matrix has a positive determinant, these are called proper rotations. Proper rotations only rotate the coordinate axes and do not perform any parity transformations on the axes. The case of determinant -1 encompasses all rotations that also include a parity transformation.

Since the Jacobian matrix of the transformation is now known, we can rewrite the gra-

[1] Reality must be enforced to ensure that the transformed position is a real coordinate.

dient operator as

$$\nabla = \frac{1}{\gamma} R^T \nabla', \tag{2.26}$$

in the primed coordinates. After some rearranging, (2.22) now becomes

$$\begin{aligned} &-\frac{\hbar^2}{2m\gamma^2}\nabla'^2\psi' + \frac{i\hbar}{m}\left[-\frac{\nabla S}{\gamma} + \frac{\vec{A}}{\gamma} - mR^T\frac{\partial \vec{x}'}{\partial t} + \frac{i\hbar}{2}R^T(\nabla^2\vec{x}')\right]\cdot(R^T\nabla'\psi') \\ &+\left[-\frac{i\hbar}{2m}\nabla^2 S + \frac{(\nabla S)^2}{2m} - \frac{1}{m}\vec{A}\cdot\nabla S + \frac{i\hbar\nabla\cdot\vec{A}+\vec{A}^2}{2m} + V - \frac{i\hbar\dot{J}}{2J} + \frac{\partial S}{\partial t}\right]\psi' = i\hbar\frac{\partial t'}{\partial t}\frac{\partial \psi'}{\partial t'}. \end{aligned} \tag{2.27}$$

Furthermore, we need the factor of γ^{-2} to be equal to $\partial_t t'$ for this to match our transformed TDSE, just as in the 1D case, to avoid the mixed time and space derivatives that are not present in the Schrödinger equation. This also means that the factor of γ is a function of time only, since t' cannot depend on position. Since γ^{-N} is the Jacobian of the transformation, the transformation must be linear in $\vec{x}$ and $\nabla^2\vec{x}' = \vec{0}$. Therefore, the only allowed coordinate transformations are of the form

$$\boxed{\vec{x}' = R(t)\left[\frac{1}{\gamma}\vec{x} + \vec{\beta}(t)\right] \quad \& \quad t' = \int_{t_0}^{t}\frac{d\tau}{\gamma^2(\tau)}} \tag{2.28}$$

where $\gamma(t)$ and $\vec{\beta}(t)$ are both arbitrary real functions of time, and $R(t) \in O(N)$ is a time-dependent orthogonal matrix.

Furthermore, comparing the terms of (2.27), we identify that the coefficient of $R^T\nabla'\psi'$ must be the rotated and scaled vector potential $\gamma^{-2}R^T\vec{A}'$ (instead of being zero as in the 1D case without vector potentials). Thus, the gradient of the phase must satisfy

$$\begin{aligned} \nabla S &= -m\gamma\vec{R}^T\frac{\partial \vec{x}'}{\partial t} + \vec{A} - \frac{1}{\gamma}R^T\vec{A}' \\ &= m\left(\frac{\dot{\gamma}}{\gamma}\vec{x} - \gamma\dot{\vec{\beta}}\right) + \vec{A} - \frac{1}{\gamma}R^T\vec{A}' - mR^T\dot{R}(\vec{x}+\gamma\vec{\beta}). \end{aligned} \tag{2.29}$$

The first part of the phase matches perfectly with the 1D case we have already seen, but the remaining part to the right is something different, which must be handled with some

care. Unlike the 1D case, we are not guaranteed that, for a given set of vector potentials and rotations, a scalar field $S(\vec{x},t)$ exists such that its gradient satisfies (2.29).

Consider the $\dot{R}R^T\vec{x}$ term. The matrix $\dot{R}R^T$ is antisymmetric for all orthogonal matrices R. By definition, the product R^TR is the identity matrix. Taking the time derivative of this equation yields

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}(R^TR) \\ &= \dot{R}^TR + R^T\dot{R} \end{aligned} \tag{2.30}$$

thus $R^T\dot{R} = -(R^T\dot{R})^T$, and the matrix is antisymmetric.

The equation $\nabla\Phi = A\vec{x}$ for a space-independent antisymmetric matrix A has no solution. To see why this is, define the circulation of the vector field $\vec{V}$ in the ij plane as $\partial_i V_j - \partial_j V_i$. If the vector field can be written as the gradient of the scalar field Φ, this results in zero circulation because the derivatives commute. Thus, in a higher dimensional analogy to the Helmholtz decomposition [30], a vector field with nonzero circulation cannot be written as the gradient of a scalar field. The circulation of $A\vec{x}$ in the ij plane, where A is an antisymmetric matrix, is $-2A_{ij}$. Therefore there does not exist a scalar field Φ so that $\nabla\Phi = A\vec{x}$.

Therefore, for S to exist, the transformed vector potential must be

$$\frac{R^T\vec{A}'}{\gamma} = \vec{A} - \nabla\alpha - mR^T\dot{R}(\vec{x}+\gamma\vec{\beta}), \tag{2.31}$$

where $\alpha(\vec{x},t)$ is an arbitrary scalar field, which represents the freedom to choose the gauge of both $\vec{A}'$ and $\vec{A}$ when we perform the coordinate transformation. It is easier to see that α can also be a gauge transform of $\vec{A}'$ if we remember that $\gamma R\nabla\alpha = \nabla'\alpha$. The phase can now be written as

$$\boxed{S(\vec{x},t) = \frac{m}{2}\left(\frac{\dot{\gamma}}{\gamma}\vec{x}^2 - 2\gamma\dot{\vec{\beta}}\cdot\vec{x}\right) + \alpha(\vec{x},t),} \tag{2.32}$$

where α is a real function of position and time.

This leaves us with the Schrödinger equation

$$\gamma^2\left[-\frac{i\hbar}{2m}\nabla^2 S+\frac{(\nabla S)^2}{2m}-\frac{1}{m}\vec{A}\cdot\nabla S+\frac{i\hbar\nabla\cdot\vec{A}+\vec{A}^2}{2m}+V-\frac{i\hbar\dot{J}}{2J}+\frac{\partial S}{\partial t}\right]\psi' - \frac{\hbar^2}{2m}\nabla'^2\psi'+\frac{i\hbar}{m}\vec{A}'\cdot\nabla'\psi'=i\frac{\partial\psi'}{\partial t'}. \quad (2.33)$$

Upon comparison with the transformed equation, we identify the coefficient of ψ' with

$$\frac{i\hbar\nabla'\cdot\vec{A}'+\vec{A}'^2}{2m}+V'. \quad (2.34)$$

Therefore, the relation between the transformed scalar potentials can be written as

$$-\frac{i\hbar}{2m}\nabla^2 S+\frac{(\nabla S)^2}{2m}-\frac{1}{m}\vec{A}\cdot\nabla S+\frac{i\hbar\nabla\cdot\vec{A}+\vec{A}^2}{2m}+V-\frac{i\hbar\dot{J}}{2J}+\frac{\partial S}{\partial t}=\frac{i\hbar\nabla'\cdot\vec{A}'+\vec{A}'^2}{2m\gamma^2}+\frac{V'}{\gamma^2}. \quad (2.35)$$

Next, we note that the Laplacian of the phase is just $\nabla^2 S = m\dot{\gamma}\mathrm{Tr}\,I/\gamma+\nabla\cdot\vec{A}-\nabla'\cdot\vec{A}'/\gamma^2$. The trace of the identity matrix I is just the number of dimensions, N. The Laplacian of the phase then cancels the divergences of the vector potentials in (2.35), and we are left with

$$\frac{1}{\gamma^2}\left(V'+\frac{\vec{A}'^2}{2m}\right)=V+\frac{\partial S}{\partial t}+\frac{(\vec{A}-\nabla S)^2}{2m}-\frac{i\hbar}{2}\left(N\frac{\dot{\gamma}}{\gamma}+\frac{\dot{J}}{J}\right). \quad (2.36)$$

But the potential function must be entirely real, so the coefficient of the imaginary term on the right-hand side must be zero since all of the functions here have been taken to be real. This is solved by setting

$$J=\gamma^{-N}, \quad (2.37)$$

which we immediately identify as the Jacobian of the transformation (2.28).

The Hamiltonian in the new coordinates is $H=(i\hbar\nabla'+\vec{A}')^2/2m+V'$, or written explic-

itly,

$$H = -\frac{\hbar^2}{2m}\nabla'^2 + \frac{i\hbar}{m}\gamma\left[R(\vec{A}-\nabla\alpha) - m\dot{R}(\vec{x}+\gamma\vec{\beta})\right]\cdot\nabla' \\ +\gamma^2\left[V + \frac{\partial\alpha}{\partial t} + \frac{m\ddot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x}\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\ddot{\gamma}\vec{\beta}) + \frac{(\vec{A}-\nabla\alpha)^2}{2m} - (\vec{A}-\nabla\alpha)\cdot\left(\frac{\dot{\gamma}}{\gamma}\vec{x} - \gamma\dot{\vec{\beta}}\right)\right]. \quad (2.38)$$

Overall, this means that the N-dimensional TDSE equation can be solved by the wave function

$$\boxed{\psi(\vec{x},t) = \frac{1}{\gamma^{N/2}}\psi'(\vec{x}',t')\exp\left[\frac{im}{2\hbar}\left(\frac{\dot{\gamma}}{\gamma}\vec{x}^2 - 2\gamma\dot{\vec{\beta}}\cdot\vec{x}\right) + \frac{i\alpha(\vec{x},t)}{\hbar}\right],} \quad (2.39)$$

where $\vec{x}'$ and t' are determined by the coordinate transformation (2.28). The transformed wave function satisfies the N-dimensional TDSE in the primed coordinates with a vector potential

$$\boxed{\vec{A}' = \gamma R(\vec{A}-\nabla\alpha) - \gamma m\dot{R}(\vec{x}+\gamma\vec{\beta}),} \quad (2.40)$$

and a scalar potential

$$\begin{aligned}\frac{V'}{\gamma^2} &= V + \frac{\partial S}{\partial t} + \frac{(\vec{A}-\nabla S)^2}{2m} - \frac{(\vec{A}'/\gamma)^2}{2m} \\ &= V + \frac{\partial\alpha}{\partial t} + \frac{m\ddot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x}\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\gamma\ddot{\vec{\beta}}) + \frac{m}{2}(\gamma\dot{\vec{\beta}})^2 \\ &\quad - (\vec{A}-\nabla\alpha)\cdot m\gamma R^T\frac{\partial\vec{x}'}{\partial t} - \frac{m}{2}[\dot{R}(\vec{x}+\gamma\beta)]^2.\end{aligned} \quad (2.41)$$

Comparing the terms of the N-dimensional transformed potential to the 1D case (2.15), we see that much is the same. However, there are some differences in the last two terms that are created by the magnetic vector potential $\vec{A}$ and the rotation of the transformation. Recall that the non-relativistic Lagrangian for a particle in a magnetic field features an interaction potential of $-\vec{A}\cdot\vec{v}$ where $\vec{v}$ is the speed of the particle. The first term of the second line is then the interaction of the moving reference frame with the magnetic field. The last term is then the kinetic energy of the rotation, which creates the centrifugal force.

We must show that the potential transformation (2.41) is invariant to gauge transforma-

tions of the vector potential in both coordinates. Beginning in the unprimed coordinate, let Λ be the gauge parameter, and let us perform the gauge transformation (2.19). The wave function will then transform as

$$e^{i\Lambda/\hbar}\psi(\vec{x},t) = e^{i(S+\Lambda)/\hbar}\psi'(\vec{x}',t'). \tag{2.42}$$

Effectively, the gauge transformation on the right-hand side can be absorbed by taking the arbitrary parameter $\alpha \to \alpha+\Lambda$. The quantity $A-\nabla\alpha$ is invariant under this transformation, since it transforms to $\vec{A}+\nabla\Lambda-\nabla(\alpha+\Lambda) = \vec{A}-\nabla\alpha$. Therefore, the transformed vector potential (2.40) is also invariant. The scalar potential (2.41) becomes

$$\frac{V'}{\gamma^2} = V - \frac{\partial\Lambda}{\partial t} + \frac{\partial(\alpha+\Lambda)}{\partial t} + \frac{m\ddot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x}\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\gamma\ddot{\vec{\beta}}) + \frac{m}{2}(\gamma\dot{\vec{\beta}})^2 \\ - (\vec{A}-\nabla\alpha)\cdot m\gamma R^T\frac{\partial\vec{x}'}{\partial t} - \frac{m}{2}[\dot{R}(\vec{x}+\gamma\beta)]^2. \tag{2.43}$$

This equation is identical to the original. Therefore, a gauge transformation of the wave function leaves the transformed scalar and vector potentials invariant if one simultaneously takes $\alpha \to \alpha+\Lambda$. Since the FPT must be identical in both directions (under interchange of the primed and unprimed variables), it follows that the FPT is also invariant to gauge transformations of ψ' in the primed coordinates.

2.2.1 3-Dimensional Considerations

In this section, we will focus on the special case of 3 spatial dimensions, and the $SO(3)$ subgroup of $O(3)$. It is only necessary to consider this subgroup, since allowing the scale factor γ to be negative will still encompass all possible transformations. Since we live within 3 spatial dimensions (insofar as we currently know), this is the most physically relevant number of dimensions to analyze in more detail. Moreover, in 3 spatial dimensions we can exploit the cross product and the nice properties of $SO(3)$ matrices.

In $SO(3)$, the rotation matrices are normally parametrized by the rotation vector $\vec{\theta}$ where

the magnitude defines the angle of rotation and the direction defines the normal vector of the plane of rotation, according to the right-hand rule [31–33]. It was already noted previously that $R^T\dot{R}$ is an antisymmetric matrix. Let the components of the matrix be $\varepsilon_{ijk}\omega_j$, which spans the space of antisymmetric matrices in three dimensions. Here ε_{ijk} is the Levi-Civita symbol (see Appendix B) and $\vec{\omega}$ is a real (pseudo)vector. Multiplying this matrix with a vector, it is obvious that this matrix has the action of taking the cross product of a vector $\vec{\omega}\times\vec{v}$. Since this matrix has the effect of taking the cross product, it is standard notation to denote it by $[\vec{\omega}]_\times$, where it is defined as the linear map $[\vec{\omega}]_\times\vec{v} = \vec{\omega}\times\vec{v}$.

Using this notation, we can now rewrite the time derivative of the rotation matrix as

$$\dot{R} = R[\vec{\omega}]_\times. \tag{2.44}$$

Furthermore, if we parametrize the rotation R about the axis $\hat{n}$ with angle θ according to the right hand rule, the *pseudovector* $\vec{\omega}$ can be shown to be (see Appendix D.5, eq. D.40)

$$\vec{\omega} = \dot{\theta}\hat{n} + \sin\theta\dot{\hat{n}} + (\cos\theta - 1)\hat{n}\times\dot{\hat{n}} \neq \frac{\mathrm{d}}{\mathrm{d}t}\vec{\theta}, \tag{2.45}$$

which is not the instantaneous angular velocity vector when the axis of rotation is time-dependent. By the properties of the rotation matrix, we may also write this as

$$\dot{R} = [\vec{\Omega}]_\times R, \tag{2.46}$$

where $\vec{\Omega} = R\vec{\omega}$ is the rotated angular velocity. The two angular velocities only differ by a minus sign on the $\hat{n}\times\dot{\hat{n}}$ component.

To see why this should be the case, consider the fixed point $\vec{x}$ in the non-rotated coordinates. The corresponding point in the rotated coordinates is $\vec{x}' = R\vec{x}$. The velocity of this point in the rotating frame is the time derivative $\vec{v} = \dot{\vec{x}}' = \dot{R}\vec{x}$, which will be seen to have rotational velocity only, with no radial component. The speed of rotational motion [32] is

$\vec{v} = \vec{\omega}' \times \vec{x}'$, where $\vec{\omega}'$ is the instantaneous angular velocity in the rotated coordinates. Since cross products preserve orientation and have unit determinant (see Appendix D), we must have $\vec{v} = (R\vec{\omega}) \times (R\vec{x}) = R(\vec{\omega} \times \vec{x})$. We already showed this is precisely the action of $\dot{R}$ on the point $\vec{x}$, thus we have $\dot{R} = R[\vec{\omega}]_\times$ as desired.

Thus we can write the transformed vector potential in 3-dimensions as

$$\begin{aligned} \vec{A}' &= \gamma R(\vec{A} - \nabla\alpha) - m\gamma\vec{\Omega} \times [R(\vec{x} + \gamma\vec{\beta})] \\ &= \gamma R\vec{A} - \nabla'\alpha - m\gamma^2\vec{\Omega} \times \vec{x}'. \end{aligned} \tag{2.47}$$

Now that we are in 3 dimensions, we can define the magnetic field as the curl of the vector potential. The transformed magnetic field should then be the curl in the primed coordinates of the new vector potential, or $\vec{B}' = \nabla' \times \vec{A}'$. This yields the transformed magnetic field

$$\vec{B}' = \gamma^2 R(\vec{B} - 2m\vec{\omega}) = \gamma^2(R\vec{B} - 2m\vec{\Omega}), \tag{2.48}$$

where $\vec{B} = \nabla \times \vec{A}$ is the magnetic field of the initial coordinates. Finally, the transformed scalar potential is

$$\begin{aligned} \frac{V'}{\gamma^2} = V + \frac{\partial\alpha}{\partial t} + \frac{m\ddot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x} \cdot (2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}) + \frac{m}{2}(\gamma\dot{\vec{\beta}})^2 \\ - \frac{m}{2}[\vec{\omega} \times (\vec{x} + \gamma\vec{\beta})]^2 - (\vec{A} - \nabla\alpha) \cdot \left[\frac{\dot{\gamma}}{\gamma}\vec{x} - \gamma\dot{\vec{\beta}} - \vec{\omega} \times (\vec{x} + \gamma\vec{\beta})\right]. \end{aligned} \tag{2.49}$$

On comparison with (2.15), the top line of the three-dimensional case is analogous, only differing by the inclusion of the additional 2 terms on the bottom. The first is the kinetic energy of the rotating frame (which creates the outward centrifugal force), and the second is the interaction potential of the moving frame with the magnetic field, as discussed earlier.

2.3 Physical Interpretation and Expectation Values

In this section, we will find a physical motivation for the transformed wave function (2.21). We consider how the measurable probability must transform in different reference frames and determine how wave functions should transform. We will see that not only do we arrive at the same form of the wave function, but that the restriction to linear frame transformations is a fundamental limitation of quantum mechanics that does not depend on the particular form of the Hamiltonian or TDSE under consideration.

Consider a wave function $\psi(\vec{x},t)$ in the Hilbert space $\mathcal{H}$ for a particle with probability density $|\psi|^2$ in the coordinates $(\vec{x},t)$. The probability of finding this particle within a volume element dV at the location $(\vec{x},t)$ is equal to the volume element multiplied by the probability density at this point, or $dP(\vec{x},t;dV) = |\psi(\vec{x},t)|^2 dV$. Next, consider the particle's wave function in the transformed coordinates $\psi'(\vec{x}',t')$, which belongs to the Hilbert space $\mathcal{H}'$. Since this is the wave function for the same particle, only in different coordinates, it must predict the same outcome for all experiments we could perform on the particle.

Let $(\vec{x},t)$ and $(\vec{x}',t')$ point to the same physical location in the two different coordinate systems, and let dV' be the volume element dV in the primed coordinates. Since the probability of finding the particle in a given volume at a fixed point in time and space must be the same irrespective of the coordinates in which we choose to perform experiments, we must require that

$$dP(\vec{x},t;dV) = dP'(\vec{x}',t';dV') \longrightarrow |\psi(\vec{x},t)|^2 dV = |\psi'(\vec{x}',t')|^2 dV'. \tag{2.50}$$

The transformed volume element is related to the original volume by the Jacobian $J(\vec{x},t)$ of the coordinate transformation $(\vec{x}',t') \to (\vec{x},t)$. It is calculated by taking the magnitude of the determinant of the Jacobian matrix $J = |\det \mathbf{J}|$, whose matrix elements are $J_{ij} = \partial_j x_i'$. This then gives the transformed volume element as $dV' = J(\vec{x},t)dV$, which means that the infinitesimal probability of finding the particle within the volume dV is $|\psi|^2 dV =$

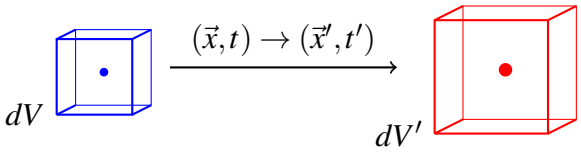

Figure 2.1: A volume element scaled by the Jacobian of a transformation. The probability density must vary inversely to the volume to preserve the outcome of experiment.

$J(\vec{x},t)|\psi'|^2 dV$. Since the states $|\psi\rangle$, $|\psi'\rangle$, and the volume dV were arbitrary, we can divide out the volume. Thus we can finally determine how the wave functions of two coordinate systems are related by taking the square root, which introduces the arbitrary phase factor $e^{iS/\hbar}$, where $S(\vec{x},t)$ is a real function. In total, we arrive at the same Ansatz we introduced in the preceding sections:

$$\psi(\vec{x},t) = \sqrt{J(\vec{x},t)}\psi'(\vec{x}',t')e^{iS(\vec{x},t)/\hbar}. \tag{2.51}$$

Therefore, to interpret the two wave functions as corresponding to the same particle, they must be identical at every point in space (up to a scale factor and phase change).

In general, for an arbitrary coordinate transformation, the Jacobian will depend on position *and* time. In §2.1 and §2.2, it was assumed that this function was only dependent on time. This was because the transformations turned out to be linear, in which case the Jacobian is necessarily independent of position. The requirement that the transformation be linear turns out to have a very important purpose: to preserve the expectation value of position.

Let the original wave function be $\psi(\vec{x},t) = \langle\vec{x}|\psi(t)\rangle$ and let the transformed one be $\psi'(\vec{x}',t') = \langle\vec{x}'|\psi'(t')\rangle$. The expectation value of the position of the particle $|\psi\rangle$ at time t is $\vec{x}_0$ in these coordinates. Physically, this corresponds to the point P in space. Since the transformed state describes an identical state, only in different coordinates, the expectation value of its position must correspond to the same point P in the primed coordinates, $\vec{x}'_p$. Let operators be denoted by upper-case letters, and their eigenvalues by lower-case letters. This

equivalent to the statement that

$$\vec{x}'_p = \left\langle \psi' \middle| \vec{X} \middle| \psi' \right\rangle = \langle \psi | \vec{X} | \psi \rangle', \tag{2.52}$$

where the prime on the right-hand-side of (2.52) denotes the coordinate transformation of $\vec{x}_p$ to $\vec{x}'_p$.

We will now evaluate the expectation value of the position operator by the transformed wave function. By resolution of the identity, we have the result

$$\begin{aligned} \left\langle \psi' \middle| \vec{X} \middle| \psi' \right\rangle &= \int \mathrm{d}^3 x' \left\langle \psi' \middle| \vec{X} \middle| \vec{x}' \right\rangle \left\langle \vec{x}' \middle| \psi' \right\rangle \\ &= \int \mathrm{d}^3 x' \, \vec{x}' \left| \psi'(\vec{x}', t') \right|^2. \end{aligned} \tag{2.53}$$

But we have already determined the form of the transformed wave function to be (2.51). We can insert this transformation into the previous equation to show that

$$\begin{aligned} \left\langle \psi' \middle| \vec{X} \middle| \psi' \right\rangle &= \int \mathrm{d}^3 x J(\vec{x}, t) \vec{x}' \frac{1}{J(\vec{x}, t)} |\psi(\vec{x}, t)|^2 \\ &= \langle \psi | \vec{X}' | \psi \rangle, \end{aligned} \tag{2.54}$$

where $\vec{X}'$ is the transformed position operator, so that $\vec{X}' |\vec{x}\rangle = \vec{x}' |\vec{x}\rangle$. If the primed position is determined by the map $\vec{x}' = T(\vec{x}, t)$, then an operator with eigenvalue $\vec{x}'$ can be constructed by the same function $\vec{X}' = T(\vec{X}, t)$.

In total, this means that the transformation function must satisfy

$$T(\langle \vec{X} \rangle, t) = \left\langle T(\vec{X}, t) \right\rangle \tag{2.55}$$

for all arbitrary states $|\psi\rangle$ in the Hilbert space. But this can only be true for general states if the function $T(\vec{x}, t)$ is linear in position. As a counterexample, consider the SHO stationary states. For these states, the position expectation value for any state $|n\rangle$ is $\langle X \rangle = 0$. If (2.55) was true for higher powers than linear, we would expect $\langle X^2 \rangle = \langle X \rangle^2$. However,

this is not the case, and instead the expectation value of the quadratic position operator is $\langle X^2 \rangle = \hbar(n+1/2)/m\omega$.

Indeed, the equation (2.55) means that the function T must satisfy

$$\int T(\vec{x},t)|\psi|^2 \mathrm{d}^N x = T\left(\int \vec{x}|\psi|^2 \mathrm{d}^N x, t\right), \tag{2.56}$$

for all wave functions ψ. This can only be true if the function T satisfies all of the same properties of linearity that the integral itself satisfies. Assume that $T(\vec{x},t)$ is representable as a power series. Then the integral (2.56) becomes

$$\begin{aligned}&\int (c^{(0)} + c^{(1)}_{ij} x_i + c^{(2)}_{ijk} x_j x_k + \ldots)|\psi|^2 \mathrm{d}^N x \\ &= c^{(0)} \int |\psi|^2 \mathrm{d}^N x + c^{(1)}_{ij} \int x_j |\psi|^2 \mathrm{d}^N x + c^{(2)}_{ijk} \left(\int x_j |\psi|^2 \mathrm{d}^N x\right)\left(\int x_k |\psi|^2 \mathrm{d}^N x\right) + \ldots \end{aligned} \tag{2.57}$$

This can only be true for an arbitrary wave function $\psi(\vec{x},t)$ if the constants $c^{(2)}_{ijk}$ and higher order terms in the power series are zero. Furthermore, $c^{(0)}$ can only be nonzero if $\langle\psi|\psi\rangle \in R$ is a normalizable state.

Thus, the only allowed coordinate transformations are linear in position. As a consequence, the Jacobian is independent of position and $\vec{x}' = M\vec{x} + \vec{b}$, where M is a time-dependent $N \times N$ matrix. Since the position operator is Hermitian, it follows that the linear map M and the translation $\vec{b}$ must both be real so that the transformed position operator is Hermitian, which guarantees that its expectation value will be a real position.

This is not to say that generalized non-linear coordinate transformations are not possible; they are. Consider the transition to spherical coordinates, as it has the position-dependent Jacobian determinant $J = r^2 \sin\theta$. The key difference between these and the transformations we have been considering is that these are transformations of the coordinate system, and not a boost into a new reference frame. This means that it should be understood that we are boosting into the primed frame, and the vector $\vec{X}$ is the same re-

gardless of the coordinate system we choose to measure it in (i.e., Cartesian, cylindrical, spherical...). It is, however, possible to apply nonlinear unitary transformations to the position and momentum operators, though doing so presents several issues, some of which we have already mentioned. For a discussion of this, see [34].

To summarize what we have shown so far, we first showed that as a consequence of the conservation of probability, the wave function must transform as (2.21). Next, we showed that to be able to transform expectation values using the same point transformation, the transformation must necessarily be linear in $\vec{x}$. These two facts are true regardless of the equation of motion for the wave functions and do not depend on the Hamiltonian of the system. They only depend on the Hilbert space structure of quantum mechanics. Then the exact form of the original and transformed Hamiltonians will only change the allowed coordinate transformations and determine the phase function $S(\vec{x},t)$.

We have so far limited ourselves to the class of Hamiltonians that are composed of a kinetic term $\vec{p}^2/2m$ plus a potential function, and have required that the resulting transformed Hamiltonian be of this same type. In some ways, we can best interpret these coordinate transformations as a transformation to a *quasi-inertial* reference frame, in that they preserve the form of the Hamiltonian and the resulting equations of motion, but do not necessarily represent an exact symmetry. In this way, physics looks the same except for additional fictitious forces.

2.3.1 Ehrenfest Theorem in the Transformed Coordinates

Next, we will introduce the equations of motion for observables in both coordinates. Consider a state vector $|\psi(t)\rangle$ that evolves in time according to the Schrödinger equation $H|\psi\rangle = i\hbar\partial_t|\psi\rangle$ where $H^\dagger = H$ is the Hamiltonian. By taking the time derivative of the

expectation value of an operator, and using the Schrödinger equation, one shows

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle &= \left\langle\frac{\partial\Omega}{\partial t}\right\rangle + \langle\psi|\,\Omega\frac{\mathrm{d}}{\mathrm{d}t}\,|\psi\rangle + \left(\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\psi|\right)\Omega\,|\psi\rangle \\ &= \left\langle\frac{\partial\Omega}{\partial t}\right\rangle + \frac{1}{i\hbar}\,\langle\psi|\Omega H|\psi\rangle - \frac{1}{i\hbar}\,\langle\psi|H\Omega|\psi\rangle \\ &= \left\langle\frac{\partial\Omega}{\partial t}\right\rangle + \frac{1}{i\hbar}\,\langle[\Omega,H]\rangle\,.\end{aligned} \tag{2.58}$$

This result is known as the Ehrenfest theorem [27, 28], and is true for any Hamiltonian.

The Hamiltonian of a spinless charged particle is $H = (\vec{P}-\vec{A})^2/2m + V(\vec{X})$. We can then find how the position expectation value changes over time in both reference frames using the Ehrenfest theorem (2.58). Denoting expectation values of the transformed wave function by $\langle\psi'|\Omega|\psi'\rangle = \langle\Omega\rangle'$, the expectation value of the kinetic momenta[2] of the two states are

$$\begin{aligned}m\frac{\mathrm{d}}{\mathrm{d}t}\,\langle\vec{X}\rangle &= \langle\vec{P}-\vec{A}\rangle \\ m\frac{\mathrm{d}}{\mathrm{d}t'}\,\langle\vec{X}\rangle' &= \langle\vec{P}-\vec{A}'\rangle'\end{aligned} \tag{2.59}$$

where $\vec{A}'(\vec{X})$ is the vector potential of the transformed Hamiltonian and is a function of the position operator.

We have already determined that the expectation value of position position for the transformed wave function must be the same point in space as the expectation value of the original state and thus must be related by the same coordinate transformation. This restricts us to the linear time-dependent transformation $M\vec{x}+\vec{b}$, where $M(t)$ is a $N\times N$ real matrix and $\vec{b}(t)$ is a real vector.

The expectation value of position for the transformed state is then

$$\langle\vec{X}\rangle' = \langle M\vec{X}+\vec{b}\rangle\,. \tag{2.60}$$

[2]Meaning the momentum due entirely to the particles velocity, as opposed to the total momentum $\vec{P}$.

Taking the time derivative of both sides of (2.60) and using (2.59), we obtain

$$\frac{\mathrm{d}t'}{\mathrm{d}t}\frac{1}{m}\langle\vec{P}-\vec{A}'\rangle' = \dot{M}\langle\vec{X}\rangle + M\frac{1}{m}\langle\vec{P}-\vec{A}\rangle + \langle\dot{\vec{b}}\rangle\,. \tag{2.61}$$

Next we will look at how the kinetic momentum $\langle\vec{P}-\vec{A}'\rangle'$ of the transformed wave function relates to operators in the original frame. We will evaluate this by taking the integral over the primed position, and then later inserting our ansatz (2.51) for the transformation of wave functions in the position basis. Expanding the expectation value as the integral over the primed position, we have

$$\langle\vec{P}-\vec{A}'\rangle' = \int \mathrm{d}^3x'\,\psi'^*(\vec{x}',t')(-i\hbar\nabla'-\vec{A}'(\vec{x}'))\psi'(\vec{x}',t'), \tag{2.62}$$

where $-i\hbar\nabla'$ is the momentum operator of the primed coordinates. We can now replace ψ' with the ansatz $\psi' = J^{-1/2}e^{-iS/\hbar}\psi(\vec{x},t)$. Next, the ith component of the gradient operator is $\partial_i = (\partial_i x'_j)\partial'_j = M_{ji}\partial_j$, which we can rewrite as $\nabla = M^T\nabla'$. Thus, since our transformation was assumed to be invertible, the primed gradient operator is $\nabla' = (M^T)^{-1}\nabla$.

Putting all of this into the integral, we find that the expectation value of the kinetic momentum in the transformed frame is

$$\langle\vec{p}-\vec{A}'\rangle' = (M^T)^{-1}\langle\vec{P}-\nabla S\rangle - \langle\vec{A}'(\vec{X}')\rangle\,. \tag{2.63}$$

Inserting (2.63) into (2.61), we have that

$$\frac{\mathrm{d}t'}{\mathrm{d}t}\left[(M^T)^{-1}\langle\vec{P}-\nabla S\rangle - \langle\vec{A}'\rangle\right] = \dot{M}\langle\vec{X}\rangle + M\frac{1}{m}\langle\vec{P}-\vec{A}\rangle + \langle\dot{\vec{b}}\rangle \tag{2.64}$$

Since the state is arbitrary, this equality must hold for all states. Therefore, in general the phase $S(\vec{x},t)$ must satisfy

$$\left(\frac{\mathrm{d}t'}{\mathrm{d}t}\right)\nabla S = -M^T\left(\dot{M}\vec{X}+\dot{\vec{b}}+M\vec{A}-\frac{\mathrm{d}t'}{\mathrm{d}t}\vec{A}'\right) + \left(\frac{\mathrm{d}t'}{\mathrm{d}t}-M^TM\right)\vec{P} \tag{2.65}$$

But since the phase is independent of momentum, the coefficient of the momentum operator must be zero:

$$M^T M = \frac{\mathrm{d}t'}{\mathrm{d}t}. \tag{2.66}$$

Let $\partial_{t'} t = \gamma^2$. Then we have $M = R/\gamma$, where R is an orthogonal matrix. Now that we have shown that the linear transformation can only be a scaling, rotation and translation, let us define $\vec{b} = R\vec{\beta}$ so that the total transformation is now $\vec{x}' = R(\vec{x}/\gamma + \vec{\beta})$. The gradient of the phase is then

$$\nabla S = m\left(\frac{\dot{\gamma}}{\gamma}\vec{X} - \gamma R^T \dot{\vec{b}}\right) + \underbrace{\vec{A} - \frac{1}{\gamma}R^T\vec{A}' - mR^T\dot{R}\vec{X}}_{\nabla\alpha} \tag{2.67}$$

The vector potentials may have nonzero curl, or in higher dimensions they may equivalently have nonzero components for the spatial indices ($\mu, \nu > 0$) of the electromagnetic tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. The spatial components of the electromagnetic tensor represents the circulation of the vector potential in the $\mu - \nu$ plane. This nonzero circulation means that we cannot write this as the gradient of a scalar field due to the higher-dimensional analogs of the Helmholtz decomposition [30]. Since the matrix $R^T\dot{R}$ is antisymmetric, the product $R^T\dot{R}\vec{x}$ has nonzero circulation and therefore it cannot be written as the gradient of a scalar field either. For the phase to exist, these terms must be equal to the gradient of a real scalar function $\alpha(\vec{x}, t)$ and all of the sources of circulation must cancel each other. This determines the phase function S and the transformed vector potential $\vec{A}'$:

$$S(\vec{X}, t) = \frac{m}{2}\left(\frac{\dot{\gamma}}{\gamma}\vec{X}^2 + \gamma R^T\dot{\vec{b}}\cdot\vec{x}\right) + \alpha, \tag{2.68}$$

$$\vec{A}'(\vec{X}') = \gamma R(\vec{A} - \nabla\alpha) - m\gamma\dot{R}\vec{X}. \tag{2.69}$$

Thus, the transformed vector potential is just the result of a gauge transformation followed by a rotation and a scaling, with the addition of the $-m\gamma\dot{R}\vec{X}$ term to introduce the fictitious rotational forces, as we have already seen.

We have shown how the Ehrenfest theorem allows us to successfully find the phase

function and the transformed vector potentials. This should perhaps not be surprising, since the theorem is equivalent to the Schrödinger equation, for which we have already derived the FPT. In principle, this can be done again to find the transformed scalar potential by taking the time derivative of the kinetic momentum operator's expectation value in both coordinates and using the Lorentz force law. Starting with

$$\frac{\mathrm{d}}{\mathrm{d}t'}\left\langle \vec{P}-\vec{A}'\right\rangle' = \gamma^2\frac{\mathrm{d}}{\mathrm{d}t}\gamma R\left\langle \vec{P}-\vec{A}-\nabla S+\nabla\alpha+mR^T\dot{R}\vec{x}\right\rangle, \tag{2.70}$$

this would result in an equation relating the gradients of both potentials, which can be solved for the transformed scalar potential. In practice this is proves to be quite difficult, and we were unable to calculate the transformed potential in this manner.

2.4 Rotating Frames

After constant linear acceleration, rotating reference frames are one of the most fundamental non-inertial reference frames. Virtually every experiment we perform is done in the rotating reference frame of the Earth's rotation. This produces fictitious forces which must be accounted for. Therefore, it is necessary to understand the rotating reference frame in both classical and quantum physics. To demonstrate the utility of the form-preserving transformation, we will use it to analyze rotating reference frames and show that it agrees with well-known results.

Let $\vec{x}$ be the position of an object in the inertial frame and $\vec{x}' = R(\vec{\theta})\vec{x}$ be the coordinates in the rotating frame. Here, the linear transformation R is a rotation about the axis $\hat{\theta}$ with angle θ. Performing the coordinate transformation in this way, transforming the components of the vector rather than the basis vectors, is called an active transformation. In this chapter, we will exclusively use active transformations. In a passive transformation, it is the basis vectors themselves, or the coordinate axes, that are rotated. This means that the active transformation about the axis $\vec{\theta}$ represents the coordinate axes of the rotating refer-

ence frame spinning in the opposite directions. Our axis of rotation in the active frame of reference is in the opposite direction to that of the usual passive transformations, such as those used in [32, 35].

To see how rotating reference frames behave in classical mechanics, we start with Newton's second law for an object located at the position $\vec{x}$:

$$\vec{F} = m\vec{a} = m\frac{\mathrm{d}^2}{\mathrm{d}t^2}\vec{x}, \tag{2.71}$$

for the net force $\vec{F}$ on the object in the inertial reference frame. We must be careful taking the time derivatives during an active transformation. We are treating vectors as lists of coordinates, and thus, if we took the total time derivative of the transformed coordinates, it would not take into account the time dependence of the new basis vectors. To counter this, let $\vec{x}' = R\vec{x}$ be the coordinates of the object in the rotating reference frame. Since the position of the object can be written as $\vec{x} = R^T\vec{x}'$, the coordinates are now in an inertial frame, and we need not worry about time-dependent basis vectors while taking the time derivative. Now, Newton's second law becomes

$$\vec{F} = m(R^T\ddot{\vec{x}}' + 2\dot{R}^T\dot{\vec{x}}' + \ddot{R}^T\vec{x}'). \tag{2.72}$$

Here $\dot{\vec{x}}' = \frac{\mathrm{d}}{\mathrm{d}t}\vec{x}'$ denotes the total time derivative of position as measured in the rotating frame. This then only includes the movement within the rotating frame and does not measure the rate of change due to the rotating basis vectors.

As noted previously, the derivative of a rotation matrix is the matrix $\dot{R} = R[\vec{\omega}]_\times$ and we can take the transpose of this to obtain $\dot{R}^T = -[\vec{\omega}]_\times R^T$ since the cross product is anti-symmetric and the time derivative commutes with the transpose operator. The second order time derivative of the rotation matrix then follows likewise, and we have the net force is

$$\vec{F} = m[R^T\ddot{\vec{x}}' - 2\vec{\omega}\times(R^T\dot{\vec{x}}') + \vec{\omega}\times(\vec{\omega}\times\vec{x}) - \dot{\vec{\omega}}\times\vec{x}]. \tag{2.73}$$

From here we obtain that the apparent force on the coordinates of the rotating frame is

$$\begin{aligned}\vec{F}_R \equiv m\ddot{\vec{x}}' &= R\left[\vec{F} - \vec{\omega}\times(\vec{\omega}\times\vec{x}) + \dot{\vec{\omega}}\times\vec{x} + 2\vec{\omega}\times(R^T\dot{\vec{x}}')\right] \\ &= R\vec{F} - \vec{\Omega}\times(\vec{\Omega}\times\vec{x}') + \dot{\vec{\Omega}}\times\vec{x}' + 2\vec{\Omega}\times\dot{\vec{x}}'\end{aligned} \tag{2.74}$$

where $\vec{\Omega} = R\vec{\omega}$ is the angular velocity in the rotated frame. Note that we do not have to be careful about which coordinates we are using to observe the time derivative of $\vec{\omega}$ since

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{\Omega} = R(\vec{\omega}\times\vec{\omega}) + R\dot{\vec{\omega}} = R\dot{\vec{\omega}}, \tag{2.75}$$

and there are no additional changes to the time derivative due to the time-dependence of the rotation itself.

Equation (2.74) shows that the coordinate transformation to the rotating reference frame has introduced the following three fictitious forces:

$$\begin{aligned}\text{Centrifugal Force:} \quad & -m\vec{\omega}\times(\vec{\omega}\times\vec{x}) \\ \text{Euler Force:} \quad & m\frac{\mathrm{d}\vec{\omega}}{\mathrm{d}t}\times\vec{x} \\ \text{Coriolis Force:} \quad & 2m\vec{\omega}\times\vec{v}_r,\end{aligned} \tag{2.76}$$

where $\vec{v}_r = R^T\dot{\vec{x}}'$ is the velocity observed in the rotating frame rotated back into the stationary frame. The vector $\vec{\omega}$ is the angular velocity vector in the non-rotating coordinates. The Euler and Coriolis forces are not conservative, unlike the centrifugal force. They cannot be written as the gradient of a scalar potential $\vec{F} = -\nabla V$ since they are of the form of an anti-symmetric matrix acting on $\vec{x}$. Indeed, if we compare these forces to the potential in (2.49), we see no such analogs of these forces by taking the gradient. We shall soon see that it is the transformed magnetic vector potential that is responsible for the introduction of these forces in quantum mechanics.

It is the goal of this section to compute the quantum analog of the fictitious forces that arise in a rotating reference frame. Consider the point transformation to the rotating

reference frame $\vec{x}' = R\vec{x}$, where $R \in SO(3)$ is a rotation and $t' = t$ leaves the time coordinate invariant. Furthermore, we will take the vector and scalar potentials to both be null in the initial reference frame. The transformed vector potential is then $\vec{A}' = -m\dot{R}(\vec{\omega} \times \vec{x}) = -m\vec{\Omega} \times \vec{x}'$ where $\vec{\Omega} = R\vec{\omega}$ is the angular velocity vector in the rotated reference frame. The transformed Schrödinger equation is then

$$\left[-\frac{\hbar^2}{2m}\nabla'^2 - i\hbar(\vec{\Omega} \times \vec{x}') \cdot \nabla + V(R^T\vec{x}')\right]\psi' = i\hbar\frac{\partial\psi}{\partial t'}. \tag{2.77}$$

We can rewrite the gradient term as $-i\hbar(\vec{\Omega} \times \vec{x}') \cdot \nabla'$ as a dot product with the angular momentum operator $\vec{\Omega} \cdot (\vec{x}' \times -i\hbar\nabla')$. Set $\psi'(\vec{x}', t') = \langle \vec{x}' | \psi'(t') \rangle$, where the transformed position basis is $|\vec{x}'\rangle = |R\vec{x}\rangle$. We will denote the position, momentum, and angular momentum operators by $\vec{X}$, $\vec{P}$ and $\vec{L} = \vec{X} \times \vec{P}$ respectively. The transformed Hamiltonian operator H' can then be written from (2.77) as

$$H' = \frac{\vec{P}^2}{2m} + \vec{\Omega} \cdot \vec{L} + V(R^T\vec{X}). \tag{2.78}$$

In the Schrödinger picture, the state evolves through time according to the Schrödinger equation $H|\psi\rangle = i\hbar|\dot{\psi}\rangle$. It follows that the time derivative of the expectation values of an operator Ξ is determined by the Ehrenfest theorem (2.58).

Dropping the prime on the position, since it is understood that the cross product of two vectors must be in the same coordinates, we have that the time evolution of position in the rotating coordinates is

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{X}\rangle' &= \frac{1}{i\hbar}\left\langle\left[\vec{X}, H'\right]\right\rangle' \\ &= \frac{1}{i\hbar}\left\langle\frac{1}{2m}\left[\vec{X}, \vec{P}^2\right] + \left[\vec{X}, \vec{\omega} \cdot \vec{L}\right]\right\rangle'. \end{aligned} \tag{2.79}$$

The ith component of the commutator with momentum squared can be written as

$$[X_i, P_j P_j] = P_j[P_i, P_j] + [X_i, P_j]P_j = 2i\hbar P_j \delta_{ij}. \tag{2.80}$$

Thus the commutator is $[\vec{X}, \vec{P}^2] = 2i\hbar\vec{P}$. Using the commutation relation $[X_i, L_j] = i\hbar\varepsilon_{ijk}X_k$, the second commutator is

$$\begin{aligned} \left[X_i, \omega_j L_j\right] &= i\hbar\varepsilon_{ijk}\omega_j X_k, \\ \rightarrow [\vec{X}, \vec{\omega}\cdot\vec{L}] &= i\hbar\vec{\omega}\times\vec{X}. \end{aligned} \tag{2.81}$$

Thus the expectation value of velocity of the state (2.79) in the rotating coordinates is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{X}\rangle' = \left\langle \frac{\vec{P}}{m} + \vec{\omega}\times\vec{X} \right\rangle'. \tag{2.82}$$

Using (2.82) as motivation, we define the velocity operator as $\vec{V} = \vec{P}/m + \vec{\omega}\times\vec{X}$. The operator $\vec{P}$ is the conjugate momentum. In the non-rotating reference frames, this is also the kinetic momentum, $m\vec{V}$ (this can be checked with the Ehrenfest theorem in the non-rotating TDSE). We can compute the expectation value of the non-rotating momentum by integrating in the position representation, which yields the result $\langle\vec{P}\rangle'/m = R\langle\vec{P}\rangle/m$. This is just the velocity of the non-rotating initial state rotated into the primed coordinates. Dropping the rotation matrices[3], this gives the classical result [32, Chapter 4.9] [35, Chapter 9.5] (with a sign difference on $\vec{\omega}$ since we are applying R in an active transformation, equivalent to a passive transformation with opposite angle)

$$\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)_r \vec{x} = \frac{\mathrm{d}}{\mathrm{d}t}\vec{x} + \vec{\omega}\times\vec{x}, \tag{2.83}$$

where the subscript r refers to the time derivative in the rotating frame.

[3]This is done for the sake of comparison. It is understood that for the two vectors to be equal, they must be compared in the same basis, so we drop the matrices and assume that statement is true irrespective of basis

Next, the acceleration in the rotating coordinates is given by the time derivative of (2.82) as determined by the Ehrenfest theorem (2.58).

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \vec{V}\right\rangle' &= \left\langle \frac{\partial}{\partial t}\vec{\omega}\times\vec{X}\right\rangle' + \frac{1}{i\hbar}\left\langle \left[\frac{\vec{P}}{m}+\vec{\omega}\times\vec{X}, \frac{\vec{P}^2}{2m}+\vec{\omega}\cdot\vec{L}+V(R^T\vec{X})\right]\right\rangle' \\ &= \left\langle \dot{\vec{\omega}}\times\vec{X}\right\rangle' + \frac{1}{i\hbar}\left\langle \frac{1}{m}\left[\vec{P},\vec{\omega}\cdot\vec{L}+V'\right] + \left[\vec{\omega}\times\vec{x}, \frac{\vec{P}^2}{2m}+\vec{\omega}\cdot\vec{L}\right]\right\rangle'\end{aligned} \tag{2.84}$$

Using the commutation relation $[P_i, L_j] = i\hbar\varepsilon_{ijk}P_k$, one can show that

$$m\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \vec{V}\right\rangle' = \left\langle -\nabla V' + \frac{\mathrm{d}\vec{\omega}}{\mathrm{d}t}\times\vec{X} + 2m\vec{\omega}\times\vec{V} - m\vec{\omega}\times(\vec{\omega}\times\vec{X})\right\rangle'. \tag{2.85}$$

The gradient term of the transformed potential $V'(\vec{X}) = V(R^T\vec{X})$ in the $\vec{x}'$ position basis is $-R\nabla V(\vec{x})$ which is the force of the non-rotating state rotated into the primed coordinates.

Comparing (2.85) with the classical result (2.74), we see that it is the simplest quantization of the classical force. Therefore, we have shown that fictitious forces arising from rotating reference frames agree with the classical result, and are the result of the introduction of a "magnetic field" from the transformed vector potential.

2.5 Free – Harmonic Equivalence

Now that we have studied the transformations in some detail, we will look at a non-trivial 1D example with a time-dependent $\gamma(t)$. Examining the transformation of the potential (2.15), we see that it is possible to introduce a quadratic term to the transformed potential. In particular, free space is equivalent to a harmonic potential, as we can always map solutions to one another. The equivalence of free space to the harmonic oscillator is already a well-known result [17–19]. This equivalence means that any solution of either the free-space or the harmonic oscillator TDSE can always be mapped to a solution of the other. We will show this fact as a result of the FPT in one dimension.

In the derivation of the transformed potential, there was no reason to prefer one set

of coordinates over the other since the equations of motion are preserved. If we were to transform from the primed coordinates back to the original, the potential V should have a symmetric equation to determine it from V'. Indeed, if we take $\varepsilon = 1/\gamma$, $\zeta = -\gamma\beta$ and switch the time derivatives for the primed time derivatives, the transformation for the potential is completely symmetric. To avoid confusion, we will not swap the labels we used previously at this point.

Consider the transformation from the harmonic potential $V = \frac{1}{2}m\omega^2 x^2$ to free space in the primed coordinates $V' = 0$. Using both of these potentials in (2.15), we may construct a differential equation for the parameters α, β, γ:

$$0 = \frac{1}{2}mx^2\left(\omega^2 + \frac{\ddot{\gamma}}{\gamma}\right) + mx(2\dot{\gamma}\dot{\beta} + \gamma\ddot{\beta}) + \frac{m}{2}\gamma^2\dot{\beta}^2 + \dot{\alpha}. \tag{2.86}$$

Since this must be zero for all $x \in \mathbb{R}$, the coefficient of the quadratic, linear, and constant terms must all be zero independently. This gives us the 3 differential equations

$$\ddot{\gamma} + \omega^2\gamma = 0 \qquad 2\dot{\gamma}\dot{\beta} + \gamma\ddot{\beta} = 0 \qquad \dot{\alpha} + \frac{1}{2}m\gamma^2\dot{\beta}^2 = 0. \tag{2.87}$$

Then the scale factor γ must solve the harmonic equation, and has the general solution $\gamma(t) = A\cos(\omega t + \varphi)$ for the real constants A and φ. Next, the translation β is solved by separating the variables and integrating. This gives $\dot{\beta} = v_0\gamma^{-2}$, where v_0 is a constant of integration. Since the time transforms as $dt' = \gamma^{-2}dt$, we immediately have $\beta = v_0 t' + x_0'$ is a constant velocity translation of the x' coordinate. Lastly the gauge parameter α integrates to $\alpha = -\frac{1}{2}mv_0^2 t'$ plus a constant of integration. This constant of integration is just a constant phase factor on the wave function, which has no impact on the physics. Therefore, we are free to set this to be zero.

The transformed time can be integrated from γ to find that $\omega t' = A\tan(\omega t + \varphi) + t_0'$. With the initial conditions of $t' = 0$ and $\dot{t}' = 1$ at $t = 0$, we choose the constants of integration as $A = 1$ and $t_0' = \varphi = 0$. Then we can rewrite the transformation parameters in terms of the

transformed time coordinates t':

$$\omega t' = \tan(\omega t), \qquad \alpha = -\frac{m}{2}v_0^2 t', \qquad \beta = v_0 t' + x_0', \qquad \gamma = \frac{1}{\sqrt{1+(\omega t')^2}}. \tag{2.88}$$

We have now shown that there exists an α, β, γ such that we can take a harmonic oscillator potential to free space. Thus, we can write a free space solution as a harmonic oscillator solution (and vice versa) with

$$\psi_{\text{free}}(x',t') = \frac{1}{[1+(\omega t')^2]^{1/4}}\psi_{\text{SHO}}\left[\frac{x'-\beta}{\sqrt{1+(\omega t')^2}}, \frac{\tan^{-1}(\omega t')}{\omega}\right] \times \exp\left[\frac{im}{2\hbar}\left(\frac{\omega^2 t'(x'-\beta)^2 + 2v_0(x'-\beta)}{1+(\omega t')^2} + v_0^2 t'\right)\right]. \tag{2.89}$$

This completes the map between solutions of free space and the harmonic oscillator.

With this map, we can calculate the free-space dispersion of any harmonic oscillator state. Specifically, we will look at the dispersion of the stationary states. Since we will no longer be comparing the coordinates, we will drop the primes on x and t for brevity.

Let $a_0 = \sqrt{\hbar/m\omega}$ be the length scale of the harmonic oscillator at $t = 0$. Then, if we choose the harmonic oscillator wave function to be the nth energy eigenstate, the free space wave function becomes

$$\psi(x,t) = \frac{1}{\sqrt{2^n n! a_0 \sqrt{\pi}}}\frac{[1+(\omega t)^2]^{n/2}}{(1+i\omega t)^{n+\frac{1}{2}}}\exp\left[-\frac{(x-\beta)^2}{2a_0^2(1+i\omega t)}\right] \times \exp\left[\frac{iv_0}{\omega a_0^2}\left(x - \frac{v_0 t}{2}\right)\right] \mathrm{H}_n\left(\frac{x-\beta}{a_0\sqrt{1+(\omega t)^2}}\right), \tag{2.90}$$

where we have used

$$e^{-i(n+1/2)\tan^{-1}(\omega t)} = \left[\frac{\sqrt{1+(\omega t)^2}}{1+i\omega t}\right]^{n+1/2}. \tag{2.91}$$

To see the results only of the spatial translation and scaling, it is advantageous to remove

the phase and look only at the probability density. The probability density $|\psi|^2$ for this wave function is

$$|\psi|^2 = \frac{1}{2^n n! a(t)\sqrt{\pi}} e^{-(x-\beta)^2/a^2(t)} \mathrm{H}_n\left(\frac{x-\beta}{a(t)}\right), \tag{2.92}$$

where $a(t)$ is the time dependent width of the probability density $a(t) = a_0\sqrt{1+(\omega t)^2}$. From the probability density, it follows that this is an oscillator eigenstate that is translating, stretching along the x-axis while being squished vertically to preserve the norm of the state. The phase that we removed is responsible for transforming the momentum of the state introduced by the time-dependent scaling and translations.

The expectation values of position and momentum, as well as the width of the distribution, can all be computed analytically for the state (2.90) using well-known recursion relations of the Hermite polynomials (see Appendix E). The expectation values of this state are summarized as:

$$\begin{aligned} \langle X\rangle = v_0 t + x_0 \quad \left\langle X^2\right\rangle &= \langle X\rangle^2 + a^2(n+1/2) \qquad \Delta X = a(t)\sqrt{n+1/2} \\ \langle P\rangle = m v_0 \qquad \left\langle P^2\right\rangle &= \langle P\rangle^2 + \frac{\hbar^2}{a_0^2}(n+1/2) \qquad \Delta P = \frac{\hbar}{a_0}\sqrt{n+1/2} \\ \Delta X \Delta P &= \hbar \frac{a(t)}{a_0}\left(n+\frac{1}{2}\right). \end{aligned} \tag{2.93}$$

Notice the lack of dispersion in the width of the momentum distribution. This is not unique to these particular states and in fact will occur for all states that obey a free Schrödinger equation. The width of a momentum distribution [28] is

$$(\Delta P)^2 = \left\langle (P - \langle P\rangle)^2\right\rangle = \left\langle P^2\right\rangle - \langle P\rangle^2. \tag{2.94}$$

We may know take the total time derivative of both sides and apply Ehrenfest's theorem. Doing this, it is easy to see that the time evolution of the width is

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta P^2 = \frac{1}{i\hbar}\left\langle [P^2, H]\right\rangle - 2\langle P\rangle \frac{1}{i\hbar}\langle [P,H]\rangle = -\left\langle P\frac{\partial V}{\partial x} + V'P\right\rangle + 2\langle P\rangle\left\langle \frac{\partial V}{\partial x}\right\rangle. \tag{2.95}$$

But the derivative of the potential $\frac{\partial V}{\partial x}$ is zero for the free particle. Note that this also implies that, for a normalized state with $\langle\psi|\psi\rangle = 1$, there is no momentum dispersion for linear potentials as noted by [36].

2.5.1 Relation to the Diffusion and Heat Equations

The heat equation is a partial differential equation that models the temperature in a medium as it conducts and equilibrates throughout the medium. It is a special case of the diffusion equation [37] without any sources or damping. The heat equation can be written as

$$k\nabla^2 u(\vec{x},t) = \frac{\partial}{\partial\tau}u(\vec{x},t), \tag{2.96}$$

where $u(\vec{x},t)$ is a real scalar field representing the temperature at the point $\vec{x}$ and at time t, and k is the constant of thermal diffusivity with dimensions of L^2/T.

The Schrödinger equation is also a special case of the diffusion equation. Consequently, the heat equation may be transformed into the free Schrödinger equation by transforming to an imaginary time $i\tau = t$ and by writing the diffusion parameter in terms of the particle mass $m = \hbar/2k$. This then becomes the Schrödinger equation for a free particle

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},\tau) = i\hbar\frac{\partial}{\partial t}\psi(\vec{x},\tau), \tag{2.97}$$

where $C\psi(\vec{x},\tau) = u(\vec{x},t)$ and C is a real normalization constant with dimensions of temperature times $L^{1/2}$. Therefore, any free-particle wave function $\psi(\vec{x},it)$ that is real will also be a solution to the heat equation (and the diffusion equation for systems with nonzero potential functions $V(\vec{x},t)$).

This means that our solution for the dispersion of the harmonic oscillator eigenstates (2.90) can also be expressed as a solution to the heat equation. To obtain our solution to the

heat equation, we take $it \to t$ in (2.90). This results in the function

$$u(\vec{x},t) = \frac{C}{\sqrt{2^n n! a_0 \sqrt{\pi}}} \frac{[1-(\omega t)^2]^{n/2}}{(1+\omega t)^{n+\frac{1}{2}}} \exp\left[-\frac{(x-\beta)^2}{2a_0^2(1+\omega t)}\right] \times \exp\left[\frac{v_0}{\omega a_0^2}\left(ix - \frac{v_0 t}{2}\right)\right] \mathrm{H}_n\left(\frac{x-\beta}{a_0\sqrt{1-(\omega t)^2}}\right), \quad (2.98)$$

where the length scale of the oscillator is now $a_0 = \sqrt{2k/\omega}$. In the dispersion example, the frequency of the oscillator was a free parameter. Interpreting this as a solution to the heat equation, the frequency or time constant of the system must then be determined by the material and the initial conditions of the temperature field. Let the length scale of the temperature field a_0 be the free parameter. Then the frequency of the system will be determined by $\omega = 2k/a_0^2$, and the time constant will be $T = 2\pi/\omega = \pi a_0^2/k$

Since the diffusion equation must be real, we must set v_0 to be zero to eliminate the complex exponential. This eliminates the constant velocity translation that was possible in the Schrödinger equation. This then limits $\beta(t)$ to be a constant offset of the position, which we may set to zero without loss of generality. Thus, a solution to the heat equation is

$$u_n(\vec{x},t) = A_n \frac{[1-(\omega t)^2]^{n/2}}{(1+\omega t)^{n+\frac{1}{2}}} \exp\left[-\frac{x^2}{2a_0^2(1+\omega t)}\right] \mathrm{H}_n\left(\frac{x}{a_0\sqrt{1-(\omega t)^2}}\right). \quad (2.99)$$

where A_n is a real constant with dimensions of temperature. However, for $n \neq 0$, the Hermite polynomials contain regions that are negative. These u_n may not then be physically relevant solutions to the heat equation, but are still valid for systems that obey this diffusion equation and allow for negative values in the scalar field.

Chapter 3

Form-Preservation with Operators

The form-preserving transformations are interpreted as all of the coordinate transformations we can perform in which quantum mechanics remains valid. Because we assume we can perform quantum mechanics in any of these reference frames equally, the outcome of experiments and thus the expectation values of observables, as well as the inner product between states must be preserved. Furthermore, since no reference frame is preferred and quantum mechanics may be performed equally in all of them, any two successive FPTs must also be an FPT, suggesting that they must form a group. Since FPTs form a group and preserve inner products and expectation values, they are representable by *unitary operators*.

In this chapter, we will provide an introduction to unitary transformations in quantum mechanics and their properties. We will then derive the Galilean and Schrödinger symmetries as unitary transformations, and will demonstrate that they are special cases of the FPT. We will conclude by determining the unitary representation of the FPT group and its algebra. We show that this is equivalent to the transformation derived for the position representation in the previous chapter. We conclude by using the unitary transformations and their corresponding algebra to extend the FPT to non-relativistic particles with spin.

3.1 Unitary Transformations

A unitary operator is an operator that satisfies the equation

$$U^\dagger U == UU^\dagger = 1, \tag{3.1}$$

meaning that the operator's Hermitian conjugate is also its inverse. To see why these operators are fundamental to QM, consider the transformed state vector $|\psi'\rangle = U|\psi\rangle$ where U is a unitary operator. A unitary transformation of this type will preserve the inner product of state vectors

$$\langle\psi'|\psi'\rangle = \langle\psi|U^\dagger U|\psi\rangle = \langle\psi|\psi\rangle\,. \tag{3.2}$$

It is easy to see from the above equation that not only does the unitary transformation preserve the inner product with the same state, but also with any other state. In this way, it is analogous to orthogonal transformations for regular vectors. Since the inner product in Hilbert space is preserved, the probabilities of measuring a certain outcome from an observable (via the Born rule) are preserved.

Furthermore, the expectation values of observables are preserved. However, the operators themselves must be transformed accordingly. To see this, we take the expectation value of an operator, Ω, and insert the identity operator $U^\dagger U$:

$$\langle\psi|\Omega|\psi\rangle = \langle\psi|U^\dagger U\Omega U^\dagger U|\psi\rangle = \langle\psi'|\Omega'|\psi'\rangle\,, \tag{3.3}$$

where Ω' is the transformed operator $U\Omega U^\dagger$. Thus all of the physical predictions in quantum mechanics remain invariant under the transformation of all state vectors $|\psi\rangle \to U|\psi\rangle$ and all observables $\Omega \to U\Omega U^\dagger$.

Unitary operators may be written as the exponentials e^{iH}, where H are Hermitian operators [27]. It can be checked that operators defined this way are always unitary. The transformation of operators $U\Omega U^\dagger$ can then be calculated by the Campbell identity [31, 33]

$$e^X Y e^{-X} = e^{\mathrm{ad}_X} Y = Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \frac{1}{3!}[X,[X,[X,Y]]] + \ldots \tag{3.4}$$

where $\mathrm{ad}_X Y = [X,Y]$ is the adjoint operator. We define $\mathrm{ad}_X^n Y$ as applying the adoint operator

to n times in succession: $[X,[X,\cdots[X,Y]\cdots]]$ and e^{ad_X} is defined as the operator

$$e^{\mathrm{adx}} = \sum_{n=0}^{\infty} \frac{1}{n!} \mathrm{ad}_X^n. \tag{3.5}$$

It is also important to note that unitary transformations of the position and momentum operators preserve the Heisenberg algebra. If $X_i' = UX_iU^\dagger$ and $P_i' = UP_iU^\dagger$, then it is trivial to verify that the algebra of the transformed operators is invariant under unitary transformations

$$[X_i', P_j'] = i\hbar\delta_{ij} \qquad [X_i', X_j'] = 0 \qquad [P_i', P_j'] = 0. \tag{3.6}$$

As noted by Dirac [38], this makes unitary transformations canonical in the sense that they preserve the fundamental commutation relations just as canonical transformations preserve the Poisson brackets between position and momentum. The Heisenberg algebra is not only invariant to unitary transformations, as Mello and Moshinsky [34] and Anderson [39] point out, but any transformation of the type $\Omega' = U\Omega U^{-1}$. However, these transformations are not considered here because they fail to preserve the hermiticity and expectation value of observables, as well as the inner product of state vectors.

Lastly, we must determine the time evolution of this transformed state and therefore its Hamiltonian operator. To obtain the Schrödinger equation for the transformed state vectors, we take the time derivative of the transformed state

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} U|\psi\rangle = i\hbar \dot{U}|\psi\rangle + i\hbar U \frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle. \tag{3.7}$$

From here we can insert the Schrödinger equation for the original state vector

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t}|\psi'\rangle &= i\hbar \dot{U}|\psi\rangle + UH|\psi\rangle \\ &= (i\hbar \dot{U}U^\dagger + UHU^\dagger)|\psi'\rangle \end{aligned} \tag{3.8}$$

Therefore, the transformed state vector obeys a Schrödinger equation with a new Hamiltonian $H' = i\hbar\dot{U}U^\dagger + UHU^\dagger$.

Note that this transformation of the Hamiltonian does not preserve its expectation value due to the time derivative of the unitary operator. This may seem odd upon first glance, but it should be an expected behavior of unitary transformations. Consider, for example, a boost into a new reference frame with constant velocity v. This will change the expected energy of our particle since the kinetic energies become shifted. Thus *energy is reference frame dependent*, just as it is in classical mechanics, and it is not a problem that the expectation value of energy is not invariant.

Instead, the reader should remind themselves that the Hamiltonian is better understood as the generator of time evolution, rather than an energy operator. With this in mind, it should be natural to predict that the reason the Hamiltonian transforms in this manner is to produce the correct time evolution of the expectation values of observables via the Ehrenfest theorem.

Let A be a quantum operator and $\langle A\rangle$ be the expectation value of the operator for the state $|\psi\rangle$. We then introduce the unitary operator U and the transformed state $|\psi'\rangle = U|\psi\rangle$. Starting from the Ehrenfest theorem, it follows that

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle &= \frac{1}{i\hbar}\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle \\ \longrightarrow \frac{\mathrm{d}}{\mathrm{d}t}\langle A'\rangle' &= \frac{1}{i\hbar}\left\langle [A', UHU^\dagger]\right\rangle' + \left\langle \frac{\partial A'}{\partial t}\right\rangle' - \left\langle \dot{U}U^\dagger A' + A'U\dot{U}^\dagger\right\rangle', \end{aligned} \tag{3.9}$$

where the rightmost term in the second line follows from the product rule of the partial derivative with respect to time. Next, we note that the operator $\dot{U}U^\dagger$ is anti-Hermitian, which follows directly from taking the time derivative of $UU^\dagger = 1$. Thus, the time evolution of the operator's expectation value becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A'\rangle' = \frac{1}{i\hbar}\langle [A', H']\rangle' + \left\langle \frac{\partial A'}{\partial t}\right\rangle', \tag{3.10}$$

where the transformed Hamiltonian $H' = UHU^\dagger + i\hbar\dot{U}U^\dagger$ is what we found previously.

3.2 Symmetries in Quantum Mechanics

Unitary transformations preserve the expectation values of operators and the probabilities of a given measurement. In this way, they mirror rotations and other coordinate transformations in classical mechanics, though Dirac argued that unitary transformations are much more general in what they are capable of representing [38].

When a system is symmetric under a unitary transformation, we mean that the equations of motion for the system are preserved. In the case of quantum mechanics, the Schrödinger equation is left invariant under the transformation. The most straightforward way to preserve the equations of motion is to leave the Hamiltonian invariant under the unitary transformation. Requiring that the Hamiltonian remain invariant, or that $H' = H = i\hbar\dot{U}U^\dagger + UHU^\dagger$, is equivalent to stating that the unitary operator must obey the von Neumann equation of motion [27, chap. 3]

$$[H,U] = i\hbar\frac{\mathrm{d}}{\mathrm{d}t}U, \tag{3.11}$$

which differs from the Heisenberg equation of motion[27, chap. 3] by a minus sign. This must be true for both discrete and continuous symmetries.

For a continuous symmetry, we consider the Lie group element $U = e^{i\varepsilon G}$, where G is a Hermitian generator of the symmetry and ε is a time-independent real parameter. Take $\varepsilon \ll 1$ and expand (3.11) to first order in ε. Then the generator of the continuous symmetry will also satisfy the von Neumann equation

$$[H,G] = i\hbar\frac{\mathrm{d}}{\mathrm{d}t}G. \tag{3.12}$$

Though this was taken from only expanding the exponential to first order, satisfying the first order condition guarantees the higher order conditions of ε are also satisfied [27].

Symmetries of the type (3.12) do not describe all symmetries of the Schrödinger equation. Let $\mathcal{D} = i\hbar\partial_t - H$ be the Schrödinger operator, and the state $|\psi\rangle$ be a state vector so that $\mathcal{D}|\psi\rangle = 0$. We will define a symmetry of the Schrödinger equation to be a unitary transformation U that does not change the Schrödinger equation. Under this condition, we have

$$\begin{aligned} 0 &= \mathcal{D}U|\psi\rangle \\ &= (U\mathcal{D} + [\mathcal{D}, U])|\psi\rangle . \end{aligned} \tag{3.13}$$

The first term vanished since $\mathcal{D}|\psi\rangle$ is zero, as before. Therefore, the second term must also annihilate the state and must therefore be proportional to the product of any operator Ω with $\mathcal{D}$ on the right.

$$[\mathcal{D}, U] \propto \Omega\mathcal{D} \tag{3.14}$$

Therefore, an infinitesimal symmetry generator G satisfies the equations

$$[\mathcal{D}, G] = i\lambda_n\Omega_n\mathcal{D} \tag{3.15}$$

for the unknown numbers λ_n and all operators Ω_n. This statement is equivalent to (3.12) when $\lambda_n = 0$.

Lastly, it is worth noting how the Schrödinger operator transforms. By an insertion of the identity, we see that $\mathcal{D}|\psi\rangle = \mathcal{D}U^\dagger|\psi'\rangle = 0$. Multiplying both sides on the left by U it is clear that the Schrödinger operator transforms as a normal operator $\mathcal{D}' = U\mathcal{D}U^\dagger$ and satisfies the transformed Schrödinger equation $\mathcal{D}'|\psi'\rangle = 0$. It can be checked that this is fully consistent with the transformed Hamiltonian we found in the previous section.

3.2.1 Conserved Quantities

Just as in classical mechanics with Noether's theorem, symmetries in the Schrödinger equation also implies the existence of conserved quantities. Let G be a Hermitian operator, which thus corresponds to some observable that could in principle be measured by exper-

iment, and denote the state by $|\psi\rangle$. The time evolution of this generator can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle G\rangle = \frac{1}{i\hbar}\langle[\mathcal{D}, G]\rangle \tag{3.16}$$

where $\mathcal{D} = i\hbar\partial_t - H$ is the Schrödinger operator. If G is a symmetry, then it will satisfy the symmetry condition $[\mathcal{D}, G] = i\lambda_n \mathcal{D}^n$. The expectation value of this is zero, since $\mathcal{D}|\psi\rangle = 0$ and the Schrödinger operator annihilates the state vector on the right-hand side. Therefore, the total time derivative of the expectation value of a symmetry generator G is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle G\rangle = 0 \tag{3.17}$$

and $\langle G\rangle$ is a conserved quantity. Just as in classical mechanics, the existence of symmetries in the equation of motion implies a corresponding conserved quantity.

3.2.2 Galilean Symmetry Group

The Galilean symmetry group (in three dimensions) is a 10-parameter group that encompasses all of the allowed coordinate transformations that transform one inertial frame into another. In classical mechanics, the Galilean symmetries are constant velocity boosts, rotations, translations, and time translations. Any of these transformations preserves the classical free Hamiltonian, and thus preserves the equations of motion in classical mechanics.

In quantum mechanics, a Galilean symmetry can be represented by the unitary transformation $U = e^{iG/\hbar}$, where G is the Hermitian generator of the symmetry. A unitary operator corresponding to a member of the Galilean symmetry group will leave the free space TDSE invariant. Therefore, they satisfy the symmetry condition (3.11) for the generator G. We follow the usual technique [10, 12, 40] for finding the Lie algebra of the Galilei group. We begin with the ansatz

$$G = \vec{a}(\vec{X}, t)\cdot\vec{P} + b(\vec{X}, t)i\hbar\partial_t + c(\vec{X}, t) \tag{3.18}$$

where $\vec{a}$, b, and c are functions of time and the position operator. Using the symmetry condition $[P^2/2m, G] = i\hbar\dot{G}$ we may solve the system of differential equations for the Galilean symmetry generators.

This ansatz is chosen because it is the most general operator we can write that is linear in momentum and ∂_t. We require these to be linear so that the transformation on position is not a function of the momentum operator, and so that the time transformation is not a function of the operator ∂_t. These would not result in a simple coordinate transformation of the arguments in the wave function.

Expanding the commutator, we have the differential equation

$$[2i(\partial_j a_k)P_j + \hbar\nabla^2 a_k]P_k + [2i(\partial_j b)P_j + \hbar\nabla^2 b]i\hbar\partial_t + [2i(\partial_j c)P_j + \hbar\nabla^2 c] \\ = -2mi(\dot{\vec{a}}\cdot\vec{P} + \dot{b}i\hbar\partial_t + \dot{c}). \quad (3.19)$$

From this, we have the following coupled differential equations:

$$\begin{gathered} \hbar(\nabla^2\vec{a}) + 2i\nabla c + 2mi\dot{\vec{a}} = 0, \qquad (\partial_j a_k)P_j P_k = 0, \quad (\nabla b)\cdot\vec{P} = 0, \\ \hbar\nabla^2 b + 2mi\dot{b} = 0, \quad \hbar\nabla^2 c + 2mi\dot{c} = 0. \end{gathered} \quad (3.20)$$

The functions b and c satisfy the free Schrödinger equation. Furthermore, we have $\nabla b\cdot\vec{P} = 0$, which implies that the gradient of b is the zero vector $\nabla b = \vec{0}$ and thus b is a function of time only. The Schrödinger equation for b then becomes $\dot{b} = 0$, or b is constant in time also. Therefore, $b = t_0$ is a real number.

The general solution to $(\partial_j a_k)P_j P_k = 0$ is $a_i = S_{ij}(t)X_j + u_i(t)$ where $S(t)$ is a real time-dependent $N\times N$ antisymmetric matrix and $\vec{u}(t)$ is a time-dependent N-dimensional vector. In three dimensions we can write the antisymmetric matrix as $S_{ij} = \varepsilon_{ikj}\theta_k(t)$ so that $\vec{a} = \vec{\theta}\times\vec{X} + \vec{u}$. Therefore, the Laplacian of $\vec{a}$ is $\vec{0}$ since $\vec{a}$ is first order in position, and the

remaining differential equations become

$$\partial_i c + m\dot{S}_{ij}X_j + m\dot{u}_i = 0 \tag{3.21a}$$

$$\nabla^2 c + 2mi\dot{c}/\hbar = 0. \tag{3.21b}$$

Taking the divergence of the top equation shows that $\nabla^2 c = 0$ and therefore the function c does not depend on time. Since c is a function of position only and $\vec{u}$ is a function of time only, $\partial_i c = -m\dot{u}_i = -mv_i$ where v_i is a constant. The time derivative of S_{ij} (and the vector $\vec{\theta}$ in three-dimensions) must then be zero. This is because the matrix $\dot{S}$ is still antisymmetric, and there does not exist a scalar function of position $f(\vec{X})$ such that its gradient is the product of position with an antisymmetric matrix.

The solutions for $\vec{a}$, b and c are therefore

$$\vec{a} = S\vec{X} + \vec{v}t + \vec{x}_0 \qquad b = t_0 \qquad c = -m\vec{v}\cdot\vec{X}, \tag{3.22}$$

for the $(N+3)(N+2)/2$ real parameters v_i, x_{0i}, S_{ij} and t_0. These parameters must be real so that the generator is Hermitian.

We can now write all generators of the Galilean symmetry as the linear combination $G = \frac{1}{2}S_{ij}L_{ji} + v_iK_i + x_{0i}P_i + t_0T$ for the boost generator $\vec{K} = t\vec{P} - m\vec{X}$, rotation generator $L_{ij} = X_iP_j - X_jP_i$, translation generator $\vec{P}$ and the time-translation generator $T = i\hbar\partial_t$. Thus, all of the symmetries for the free Hamiltonian in classical mechanics are present in quantum mechanics as well. The Galilean algebra in three-dimensions is defined by the $\binom{10}{2} = 45$ commutation relations

$$\begin{aligned}
&[P_a, P_b] = 0 \qquad [P_a, L_b] = i\hbar\varepsilon_{abc}P_c \quad [P_a, K_b] = im\hbar\delta_{ab} \\
&[T, P_a] = 0 \qquad [T, L_a] = 0 \qquad [T, K_a] = i\hbar P_a \\
&[L_a, L_b] = i\hbar\varepsilon_{abc}L_c \quad [K_a, L_b] = i\hbar\varepsilon_{abc}K_c \qquad .
\end{aligned} \tag{3.23}$$

In higher dimensions, the angular momentum tensor instead satisfies the commutation relations

$$\begin{aligned}[L_{ij},L_{ab}] &= i\hbar(\delta_{jb}L_{ia}+\delta_{ia}L_{jb}-\delta_{ja}L_{ib}-\delta_{ib}L_{ja}) \qquad [T,L_{ab}]=0\\ [K_a,L_{bc}] &= i\hbar(\delta_{ac}K_b-\delta_{ab}K_c) \qquad [P_a,L_{bc}]=i\hbar(\delta_{ac}P_b-\delta_{ab}P_c).\end{aligned} \tag{3.24}$$

Using these commutation relations, we can construct unitary operators of the form $U = e^{ia_bG_b/\hbar}$ where a_b are real constants and $G_b = \{\vec{P}, L_{ij}, \vec{K}, T\}$ are the generators of the Galilean symmetry group. The free Hamiltonian will be invariant to any of these transformations.

Temporal and spatial translation invariance and rotational invariance are all trivial to show for the free Hamiltonian, since they commute with it and feature no time-dependence. Boosts, however, feature the time-dependent generator $\vec{K}$ which commutes with neither the Hamiltonian or the time Translation generator. We will show that the Schrödinger operator is invariant to boosts, regardless of its noncommutativity.

Consider the operator $U = e^{i\vec{v}\cdot\vec{K}/\hbar}$. The transformed Schrödinger operator $\mathcal{D} = T - H$ is

$$\mathcal{D}' = UTU^\dagger - \frac{1}{2m}(U\vec{P}U^\dagger)^2. \tag{3.25}$$

The time-translation operator has the commutation relation $[iK_a, T] = \hbar P_a$, and $[iK_b, \hbar P_a] = m\hbar^2\delta_{ab}$ which commutes with $\vec{K}$. Thus, we only retain the first 3 terms in the Campbell identity (3.4). The time translation operator thus transforms as

$$UTU^\dagger = T + \frac{v_a}{\hbar}[iK_a,T] + \frac{v_av_b}{2!\hbar^2}[iK_b,[iK_a,T]] = T + \vec{v}\cdot\vec{P} + \frac{m}{2}\vec{v}^2 \tag{3.26}$$

Similarly, from the commutation relation $[i\vec{v}\cdot\vec{K}/\hbar, \vec{P}] = m\vec{v}$, the momentum operator transforms as

$$\vec{P} \to U\vec{P}U^\dagger = \vec{P} + m\vec{v} \tag{3.27}$$

under a Galilean boost. Thus, the transformed Schrödinger operator is

$$\mathcal{D}' = T + \vec{v}\cdot\vec{P} + \frac{m}{2}\vec{v}^2 - \frac{(\vec{P}+m\vec{v})^2}{2m} = T - \frac{\vec{P}^2}{2m}, \tag{3.28}$$

which is exactly equal to the original Schrödinger operator. Therefore, boosts leave the free Schrödinger equation invariant.

Lastly, we must determine how the Galilean operators transform the coordinates of a wave function. Starting with space and time transformations, it is easy to see via Taylor expansion that

$$\langle\vec{x}|\, e^{i\vec{a}\cdot\vec{P}/\hbar}\,|\psi(t)\rangle = \psi(\vec{x}+\vec{a},t), \tag{3.29}$$

$$\text{and} \quad \langle\vec{x}|\, e^{iTs/\hbar}\,|\psi(t)\rangle = \psi(\vec{x},t-s). \tag{3.30}$$

Rotations and boosts must be handled with slightly more care.

Starting with 3-dimensional rotations, we have

$$\langle\vec{x}|\, e^{i\vec{\theta}\cdot\vec{L}/\hbar}\,|\psi(t)\rangle = e^{(\vec{\theta}\times\vec{x})\cdot\nabla}\psi(\vec{x},t). \tag{3.31}$$

This is a differential operator acting on the wave function, which we expect to be a rotation. Expanding the exponential to second order, we have

$$e^{(\vec{\theta}\times\vec{x})\cdot\nabla} = 1 + (\vec{\theta}\times\vec{x})\cdot\nabla + \frac{1}{2!}(\varepsilon_{ijk}\theta_j\theta_k\partial_i)(\varepsilon_{abc}\theta_b\theta_c\partial_a) + \ldots \tag{3.32}$$

$$= 1 + (\vec{\theta}\times\vec{x})\cdot\nabla + \frac{1}{2!}(\varepsilon_{abi}\theta_b\varepsilon_{ijk}\theta_j x_k\partial_a + \varepsilon_{ijk}\varepsilon_{abc}\theta_j x_k\theta_b x_c\partial_i\partial_k) + \ldots \tag{3.33}$$

$$= 1 + \left[\vec{\theta}\times\vec{x} + \frac{1}{2!}\vec{\theta}\times(\vec{\theta}\times\vec{x})\right]\cdot\nabla + \frac{1}{2!}(\vec{\theta}\times\vec{x})_i(\vec{\theta}\times\vec{x})_j\frac{\partial^2}{\partial x_i\partial x_j} + \ldots \tag{3.34}$$

The third-order term will introduce a $(\vec{\theta}\times)^3\vec{x}/3!$ into the coefficient of the first-order gradient and so on. Expanding higher order terms it is clear that the pattern becomes a translation

by[4] $[\exp\left(\vec{\theta}\times\right)-1]\vec{x}$. Thus, the rotation operator is

$$\langle\vec{x}|\, e^{i\vec{\theta}\cdot\vec{L}/\hbar}\,|\psi(t)\rangle = \psi\left(e^{\vec{\theta}\times}\vec{x},t\right) = \psi(R\vec{x},t) \tag{3.35}$$

where R is the rotation about the angle $\vec{\theta}$ (see Appendix D), giving the expected result of a rotation on the position coordinate of the wave function.

For general, higher-dimensional rotations,

$$\begin{aligned}\langle\vec{x}|\exp\left(-\frac{i}{2\hbar}S_{ij}L_{ij}\right)|\psi(t)\rangle &= \exp\left[\frac{1}{2}S_{ij}(x_i\partial_j - x_j\partial_i)\right]\psi(\vec{x},t)\\ &= \exp\left(\mathrm{ad}_{\frac{1}{2}S_{ij}(x_i\partial_j-x_j\partial_i)}\right)\psi(\vec{x},t)\end{aligned} \tag{3.36}$$

since $[\partial_i, f(\vec{x})] = \partial_i f(\vec{x})$. Furthermore, the exponential is entirely real, so there is no way to introduce a phase shift $e^{i\phi}$. Since the argument of all functions transforms in the same manner, it is sufficient to consider the simplest scalar function, $\psi(\vec{x},t) = x_i x_i$. Let $\Omega = \frac{\hbar}{2i}S_{ij}(x_i\partial_j - x_j\partial_i)$. Then we have

$$e^{\mathrm{ad}_{i\Omega/\hbar}}x_i x_i = e^{i\Omega/\hbar}x_i e^{-i\Omega/\hbar}e^{i\Omega/\hbar}x_i e^{-i\Omega/\hbar}. \tag{3.37}$$

But since the algebra is the same for $[\Omega, x_i]$ as $[-\frac{1}{2}S_{ab}L_{ab}, X_i]$, the position will transform the same way as the position operator. That is, we have

$$e^{\mathrm{ad}_{i\Omega/\hbar}}x_i x_i = R_{ij}x_j R_{ik}x_k, \tag{3.38}$$

where R is the rotation matrix e^{-S}. Therefore, the wave function transforms identically to the 3-dimensional case; as $\psi(\vec{x},t) \to \psi(R\vec{x},t)$.

Lastly, we will examine the effect of boosts on wave functions. Making use of the Baker-Campbell-Hausdorff (BCH) formula [33], we may break the boost operator into the

[4] This can also be seen by applying n first order rotations $\psi(\vec{x}) \to \psi(\vec{x}+\vec{d\theta}\times\vec{x})$ where $\vec{d\theta} = \vec{\theta}/n$ and taking the limit as $n \to \infty$.

separate exponential operators

$$e^{i\vec{v}\cdot\vec{K}/\hbar} = e^{im\vec{v}^2 t/2\hbar} e^{it\vec{v}\cdot\vec{P}/\hbar} e^{-im\vec{v}\cdot\vec{X}/\hbar}. \tag{3.39}$$

It is then easy to perform the translation on the rightmost exponential and the wave function. This yields the transformation

$$\langle\vec{x}| e^{i\vec{v}\cdot\vec{K}/\hbar} |\psi(t)\rangle = e^{-im\vec{v}\cdot(\vec{x}+\frac{1}{2}\vec{v}t)/\hbar}\psi(\vec{x}+\vec{v}t,t). \tag{3.40}$$

This contains the phase factor $\exp(-im\vec{v}\cdot\vec{x}/\hbar)$ which is responsible for shifting the momentum of the state by $-m\vec{v}$ to keep the expectation value of momentum invariant, as well as a phase $-m\vec{v}^2 t/2\hbar$ corresponding to the modified kinetic energy of the wave function in the boosted frame.

The elements of the 10-parameter Galilean symmetry group and their effects are summarized in Table 3.1.

Table 3.1: The generators of the Galilean symmetry group.

	Generator	U	Effect	Phase Shift
3D Rotations	$\vec{L}$	$e^{i\vec{\theta}\cdot\vec{L}/\hbar}$	$\psi(R\vec{x},t)$	–
ND Rotations	L_{ij}	$e^{-\frac{i}{2\hbar}S_{ij}L_{ij}}$	$\psi(R\vec{x},t)$	–
Translations	$\vec{P}$	$e^{i\vec{a}\cdot\vec{P}/\hbar}$	$\psi(\vec{x}+\vec{a},t)$	–
Boosts	$\vec{K}$	$e^{i\vec{v}\cdot\vec{K}/\hbar}$	$\psi(\vec{x}+\vec{v}t,t)$	$-\frac{im}{\hbar}\vec{v}\cdot(\vec{x}+\frac{1}{2}\vec{v}t)$
Time Shifts	T	$e^{isT/\hbar}$	$\psi(\vec{x},t-s)$	–

3.2.3 Free Schrödinger Group

We have seen that the Galilean symmetry group leaves the free Hamiltonian invariant, and thus any valid state vector $|\psi(t)\rangle$ that solves the Schrödinger equation will remain a solution if it is transformed by a Galilean transformation. The Galilean symmetries are not the only symmetries of the free Schrödinger equation, however. There exist additional symmetries that are present in the Schrödinger equation. These symmetries will act on both

the space and time coordinates, transforming not only the Hamiltonian but the time derivative as well. The totality of this group, the Galilean symmetries as well as its extensions, is called the *Schrödinger group* or sometimes the *maximal kinetic invariance group* of the Schrödinger equation, found by Niederer [12]. For a historical review of the Schrödinger symmetry, see [16].

The free Schrödinger equation contains a global scale symmetry. To see the existence of this symmetry, take $\vec{x} \to \vec{x}' = a\vec{x}$ and $t \to t' = a^2 t$ where a is a real number. With this transformation we have the partial derivatives rescale as $\nabla = a\nabla'$ and $\partial_t = a^2\partial'_t$, thus the scale factors in the transformed Schrödinger equation

$$-\frac{\hbar^2}{2m}a^2\nabla'^2\psi = i\hbar a^2\frac{\partial}{\partial t'}\psi \tag{3.41}$$

can be divided out, and the Schrödinger equation is symmetric under these global scale transformations. The additional symmetries of the Schrödinger group are found by making the global scale symmetry of the Schrödinger equation local in time.

The reason we missed the global and local scale symmetry of the Schrödinger group in our analysis of the Galilean symmetry is because we limited our symmetries to ones that leave the Hamiltonian invariant. Any symmetry that transforms the time derivative $i\hbar\partial_t$ in an equivalent way to the Hamiltonian will have been missed by this analysis, even though this will still preserve the Schrödinger equation. Therefore, instead of using the symmetry condition $[H,G] = i\hbar\dot{G}$, we must perform the same analysis as in [12, 17] and consider solving the equation $[\mathcal{D},G] = i\lambda\mathcal{D}$ where $\lambda(t)$ is a real function.

For the free Hamiltonian, the symmetry condition $[\mathcal{D},G] = i\lambda\mathcal{D}$ becomes

$$2m\dot{G} + 2\nabla G\cdot\vec{P} - i\hbar\nabla^2 G = \lambda\left(2mi\partial_t - P^2/\hbar\right). \tag{3.42}$$

Using the same ansatz as (3.18), we find the general solution to this symmetry condition:

$$\begin{aligned} b &= -\alpha t^2 + 2\eta t + t_0 \quad \vec{a} = (\alpha t - \eta)\vec{X} + S\vec{X} + \vec{v}t + \vec{x}_0 \\ \lambda &= \dot{b} = -2\alpha t + 2\eta \quad c = \frac{iN}{2}(-\alpha t + \eta) - \frac{m\alpha}{2}\vec{X}^2 - m\vec{v}\cdot\vec{X}, \end{aligned} \tag{3.43}$$

for the real constants α, η, t_0, $\vec{v}$, $\vec{x}_0$ and the real antisymmetric matrix S. In $3+1$ dimensions, these total 11 parameters, which again must be real so that the generator is Hermitian. We may now write the most general symmetry generator of the free Schrödinger equation as

$$G = v_i K_i - \frac{1}{2}S_{ij}L_{ij} + x_{0i}P_i + t_0 T + \alpha A - \eta D \tag{3.44}$$

which is identical to the Galilean symmetry with the two additional operators

$$A = -t^2 T + \frac{t}{2}(\vec{X}\cdot\vec{P} + \vec{P}\cdot\vec{X}) - \frac{m}{2}\vec{X}^2, \quad \text{and} \quad D = -2tT + \frac{1}{2}(\vec{X}\cdot\vec{P} + \vec{P}\cdot\vec{X}). \tag{3.45}$$

The generator D is called the *dilation* generator and is responsible for the scale transformations $\vec{X} \to e^{\eta}\vec{X}$ and $t \to e^{2\eta}t$. Dilation generators and why their algebra generates scale transformations are covered in more detail in section 3.3.1. The presence of the dilation operator captures the scale invariance of the TDSE that we pointed out was missing from the Galilean symmetry group.

We have also found another symmetry generator A, which Niederer [12] calls the *expansion generator*. He notes that this is similar to the generator for special conformal transformations; it is a type of time-dependent scale transformation that leaves the free equation invariant. It is the infinitesimal generator for the scale transformations

$$(\vec{x}, t) \to \left(\frac{\vec{x}}{1-\alpha t}, \frac{t}{1-\alpha t}\right) \tag{3.46}$$

with a real Lie parameter α and on the domain $t \in \mathbb{R} \setminus \{1/\alpha\}$.

We can compute the commutators directly from the symmetry generators. Doing this,

we get the algebra in three dimensions as

$$\begin{aligned}
&[P_a,P_b]=0 \qquad [P_a,L_b]=i\hbar\varepsilon_{abc}P_c \quad [P_a,K_b]=im\hbar\delta_{ab} \qquad [T,\vec{P}]=0\\
&[T,\vec{L}]=0 \qquad [T,\vec{K}]=i\hbar\vec{P} \qquad [K_a,L_b]=i\hbar\varepsilon_{abc}K_c \quad [L_a,L_b]=i\hbar\varepsilon_{abc}L_c\\
&[K_a,K_b]=0\\
&[A,\vec{P}]=i\hbar\vec{K} \qquad [A,\vec{K}]=0 \qquad [A,\vec{L}]=\vec{0} \qquad [D,\vec{L}]=\vec{0}\\
&[A,T]=-i\hbar D \qquad [A,D]=2i\hbar A \qquad [D,T]=2i\hbar T \qquad [\vec{K},D]=i\hbar\vec{K}
\end{aligned} \tag{3.47}$$

of which the Galilean algebra is a sub-algebra. In N-dimensions, we replace the angular momentum vector with the angular momentum tensor. These have the commutation relations

$$\begin{aligned}
&[L_{ij},L_{ab}]=i\hbar(\delta_{jb}L_{ia}+\delta_{ia}L_{jb}-\delta_{ja}L_{ib}-\delta_{ib}L_{ja}) \qquad [D,L_{ab}]=0\\
&[K_a,L_{bc}]=i\hbar(\delta_{ac}K_b-\delta_{ab}K_c) \qquad [P_a,L_{bc}]=i\hbar(\delta_{ac}P_b-\delta_{ab}P_c)\\
&[T,L_{ab}]=0 \qquad [A,L_{ab}]=0.
\end{aligned} \tag{3.48}$$

As noted in [12], the operators A, D, and T form an $SL(2,\mathbb{R})$ sub-algebra. To see this, let us transform the operators as $A'=iA/\hbar$, $D'=-iD/\hbar$, and $T'=iT/\hbar$. Together, these operators have the algebra

$$[T',A']=D' \qquad [D',A']=-2A' \qquad [D',T']=2T', \tag{3.49}$$

which makes $\{A',D',T'\}$ an sl_2-triple, i.e. they are isomorphic to the Lie group of $SL(2,\mathbb{R})$ (see Appendix C.1).

Like the Galilean group, we now wish to compute the action of the additional two operators, A and D, on the wave function. Starting with the operator $U=e^{i\eta D/\hbar}$ and the transformed state $|\psi'\rangle=U|\psi\rangle$, we have that in the position basis

$$\psi'(\vec{x},t)=e^{\eta N/2}e^{2\eta t\partial_t}e^{\eta\vec{x}\cdot\nabla}\psi(\vec{x},t). \tag{3.50}$$

Expanding the exponential and comparing it to a Taylor series, we see that the operator $e^{\eta\vec{x}\cdot\nabla}$ takes a function of $\vec{x}$ to a function of $e^{\eta}\vec{x}$. The exponential with the time derivative behaves in the same way, but with η scaled by a factor of two. Thus in the position basis

$$\psi'(\vec{x},t) = e^{\eta N/2}\psi\left(e^{\eta}\vec{x}, e^{2\eta}t\right). \tag{3.51}$$

Finding the action of A on the state vector is considerably more difficult to do directly. However, we can learn a lot about how this behaves by seeing how it transforms the position operator. We begin with the transformed position operator

$$\vec{X}' = e^{\alpha \mathrm{ad}_{iA/\hbar}}\vec{X}. \tag{3.52}$$

For the first-order adjoint, we have

$$\frac{1}{\hbar}[iA,\vec{X}] = \frac{itX_b}{\hbar}[P_b,\vec{X}] = t\vec{X}. \tag{3.53}$$

The only other commutator we must consider is

$$\frac{1}{\hbar}[iA,t^n\vec{X}] = \frac{1}{\hbar}[-it^2T,t^n]\vec{X} + t^{n+1}\vec{X} = (n+1)t^{n+1}\vec{X}. \tag{3.54}$$

It then follows that $\mathrm{ad}^n_{iA/\hbar}\vec{X} = n!t^n\vec{X}$. Therefore, the transformed position operator must be

$$\vec{X}' = e^{\alpha \mathrm{ad}_{iA/\hbar}}\vec{X} = \vec{X}\sum_{n=0}^{\infty}(\alpha t)^n = \frac{\vec{X}}{1-\alpha t}. \tag{3.55}$$

Likewise, we can compute how the time "operator" transforms as $UtU^{\dagger}$. Since $\mathrm{ad}^n_{iA/\hbar}t = n!t^n$, it is trivial to compute the transformation. It is

$$t' = e^{\alpha\,\mathrm{ad}_{iA/\hbar}}t = \frac{t}{1-\alpha t}. \tag{3.56}$$

Now we wish to compute the transformed wave function in the position basis $\psi'(\vec{x},t) = \langle\vec{x}|U|\psi\rangle$. We can expand the expansion operator to first order in α using the exponential function and compute its resulting action on the wave function in this manner. Doing so results in

$$\langle\vec{x}|U|\psi\rangle = \exp\left\{\alpha t^2\partial_t + \alpha t\vec{x}\cdot\nabla + \alpha t\frac{N}{2} - i\alpha\frac{m}{2\hbar}\vec{x}^2\right\}\psi(\vec{x},t) \tag{3.57}$$

$$\sim \left(1+\frac{\alpha tN}{2}\right)\left(1-i\frac{\alpha m\vec{x}^2}{2\hbar}\right)\psi[\vec{x}(1+\alpha t),t(1+\alpha t)], \tag{3.58}$$

for $\alpha \ll 1$. As we mentioned in §2.3, the operator $\vec{X}'$ transforms in the same way as the position coordinate in the argument of the wave function. Thus we expect that $\vec{x} \to \vec{x}/(1-\alpha t) \sim \vec{x}(1+\alpha t)$. This asymptotic expansion agrees with (3.58) to first order. Expanding this operator past first order is a tedious exercise, and instead, we may find the action of the expansion generator by different means.

Assuming that this is the correct asymptotic expansion, we can instead use the form-preserving transformation to calculate the time transformation, scale factor, and phase function. The corresponding functions are $\gamma = 1-\alpha t$, $\beta = 0$ and we will set the phase to $\alpha(t) = 0$. With these parameters, the transformed time variable is

$$t' = \int \frac{\mathrm{d}t}{(1-\alpha t)^2} = \frac{1}{\alpha}\left(\frac{1}{1-\alpha t}+C\right). \tag{3.59}$$

where C is a constant of integration that corresponds to the freedom of time translation. Setting $C=-1$ results in the desired time transformation $t' = t/(1-\alpha t)$. The wave function would then transform as

$$\psi'(\vec{x},t) = (1-\alpha t)^{-N/2}\exp\left(\frac{im}{2\hbar}\frac{-\alpha\vec{x}^2}{1-\alpha t}\right)\psi\left(\frac{\vec{x}}{1-\alpha t},\frac{t}{1-\alpha t}\right), \tag{3.60}$$

which does indeed agree with the first order expansion of (3.58). It may also be checked that these parameters leave the free particle invariant in (2.41).

Table 3.2: The generators of the Schrödinger symmetry group. In the last row, the alternate expansion parameter is $\sigma(t) = (1-\alpha t)^{-1}$.

	Generator	U	Effect	Phase Shift	Scale Factor
3D Rotations	$\vec{L}$	$e^{i\vec{\theta}\cdot\vec{L}/\hbar}$	$\psi(R\vec{x},t)$	–	–
ND Rotations	L_{ij}	$e^{-\frac{i}{2\hbar}S_{ij}L_{ij}}$	$\psi(R\vec{x},t)$	–	–
Translations	$\vec{P}$	$e^{i\vec{a}\cdot\vec{P}/\hbar}$	$\psi(\vec{x}+\vec{a},t)$	–	–
Boosts	$\vec{K}$	$e^{i\vec{v}\cdot\vec{K}/\hbar}$	$\psi(\vec{x}+\vec{v}t,t)$	$-\frac{im}{\hbar}\vec{v}\cdot(\vec{x}+\frac{1}{2}\vec{v}t)$	–
Time Shifts	T	$e^{isT/\hbar}$	$\psi(\vec{x},t-s)$	–	–
Dilations	D	$e^{i\eta D/\hbar}$	$\psi(e^{\eta}\vec{x},e^{2\eta}t)$	–	$e^{\eta N/2}$
Expansions	A	$e^{i\alpha A/\hbar}$	$\psi(\sigma\vec{x},\sigma t)$	$\frac{im\sigma}{2\hbar}\vec{x}^2$	$\sigma^{N/2}$

Schrödinger Group as Form Preservation

We have shown the usual Lie method for finding the Schrödinger group. However, the form-preserving transformation proves to be a convenient alternative way to derive the free Schrödinger group. Setting both the scalar and vector potentials in (2.40) and (2.41) to be zero, we arrive at the following symmetry conditions:

$$\vec{0} = -\gamma R\nabla\alpha - m\gamma\dot{R}(\vec{x}+\gamma\vec{\beta}), \tag{3.61}$$

$$0 = \frac{\partial\alpha}{\partial t} + \frac{m\ddot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x}\cdot(2\dot{\gamma}\vec{\beta}+\gamma\ddot{\vec{\beta}}) + \frac{m}{2}(\gamma\dot{\vec{\beta}})^2 + \nabla\alpha\cdot m\gamma R^T\frac{\partial\vec{x}'}{\partial t} - \frac{m}{2}[\gamma\dot{R}\vec{x}']^2. \tag{3.62}$$

The general solution is the coordinate transformation

$$\vec{x}' = \frac{R}{ct+d}(\vec{x}+\vec{v}_0t+\vec{x}_0) \qquad\qquad t' = \frac{at+b}{ct+d}. \tag{3.63}$$

Where $\vec{v}_0,\vec{x}_0 \in \mathbb{R}^N$, $R \in O(N)$ and $ad-bc=1$ are all real numbers. Since the numbers $ad-bc=1$, the time transformation is a Möbius transformation on the real time t. Möbius transformations are a type of conformal transformation. The connection of the Schrödinger group to the conformal group is discussed in [8]. As Niederer in [12] mentions, this transformation results directly from the fact that the generators $\{A,D,T\}$ form an sl_2 triple, and thus the matrix formed by these constants $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ is a element of $SL(2,\mathbb{R})$.

The parameters of the FPT that generate this transformation are

$$\alpha = -\frac{m}{2a^2}\vec{v}^2 t + \alpha_0 \qquad \vec{\beta} = \frac{1}{\gamma}(\vec{v}_0 t + \vec{x}_0) \qquad \gamma = ct + d, \tag{3.64}$$

where $\alpha_0 \in \mathbb{R}$. The phase of the transformation is then computed as

$$S = \frac{m}{ct+d}\left(\frac{c}{2}\vec{x}^2 + \frac{1}{a}\vec{x}\cdot\vec{v}_0\right) - \frac{m}{2a^2}\vec{v}_0^2 t + \alpha_0. \tag{3.65}$$

It is easy to check that (3.60) is a special case of this transformation with $c = -\alpha$ and the rest of the constants set to either zero or one as appropriate. The entire Schrödinger group is covered by these transformations, thus showing that it is a valuable tool in identifying symmetry transformations in Schrödinger equations. This approach also works for the "maximal kinetic invariance group" of the harmonic oscillator, which, thanks to the oscillator–free space equivalence, is isomorphic to the free symmetry group [17].

3.3 Unitary Representation of Form Preservation

Unlike the usual symmetry groups, such as the Galilean and Schrödinger groups, the form-preserving group does not necessarily leave the Schrödinger equation invariant. Instead, the form-preserving group is a *quasi-symmetry group* that guarantees a Schrödinger equation for one potential will be transformed to another. In this way, we guarantee that a solution to a Schrödinger equation can always be transformed into a solution of a different equation, rather than the same one in the case of the symmetry groups.

There is another key difference between the form-preserving group, the Schrödinger group and the SHO groups. Since time is a parameter and not an operator in QM, there is no reason for us to treat it as one for the general case, as we have done for the previous symmetry groups. Forcing the time coordinate to be a parameter means that it must commute with all of the infinitesimal generators in the Lie group. Since time commutes, we will lose all generators of time transformations in the algebra, such as the generator of time

translations $i\hbar\partial_t$. Consequently, we are free to let the parameters of the group depend on time. As we shall see later in §3.3.6, the time transformations do form a group that is not necessarily continuous.

Despite these differences, we will show that all of the FPTs form a Lie group, whose representation is unitary. We will derive the group from the infinitesimal generators and show that the entire transformation and the phase factor can be attained in this manner.

3.3.1 The Dilation Generator

The Lie theory of translations and rotations is well understood (see Appendix D for rotations). The next generator that we must introduce in detail is the dilation generator D to generate the γ scaling transformations. We will determine the form of the dilation generator by deducing its commutation relations.

Assume that a hermitian operator D exists so that we can construct a unitary scaling operator by the exponential map $U = e^{iaD/\hbar}$, where a is a real parameter. According to (3.4), this operator will transform the position operator as

$$e^{iaD/\hbar} X e^{-iaD/\hbar} = X + \frac{ia}{\hbar}[D,X] - \frac{a^2}{2!\hbar^2}[D,[D,X]] - \frac{ia^3}{3!\hbar^2}[D,[D,[D,X]]] + \dots \tag{3.66}$$

First, we consider this to first order in a. To scale the position operator, we require that it transforms to a real scalar multiple of the position operator $bX = X + ia[D,X]/\hbar$. If we restrict b to be real, then the commutator $[D,X]$ must be proportional to iX. Thus, we set the commutator to

$$[D,X] = -i\hbar X \tag{3.67}$$

so that to first order, $X \to X(1+a)$.

Since the commutator is proportional to X, all the terms in the series (3.66) will contribute to the final sum. Using $[D,X] = -i\hbar X$, it follows that applying the commutator successive times will only multiply the position operator by the constant $-i\hbar$, or $\mathrm{ad}_D^n(X) =$

$(-i\hbar)^n X$. Thus we have

$$e^{iaD/\hbar} X e^{-iaD/\hbar} = X\left(1 + a + \frac{a^2}{2!} + \frac{a^3}{3!} + \ldots\right) = Xe^a. \tag{3.68}$$

This can also be determined from the fact that $X' = e^{\mathrm{ad}_{iaD/\hbar}} X = e^{(ia/\hbar)(-i\hbar)} X = e^a X$.

Since unitary transformations preserve the canonical commutation relation $[X,P] = i\hbar$, the momentum operator must be scaled inversely to the position operator, up to the addition of an operator that commutes with position. In other words, P must transform to $e^{-a}P + \Omega$ where Ω is an operator that commutes with position $[X,\Omega] = 0$. If we assume that the operator Ω is zero, then this would suggest that the commutator of the dilation operator with the momentum operator is analogous to the position commutator, only differing in sign $[D,P] = i\hbar P$.

To fully determine the commutation relation between D and P, consider the unitary operator

$$U = e^{-iaP/\hbar} e^{-iaD/\hbar} e^{iaP/\hbar} e^{iaD/\hbar} \tag{3.69}$$

which corresponds to first dilating the position by e^a, then translating the position by a, reversing the dilation, and then reversing the translation. Written explicitly, we have the transformation

$$X \underset{e^{iaD/\hbar}}{\longrightarrow} e^a X \underset{e^{iaP/\hbar}}{\longrightarrow} e^a(X+a) \underset{e^{-iaD/\hbar}}{\longrightarrow} X + ae^a \underset{e^{-iaP/\hbar}}{\longrightarrow} X + a(e^a - 1) = X + a^2 + O\big(a^3\big), \tag{3.70}$$

which is a translation by a^2 (to all orders it is a translation by $a(e^a - 1)$). Thus, for small a, we can write the transformation as the translation operator $U \sim e^{ia^2 P/\hbar}$.

Expanding the unitary operator to second order in a, we have

$$\begin{aligned} U &= e^{-iaP/\hbar}\left(e^{iaP/\hbar} - \frac{ia}{\hbar}[D, e^{iaP/\hbar}] + \ldots\right) \\ &= 1 + \frac{a^2}{\hbar^2}[D,P] + O\big(a^3\big), \end{aligned} \tag{3.71}$$

where the first line follows from the Campbell identity. Comparing orders of a to the operator $e^{ia^2P/\hbar}$, we find that the commutator of the dilation operator with the momentum is

$$[D,P] = i\hbar P, \tag{3.72}$$

as expected.

One can check that two operators that satisfy both (3.67) and (3.72) are XP and PX. Since neither of these operators are Hermitian on their own, we set the dilation operator to be the symmetrized sum

$$D = \frac{1}{2}(XP+PX) + D_0, \tag{3.73}$$

where D_0 is an operator that commutes with both P and X (which will be responsible for time dilation in subsequent sections).

Generalizing to higher dimensions requires no significant alterations to the derivation of the dilation operator in 1D. If we follow the same arguments for general dimensions, the commutations relations become

$$[D,\vec{X}] = -i\hbar\vec{X} \qquad\qquad [D,\vec{P}] = i\hbar\vec{P}. \tag{3.74}$$

This is satisfied by the operator

$$D = \frac{1}{2}(\vec{X}\cdot\vec{P}+\vec{P}\cdot\vec{X}) + D_0, \tag{3.75}$$

where again D_0 commutes with $\vec{X}$ and $\vec{P}$.

Lastly, we must determine how the dilation operator transforms eigenstates of the position and momentum operators. First, consider an eigenstate of position $|\vec{x}\rangle$ and the unitary operator $U = e^{i\ln\gamma D/\hbar}$. We note that

$$U\vec{X}\,|\vec{x}\rangle = \vec{X}'(U\,|\vec{x}\rangle) = \vec{x}(U\,|\vec{x}\rangle). \tag{3.76}$$

Therefore, $\vec{x}$ is the eigenvalue of the operator $\vec{X}' = \gamma\vec{X}$ on the state $U|\vec{x}\rangle$. We then conclude that the transformed state must be

$$U|\vec{x}\rangle = A_\gamma|\vec{x}/\gamma\rangle \tag{3.77}$$

for a complex constant A_γ.

To determine the constant A_γ, we start with the orthogonality condition for the two non-normalizable states $\langle\vec{x}|\vec{y}\rangle = \delta^N(\vec{x}-\vec{y})$ for the two positions $\vec{x}$ and $\vec{y}$. Next, via an insertion of the identity $I = U^\dagger U$, we have

$$\begin{aligned}\langle\vec{x}|\vec{y}\rangle &= \langle\vec{x}|U^\dagger U|\vec{y}\rangle \\ &= \langle\vec{x}/\gamma|A_\gamma^* A_\gamma|\vec{y}/\gamma\rangle \\ &= |A_\gamma|^2\gamma^n\delta^n(\vec{x}-\vec{y}).\end{aligned} \tag{3.78}$$

Consequently, we have $|A_\gamma|^2 = \gamma^{-N}$, or that the constant of proportionality is determined to be $A_\gamma = \gamma^{-N/2}e^{i\phi}$ for an as yet undetermined real phase factor, ϕ.

To determine the phase factor, we consider the precise form of the dilation operator

$$D = \frac{1}{2}(\vec{X}\cdot\vec{P}+\vec{P}\cdot\vec{X})/2 + D_0 = \vec{X}\cdot\vec{P} - N\frac{i\hbar}{2} + D_0 \tag{3.79}$$

where N is the number of dimensions. Next, we look at the transformed state $U^\dagger|\psi\rangle$ in the position representation. This is

$$\begin{aligned}\langle\vec{x}|U^\dagger|\psi\rangle &= \langle\vec{x}|e^{-i\ln\gamma(\vec{X}\cdot\vec{P}-in\hbar/2+D_0)/\hbar}|\psi\rangle \\ &= \gamma^{-n/2}e^{-i\ln\gamma D_0/\hbar}e^{-\ln\gamma\vec{x}\cdot\nabla}\psi(\vec{x},t)\end{aligned} \tag{3.80}$$

where the second line follows since $-in\hbar/2$ and D_0 commutes with $\vec{X}\cdot\vec{P}$.

Lastly, we must consider the action of the operator $e^{ax\partial_x}$, which is similar to a translation operator. Naïvely we might expect this to take the function $f(x) \to f(x+ax)$, which is not

too far from correct. Taylor expanding this operator acting on the function $f(x)$ in orders of the parameter a yields

$$\left[1+ax\partial_x+\frac{a^2}{2}(x\partial_x+x^2\partial_x^2)+\frac{a^3}{3!}(x\partial_x+3x^2\partial_x^2+x^3\partial_x^3)+\ldots\right]f(x)$$
$$=\left[1+\left(a+\frac{a^2}{2}+\frac{a^3}{3!}+\ldots\right)x\partial_x+\frac{1}{2!}\left(a^2+a^3+\ldots\right)x^2\partial_x^2+\ldots\right]f(x). \quad (3.81)$$

We can compare this to the Taylor series of the function $f(e^a x)$ near x, which is the equation

$$f(e^a x)=\left[1+\left(a+\frac{a^2}{2}+\ldots\right)x\partial_x+\frac{1}{2!}\left(a+\frac{a^2}{2}+\ldots\right)^2 x^2\partial_x^2+\ldots\right]f(x). \quad (3.82)$$

Comparing orders of a and $x\partial_x$ of equations (3.81) and (3.82), we find that the two equations are equal (as can be checked to higher orders).

To prove this for all orders, we assume that the function $f(x)$ can be represented by a power series in x. Then

$$e^{ax\partial_x}x^n=\sum_{k=0}^{\infty}\frac{1}{k!}(na)^k x^n=(e^a x)^n, \quad (3.83)$$

and each power of x in the power series is transformed to $e^a x$. Therefore, $e^{a\partial_x}f(x)=f(e^a x)$ for all functions f that may be written as a power series. This result generalizes to higher dimensions for the operator $e^{a\vec{x}\cdot\nabla}$ as we might have expected, since the transformed position eigenstate must be proportional to $\vec{x/\gamma}$, as we saw previously.

Returning to the transformed state vector in the position basis, we now have

$$\langle\vec{x}|\,U^\dagger\,|\psi\rangle=\gamma^{-n/2}e^{-i\ln\gamma D_0/\hbar}\psi(\vec{x}/\gamma,t)\,. \quad (3.84)$$

From this transformed state in the position basis, we can determine the position eigenstate

from the Hermitian conjugate $(U|\vec{x}\rangle)^\dagger = \langle\vec{x}|U^\dagger$. Therefore, the transformed state must be

$$\boxed{e^{-i\ln\gamma D/\hbar}|\vec{x}\rangle = \gamma^{-n/2}e^{-i\ln\gamma D_0/\hbar}|\vec{x}/\gamma\rangle\,.} \tag{3.85}$$

The constant phase factor introduced by a dilation transformation of the position eigenstate can then be arbitrarily determined by adding multiples of the identity to D_0. In the case of the free Schrödinger group, the operator D_0 is responsible for time dilations. However, time is not treated as an operator in the form-preserving group. Then for the form-preserving group, D_0 is an arbitrary constant. Since this is just a constant phase transformation, we are free to set it to be zero without loss of generality.

3.3.2 Momentum translation by position

In addition to the dilation operator, to completely encompass the FPT, we need a way to take $\vec{P}$ and add the position operator to it $\vec{P}+a\vec{X}$, as was present in the position basis. Let us denote the generator of infinitesimal momentum translation by position by the operator Q so that

$$e^{-iaQ/\hbar}\vec{P}e^{iaQ/\hbar} = \vec{P} - \frac{ia}{\hbar}[Q,\vec{P}] + O\big(a^2\big) = \vec{P} + a\vec{X}. \tag{3.86}$$

Comparing the first-order terms in a, we see that the commutator must be $[Q,\vec{P}] = i\hbar\vec{X}$.

Next, to see how Q must commute with the position operator, we construct the operator

$$U = e^{iaX_i/\hbar}e^{iaQ/\hbar}e^{-iaX_i/\hbar}e^{-iaQ/\hbar} = 1 + \frac{a^2}{\hbar^2}[Q,X_i] + O\big(a^3\big), \tag{3.87}$$

This unitary operator will transform the momentum as

$$P_i \underset{e^{-iaQ/\hbar}}{\longrightarrow} P_i + aX_i \underset{e^{-iaX_i/\hbar}}{\longrightarrow} P_i + a + aX_i \underset{e^{iaQ/\hbar}}{\longrightarrow} P_i + a \underset{e^{iaX_i/\hbar}}{\longrightarrow} P_i, \tag{3.88}$$

which is the same effect as the identity operator. So comparing orders of a leads us to the conclusion that $[Q,X_i]$ is zero. Thus, since the Q operator commutes with position, all of

the higher-order commutators in the Campbell identity (3.86) are zero.

Next, we repeat this procedure to compute the commutation relation with the dilation operator. By considering the operator

$$U = e^{iaD/\hbar} e^{iaQ/\hbar} e^{-iaD/\hbar} e^{-iaQ/\hbar}, \tag{3.89}$$

one can show that $[Q,D] = 2i\hbar Q$. Repeating this procedure with the rotation generator $\vec{L}$ shows that it commutes with Q, as expected since Q is a scalar. An operator that satisfies all of these commutation relations is

$$Q = \frac{1}{2}\vec{X}^2 \tag{3.90}$$

3.3.3 The Form Preserving Algebra

These two additional operators we have looked at are, in fact, all that is necessary to recreate all of the FPTs, save the time transformation, which will be discussed later. Now that we have computed all of the commutation relations in three-dimensions for the 11 operators $\vec{X}$, $\vec{P}$, $\vec{L}$, Q, and D, we can write the $\binom{11}{2} = 55$ commutation relations of the algebra.

$$\begin{array}{lll}
[X_a, X_b] = 0 & [P_a, P_b] = 0 & [X_a, P_b] = i\hbar\delta_{ab} \\
[X_a, L_b] = i\hbar\varepsilon_{abc} X_c & [P_a, L_b] = i\hbar\varepsilon_{abc} P_c & [L_a, L_b] = i\hbar\varepsilon_{abc} L_c \\
[D, \vec{X}] = -i\hbar\vec{X} & [D, \vec{p}] = i\hbar\vec{P} & [D, Q] = -2i\hbar Q \\
[D, \vec{L}] = [Q, \vec{L}] = 0 & [Q, \vec{X}] = 0 & [Q, \vec{P}] = i\hbar\vec{X}.
\end{array} \tag{3.91}$$

In higher dimensions, we may no longer use the angular momentum vector and must use the angular momentum tensor. The angular momentum tensor satisfies the commutation

relations

$$\begin{aligned}
[L_{ij}, L_{ab}] &= i\hbar(\delta_{jb}L_{ia} + \delta_{ia}L_{jb} - \delta_{ja}L_{ib} - \delta_{ib}L_{ja}) \\
[X_a, L_{bc}] &= i\hbar(\delta_{ac}X_b - \delta_{ab}X_c) \quad [P_a, L_{bc}] = i\hbar(\delta_{ac}P_b - \delta_{ab}P_c) \\
[Q, L_{ab}] &= 0 \qquad\qquad\qquad [D, L_{ab}] = 0.
\end{aligned} \tag{3.92}$$

In addition to these operators, we may show that the algebra closes with any real scalar function of the position operator. The function itself must be real so that the generators remain Hermitian. The closure of these functions within the algebra is necessary to ensure gauge transformations are contained within the FPT. Let $f(\vec{X})$ and $g(\vec{X})$ be real scalar functions of the position operator. Then the algebra is

$$\begin{aligned}
[\vec{X}, f] &= 0 \quad [\vec{P}, f] = -i\hbar\nabla f \qquad [\vec{L}, f] = i\hbar\nabla f \times \vec{X} \\
[Q, f] &= 0 \quad [D, f] = -i\hbar\vec{X}\cdot\nabla f \quad [f, g] = 0,
\end{aligned} \tag{3.93}$$

which closes since each of the $\partial_i f$ is an arbitrary scalar function of position.

It is worth paying attention to the commutation relation $[\vec{L}, f]$, since this is not zero for all functions f. This commutator is zero for rotationally invariant, or central, functions $f(\vec{X}^2)$ since the gradient of a central function is parallel to the position vector. That argument only works for three dimensions, however. In higher dimensions, we have

$$[L_{ab}, f] = i\hbar(X_a\partial_b f - X_b\partial_a f) \tag{3.94}$$

This is also zero for central functions. Let the central function $f(\vec{X}) = f(u)$ where $u = \vec{X}^2$. Then the partial derivative is $\partial_a f = 2x_a \frac{\mathrm{d}}{\mathrm{d}u} f$, and the commutator (3.94) becomes

$$[L_{ab}, f] = 2i\hbar\left(X_a X_b \frac{\mathrm{d}f}{\mathrm{d}u} - X_b X_a \frac{\mathrm{d}f}{\mathrm{d}u}\right) = 0. \tag{3.95}$$

The fact that central functions commute with the angular momentum vector and tensor

Table 3.3: The transformation of operators $\vec{A}' = U\vec{A}U^\dagger$ under the form preserving group where $U = \exp(i\Omega/\hbar)$ is an element of the group, and Ω and A are elements of the Lie algebra. The rotation matrix R is $R = \exp(\vec{\theta}\times) = \exp(S)$. All scalar functions of position transform as $[g(\vec{X})]' = g(\vec{X}')$.

Ω	$\vec{X}'$	$\vec{P}'$	$\vec{L}'$	L'_{ij}	Q'	D'
$\vec{a}\cdot\vec{X}$	$\vec{X}$	$\vec{P}-\vec{a}$	$\vec{L}+\vec{a}\times\vec{X}$	$L_{ij}+a_iX_j-a_jX_i$	Q	$D-\vec{a}\cdot\vec{X}$
$\vec{b}\cdot\vec{P}$	$\vec{X}+\vec{b}$	$\vec{P}$	$\vec{L}+\vec{b}\times\vec{P}$	$L_{ij}+b_iP_j-b_jP_i$	$Q+\vec{b}\cdot\vec{X}+\frac{b^2}{2}$	$D+\vec{b}\cdot\vec{P}$
$\vec{\theta}\cdot\vec{L}$	$R\vec{X}$	$R\vec{P}$	$R\vec{L}$	–	Q	D
$\frac{1}{2}S_{ij}L_{ji}$	$R\vec{X}$	$R\vec{P}$	–	$R_{ia}R_{jb}L_{ab}$	Q	D
λQ	$\vec{X}$	$\vec{P}-\lambda\vec{X}$	$\vec{L}$	L_{ij}	Q	$D-2\lambda Q$
δD	$e^{\delta}\vec{X}$	$e^{-\delta}\vec{P}$	$\vec{L}$	L_{ij}	$e^{2\delta}Q$	D
$f(\vec{X})$	$\vec{X}$	$\vec{P}-\nabla f$	$\vec{L}+\nabla f\times\vec{X}$	$L_{ij}+X_i\partial_j f-X_j\partial_i f$	Q	$D-\vec{X}\cdot\nabla f$

operators is important because this shows that central potentials are invariant to rotations.

The presence of arbitrary scalar functions of position is important to ensure that all gauge transformations of the vector potentials are valid parts of the algebra. Thus, we have the generators of the form-preserving transformations are $\vec{X}$, $\vec{P}$, $\vec{L}$, Q, D, and all other real scalar functions $f(\vec{X})$. The generator Q itself is a real scalar function of the type described, but it has particular importance in the 1D case where we wish not to introduce a vector potential, and thus it will keep its independent name.

Now that we have specified the algebra of the form-preserving group, we may compute the transformations of the Lie algebra under the unitary transformations it generates. These transformations are summarized in Table 3.3. All members of the group may be, in principle, separated into individual unitary operators like the ones in Table 3.3 by the use of the BCH formula.

3.3.4 Unitary Form-Preservation in 1D

The one-dimensional case can be derived from the form-preserving group. In this case, we limit the Hamiltonian to $P^2/2m + V(X)$. Unlike the full N-dimensional case, where we consider the effect of vector potentials and time-dependent rotations, the 1D case only considers a scalar potential. Limiting transformations to those that do not introduce a vector potential means that there will be some restrictions on the parameters of the transformation.

When we discuss the N-dimensional case, we will see that this is no longer a problem.

For the one-dimensional case, consider the unitary operator

$$U = e^{-i\lambda/\hbar} e^{-iaQ/\hbar} e^{-ibX/\hbar} e^{-i\beta P/\hbar} e^{i\ln\gamma D/\hbar}, \tag{3.96}$$

where λ, a, b, β and $\gamma > 0$ are real functions that depend on time only. This operator is a dilation followed by a translation in position, momentum, and then lastly a translation of momentum by position.

Under the unitary transformation (3.96), the position and momentum operators transform as

$$X' = UXU^\dagger = \gamma(X-\beta); \qquad P' = UPU^\dagger = \frac{1}{\gamma}(P+b+aX). \tag{3.97}$$

Next, we consider the time derivative of the unitary operator. If we use the series definition of the exponential, since none of the operators depend on time, we find $\partial_t e^{ia\Omega} = i\dot{a}\Omega e^{ia\Omega}$. Thus, through an application of the chain rule, we have

$$\begin{aligned} i\hbar\dot{U}U^\dagger = \dot{\lambda} + \dot{a}Q + \dot{b}e^{-iaQ/\hbar}Xe^{iaQ/\hbar} + \dot{\beta}e^{-iaQ/\hbar}e^{-ibX/\hbar}Pe^{ibX/\hbar}e^{iaQ/\hbar} \\ - \frac{\dot{\gamma}}{\gamma}e^{-iaQ/\hbar}e^{-ibX/\hbar}e^{-i\beta P/\hbar}De^{i\beta P/\hbar}e^{ibX/\hbar}e^{iaQ/\hbar}. \end{aligned} \tag{3.98}$$

The above transformations on X and P are trivial since we have already discussed them. The transformations on the dilation operator can be determined by the algebra (3.91).

As per Table 3.3, the commutation relation $[P,D] = -i\hbar P$ means the operator $e^{-i\beta P/\hbar}$ takes $D \to D - \beta P$ and translates it by the momentum operator. Similarly $[X,D] = i\hbar X$ so we now have in total $D \to D + bX - \beta(P+b)$. Lastly, the commutation relation $[Q,D] = 2i\hbar Q$ means that the final operator will translate D by $2Q$, ie. $D \to D + 2aQ + bX - \beta(P+b+aX)$.

Now we can finally write the transformed Hamiltonian from (3.8) as

$$H' = \frac{P^2}{2m\gamma^2} + D\left(\frac{a}{m\gamma^2} - \frac{\dot\gamma}{\gamma}\right) + P\left(\frac{b}{m\gamma^2} + \dot\beta + \beta\frac{\dot\gamma}{\gamma}\right) + X\left(\dot b - b\frac{\dot\gamma}{\gamma} + a\dot\beta + a\beta\frac{\dot\gamma}{\gamma}\right) + Q\left(\frac{a^2}{m\gamma^2} + \dot a - 2a\frac{\dot\gamma}{\gamma}\right) + b\left(\dot\beta + \beta\frac{\dot\gamma}{\gamma}\right) + \frac{b^2}{2m\gamma^2} + V(X') + \dot\lambda. \quad (3.99)$$

Under the restrictions of the 1D case, the transformed Hamiltonian must not contain momentum contributions of linear order or mixed terms of position and momentum. Thus, we must choose the parameters a and b such that the coefficients of D and P are zero. The former requires that

$$a = m\gamma\dot\gamma, \quad (3.100)$$

and the latter requires

$$b = -m\gamma(\dot\gamma\beta + \gamma\dot\beta). \quad (3.101)$$

With these two coefficients chosen, the Hamiltonian can be simplified with a bit of algebra. This yields the transformed Schrödinger equation

$$\left[\frac{P^2}{2m} + \frac{m\gamma^3\ddot\gamma}{2}X^2 - m\gamma^3\ddot\zeta X - \frac{m}{2}\gamma^2\dot\zeta^2 + \gamma^2 V(X') + \gamma^2\dot\lambda\right]\left|\psi'\right\rangle = i\hbar\frac{\mathrm{d}}{\mathrm{d}t'}\left|\psi'\right\rangle, \quad (3.102)$$

where we have substituted $\zeta = \gamma\beta$ and $dt' = \gamma^{-2}dt$.

The original wave function can be recovered by taking $|\psi\rangle = U^\dagger|\psi'\rangle$. In the position basis, this is

$$\begin{aligned}\psi(x,t) &= \langle\vec{x}|\, e^{-i\ln\gamma D/\hbar}e^{i\beta P/\hbar}e^{ibX/\hbar}e^{iaQ/\hbar}e^{i\lambda/\hbar}\left|\psi'(t')\right\rangle \\ &= \frac{1}{\sqrt{\gamma}}e^{\gamma\beta\partial_x}e^{ibx/\gamma\hbar}e^{iax^2/2\gamma^2\hbar}e^{i\lambda/\hbar}\psi'(x/\gamma,t') \\ &= \frac{1}{\sqrt{\gamma}}\exp\left\{\frac{im}{2\hbar}\left[\frac{\dot\gamma}{\gamma}x^2 - 2\gamma x\dot\beta - \gamma\beta(\dot\gamma\beta + 2\gamma\dot\beta)\right] + \frac{i\lambda}{\hbar}\right\}\psi'(x/\gamma+\beta,t')\end{aligned} \quad (3.103)$$

which only differs from (2.16) by the addition of a function of time in the phase, which we can remove by absorbing it into the function λ. Let $\lambda = \alpha + m\gamma\beta(\dot\beta + 2\gamma\dot\beta)/2$ where α is an

arbitrary function of time. The wave function now matches (2.16) exactly

$$\psi(x,t) = \frac{1}{\sqrt{\gamma}} \exp\left[\frac{im}{2\hbar}\left(\frac{\dot{\gamma}}{\gamma}x^2 - 2\gamma\dot{\beta}x\right) + \frac{i\alpha}{\hbar}\right]\psi'(x/\gamma+\beta,t'). \tag{3.104}$$

Finally, by computing the time derivative of λ it is easy to show that the transformed potential is

$$\frac{1}{\gamma^2}V'(X) = \frac{m\ddot{\gamma}}{2\gamma}X'^2 - mX'(2\dot{\gamma}\dot{\beta}+\gamma\ddot{\beta}) + V(X') + \dot{\alpha} + \frac{m}{2}\gamma^2\dot{\beta}^2, \tag{3.105}$$

where $X' = \gamma(X-\beta)$. This is in agreement with what we found during the previous chapter in equation (2.15).

3.3.5 Unitary Form-Preservation in Higher Dimensions

Unlike the one-dimensional case, for higher dimensions we must include rotations that are time dependent in general. Let them be of the form

$$U = \begin{cases} \exp\left(\frac{-i}{\hbar}\vec{\theta}\cdot\vec{L}\right) & N = 3 \\ \exp\left(\frac{i}{2\hbar}S_{ij}L_{ij}\right) & N \neq 3 \end{cases}. \tag{3.106}$$

Where the real, time dependent parameters $S_{ij}(t)$ and $\vec{\theta}(t)$ parametrize the rotation matrices for general dimensions $R = e^S$ and 3-dimensions $R = e^{[\vec{\theta}]_\times}$, respectively. Unlike the other algebra generators, the operators $\vec{\theta}\cdot\vec{L}$ and $\frac{1}{2}S_{ij}L_{ij}$ do not commute with their time derivative. This makes computing the time derivative $\dot{U}$ more complicated than the other transformation generators in the FPT. The time derivatives are computed explicitly in Appendix D.5.

Now that we have seen the one-dimensional case and have briefly discussed time-dependent rotations, we now have all of the information required to perform a transformation under the most general element of the group. There are only four unique transformations that we must consider to encompass the entire general case for the form-preserving transformations. They are:

1. Gauge transformations $e^{-i\alpha/\hbar}$ for a scalar function of position and time α. These leave the position operator invariant and transform the momentum as $\vec{P} \to \vec{P} + \nabla\alpha$. Thus, the entire Hamiltonian will transform as

$$H(\vec{X},\vec{P}) \to H(\vec{X},\vec{P}+\nabla\alpha) + \dot{\alpha}. \tag{3.107}$$

   For the Hamiltonian of a spinless charged particle, this has the net effect of transforming the vector potential as $\vec{A} \to \vec{A} - \nabla\alpha$ and the scalar potential as $V \to V + \dot{\alpha}$.

   These gauge transformations encompass both operators of the type $\vec{a}\cdot\vec{X}$ and Q since they are both scalar functions of position and their effects can be considered in this class of transformations.

2. Position translations $e^{-i\vec{\beta}\cdot\vec{P}/\hbar}$ for a real vector $\vec{\beta}$. These leave the momentum operator invariant and instead translates the position operator $\vec{X} \to \vec{X} - \vec{\beta}$. The Hamiltonian transforms as

$$H(\vec{X},\vec{P}) \to H(\vec{X}-\vec{\beta},\vec{P}) + \dot{\vec{\beta}}\cdot\vec{P}. \tag{3.108}$$

3. Rotations of the form $e^{-i\vec{\theta}\cdot\vec{L}/\hbar}$ in three dimensions or $e^{iS_{ij}L_{ij}/2\hbar}$ in general. This transformation will rotate the position and momentum vectors by applying the linear transformation R^T. According to (D.52), the overall Hamiltonian will become

$$H(\vec{X},\vec{P}) \to H(R^T\vec{X},R^T\vec{P}) + (\dot{R}R^T\vec{X})\cdot\vec{P} \tag{3.109}$$

4. Dilations $e^{i\ln\gamma D/\hbar}$ where γ is a real function of time. As already discussed, the dilation operator scales the position and momentum operator opposite to one another $\gamma\vec{X}$ and $\vec{P}/\gamma$. The Hamiltonian is

$$H(\vec{X},\vec{P}) \to H\left(\gamma\vec{X},\frac{1}{\gamma}\vec{P}\right) - \frac{\dot{\gamma}}{\gamma}D \tag{3.110}$$

The strategy we will employ is to perform each of these transformations individually and then build up the entire general transformation from the algebra. The precise order of these transformations does not matter, except as a matter of convenience to compare to the results we obtained in the position basis.

The order we will perform the transformations is a gauge transformation, followed by the dilation, the translation, and lastly the rotation. This will have the net effect on the position operator transforming it to

$$\vec{X} \to \vec{\xi} = \gamma(R^T \vec{X} - \vec{\beta}) \tag{3.111}$$

We begin with a general gauge transformation on the original Hamiltonian with a gauge parameter $\alpha(\vec{X},t)$. In accordance with (3.107), the transformed Hamiltonian will be

$$H = \frac{(\vec{P} + \nabla\alpha - \vec{A})^2}{2m} + V + \dot{\alpha}, \tag{3.112}$$

where all functions of position $\vec{A}$, V and α are evaluated at the original position $\vec{X}$. We will denote the gauged vector potential as $\vec{A}_\alpha$ for convenience.

Next we will apply the dilation $e^{i\ln\gamma D/\hbar}$, which will transform the Hamiltonian as

$$\begin{aligned} H &= \frac{(\vec{P} - \gamma\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \frac{\dot{\gamma}}{\gamma} D \\ &= \frac{(\vec{P} - \gamma\vec{A}_\alpha - m\gamma\dot{\gamma}\vec{X})^2}{2m\gamma^2} + V + \dot{\alpha} - \dot{\gamma}\vec{A}_\alpha \cdot \vec{X} - \frac{1}{2} m\dot{\gamma}^2\vec{x}^2, \end{aligned} \tag{3.113}$$

where the arguments of all the functions of position are with respect to the total transformation on the position operator, which is currently $\gamma\vec{X}$. Although it appears that we have altered the vector potential, the curl of this addition is zero[5] so it can be removed with a gauge transformation. Performing the transformation $e^{-im\gamma\dot{\gamma}\vec{x}^2/2}$ transforms the Hamiltonian

[5] In higher dimensions, the antisymmetric derivative $\partial_i\gamma X_j - \partial_j\gamma X_i = \gamma(\delta_{ij} - \delta_{ji})$ is zero, since there is no rotational component of the vector field $\vec{X}$ in any plane. Therefore this gauge transformation leaves the electromagnetic tensor invariant.

to

$$H = \frac{(\vec{P} - \gamma\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \dot{\gamma}\vec{A}_\alpha \cdot \vec{X} + \frac{1}{2}m\gamma\ddot{\gamma}\vec{X}^2 \tag{3.114}$$

and removes the gauge transformation to the vector potential.

The third transformation is the translation by the time-dependent vector $-\vec{\beta}$. The Hamiltonian, according to (3.108), will become

$$\begin{aligned} H &= \frac{(\vec{P} - \gamma\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \dot{\gamma}\vec{A}_\alpha \cdot (\vec{X} - \vec{\beta}) + \frac{1}{2}m\gamma\ddot{\gamma}(\vec{X} - \vec{\beta})^2 + \dot{\vec{\beta}} \cdot \vec{P} \\ &= \frac{(\vec{P} + m\gamma^2\dot{\vec{\beta}} - \gamma\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \frac{m}{2}\gamma^2\dot{\vec{\beta}}^2 + \vec{A}_\alpha \cdot [\gamma\dot{\vec{\beta}} - \dot{\gamma}(\vec{X} - \vec{\beta})] + \frac{1}{2}m\gamma\ddot{\gamma}(\vec{X} - \vec{\beta})^2, \end{aligned} \tag{3.115}$$

where again we have absorbed the $\dot{\vec{\beta}} \cdot \vec{P}$ term into the kinetic momentum squared term in the front. This again is the gradient of a scalar function, so we can remove it with the gauge parameter $-m\gamma^2\dot{\vec{\beta}} \cdot \vec{X}$, which will further transform the Hamiltonian to

$$\begin{aligned} H = \frac{(\vec{P} - \gamma\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \frac{m}{2}\gamma^2\dot{\vec{\beta}}^2 + \vec{A}_\alpha \cdot [\gamma\dot{\vec{\beta}} - \dot{\gamma}(\vec{X} - \vec{\beta})] \\ + \frac{1}{2}m\gamma\ddot{\gamma}(\vec{X} - \vec{\beta})^2 - m\gamma\vec{X} \cdot (2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}). \end{aligned} \tag{3.116}$$

Finally, we will now apply the appropriate rotation $e^{-i\vec{\theta}\cdot\vec{L}/\hbar}$ or $e^{\frac{i}{2\hbar}S_{ij}L_{ij}}$, yielding

$$\begin{aligned} H = \frac{(\vec{P} - \gamma R\vec{A}_\alpha)^2}{2m\gamma^2} + V + \dot{\alpha} - \frac{m}{2}\gamma^2\dot{\vec{\beta}}^2 + \vec{A}_\alpha \cdot [\gamma\dot{\vec{\beta}} - \dot{\gamma}(R^T\vec{X} - \vec{\beta})] \\ + \frac{1}{2}m\gamma\ddot{\gamma}(R^T\vec{X} - \vec{\beta})^2 - m\gamma R^T\vec{X} \cdot (2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}) + (R\vec{\omega} \times \vec{X}) \cdot \vec{P} \end{aligned} \tag{3.117}$$

where $R\vec{\omega} \cdot L = (R\vec{\omega} \times \vec{X}) \cdot \vec{P}$ follows from the cyclic property of the scalar triple product (while keeping the order of position and momentum the same). Since the divergence of

$R\vec{\omega}\times\vec{X}$ is zero, the dot product with momentum commutes and we can write

$$H=\frac{(\vec{P}-\vec{A}')^2}{2m\gamma^2}+V+\dot{\alpha}-\frac{m}{2}\gamma^2\dot{\vec{\beta}}^2+\vec{A}_\alpha\cdot[\gamma\vec{\omega}\times R^T\vec{X}+\gamma\dot{\vec{\beta}}-\dot{\gamma}(R^T\vec{X}-\vec{\beta})]$$
$$-\frac{1}{2}m\gamma^2(R\vec{\omega}\times\vec{X})^2+\frac{1}{2}m\gamma\ddot{\gamma}(R^T\vec{X}-\vec{\beta})^2-m\gamma R^T\vec{X}\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\gamma\ddot{\vec{\beta}}) \quad (3.118)$$

where $\vec{A}'$ is the transformed vector potential

$$\vec{A}'(\vec{X},t)=\gamma R[\vec{A}(\vec{\xi},t)-(\nabla\alpha)(\vec{\xi},t)]-m\gamma^2R\vec{\omega}\times\vec{X}. \quad (3.119)$$

Unlike the previous times, the cross product cannot be written as the gradient of a scalar field and so cannot be absorbed by a gauge transformation. Thus, time-dependent rotations create an apparent magnetic field.

The last transformation we will make is a gauge transformation by the gauge parameter $m\gamma^2\vec{\beta}\cdot\dot{\vec{\beta}}$, which finally takes our Hamiltonian to

$$H=\frac{(\vec{P}-\vec{A}')^2}{2m\gamma^2}+V+\dot{\alpha}+\frac{m}{2}\gamma^2\dot{\vec{\beta}}^2+\vec{A}_\alpha\cdot[\gamma\vec{\omega}\times R^T\vec{X}+\gamma\dot{\vec{\beta}}-\dot{\gamma}(R^T\vec{X}-\vec{\beta})]$$
$$-\frac{1}{2}m\gamma^2(R\vec{\omega}\times\vec{X})^2+\frac{1}{2}m\gamma\ddot{\gamma}(R^T\vec{X}-\vec{\beta})^2-m\gamma(R^T\vec{X}-\vec{\beta})\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\gamma\ddot{\vec{\beta}}). \quad (3.120)$$

This can now be rewritten in terms of the transformed coordinate $\vec{\xi}$ as

$$H=\frac{(\vec{P}-\vec{A}')^2}{2m\gamma^2}+V(\vec{\xi})+\dot{\alpha}(\vec{\xi})+[\vec{A}(\vec{\xi})-(\nabla\alpha)(\vec{\xi})]\cdot\gamma R^T\frac{\partial\vec{\xi}}{\partial t}-\frac{1}{2}m[\vec{\omega}\times(\vec{\xi}+\gamma\vec{\beta})]^2+\frac{m\ddot{\gamma}}{2\gamma}\vec{\xi}^2$$
$$-m\vec{\xi}\cdot(2\dot{\gamma}\dot{\vec{\beta}}+\gamma\ddot{\vec{\beta}})+\frac{1}{2}m\gamma^2\dot{\vec{\beta}}^2. \quad (3.121)$$

Equation (3.121) can be written as $H=\gamma^{-2}[(\vec{P}-\vec{A}')^2/2m+V']=\gamma^{-2}H'$. The TDSE for the transformed state is then

$$H'\left|\psi'\right\rangle=i\hbar\gamma^2\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi'\right\rangle. \quad (3.122)$$

Let $dt' = \gamma^{-2} dt$ so that $\gamma^2 \frac{\mathrm{d}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t'}$. Then the time evolution of the transformed state is just the Schrödinger equation of a spinless charged particle in an electromagnetic field

$$\left[\frac{(\vec{P}-\vec{A}')^2}{2m} + V'\right] |\psi'\rangle = i\hbar \frac{\mathrm{d}}{\mathrm{d}t'} |\psi'\rangle, \tag{3.123}$$

where the vector potential is (3.119) and the scalar potential is

$$\begin{aligned}\frac{1}{\gamma^2} V'(\vec{X},t') = V + \dot{\alpha} + (\vec{A} - \nabla\alpha)\cdot\gamma R^T \frac{\partial\vec{\xi}}{\partial t} - \frac{1}{2}m[\vec{\omega}\times(\vec{\xi}+\gamma\vec{\beta})]^2 + \frac{m\dot{\gamma}}{2\gamma}\vec{\xi}^2 \\ - m\vec{\xi}\cdot(2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}) + \frac{1}{2}m\gamma^2\dot{\vec{\beta}}^2.\end{aligned} \tag{3.124}$$

The functions $\vec{A}$, V and α and its derivatives are all evaluated at the point $(\vec{\xi},t)$. This is identical to what was found in the position basis in (2.41) with $\vec{X}$ swapped with $\vec{x}'$ and $\vec{\xi}$ swapped with $\vec{x}$.

In total, the unitary transformation that we applied to get to this point is the transformation

$$U = e^{-\frac{im}{\hbar}\gamma^2\vec{\beta}\cdot\dot{\vec{\beta}}} e^{-\frac{i}{\hbar}\vec{\theta}\cdot\vec{L}} e^{\frac{im}{\hbar}\gamma^2\dot{\vec{\beta}}\cdot\vec{X}} e^{-\frac{i}{\hbar}\vec{\beta}\cdot\vec{P}} e^{-\frac{im}{2\hbar}\dot{\gamma}\gamma\vec{X}^2} e^{\frac{i}{\hbar}\ln\gamma D} e^{-\frac{i\alpha}{\hbar}}. \tag{3.125}$$

This unitary operator transforms the position and momentum[6] as

$$\vec{X} \to \vec{\xi} = \gamma(R^T\vec{X} - \vec{\beta}) \qquad \vec{P} \to \vec{\Pi} = \frac{1}{\gamma}R^T\vec{P} - m\gamma\dot{\vec{\beta}} + m\frac{\dot{\gamma}}{\gamma}\vec{\xi} + \nabla\alpha(\vec{\xi}) \tag{3.126}$$

Then, in the position basis, the transformed state vector is $|\psi'[t'(t)]\rangle \equiv |\psi'(t)\rangle = U|\psi(t)\rangle$, is

$$\begin{aligned}\psi'(\vec{x},t') &= e^{-\frac{im}{\hbar}\gamma^2\vec{\beta}\cdot\dot{\vec{\beta}}} e^{-(\vec{\theta}\times\vec{x})\cdot\nabla} e^{\frac{im}{\hbar}\gamma^2\dot{\vec{\beta}}\cdot\vec{x}} e^{-\vec{\beta}\cdot\nabla} e^{-\frac{im}{2\hbar}\dot{\gamma}\gamma\vec{x}^2} \gamma^{3/2} e^{\ln\gamma\vec{x}\cdot\nabla} e^{-\frac{i\alpha}{\hbar}} \psi(\vec{x},t) \\ &= \gamma^{3/2}\exp\left[-\frac{im}{2\hbar}\left(\frac{\dot{\gamma}}{\gamma}\vec{\xi}^2 - 2\gamma\dot{\vec{\beta}}\cdot\vec{\xi}\right) - \frac{i}{\hbar}\alpha(\vec{\xi})\right]\psi(\vec{\xi},t)\end{aligned} \tag{3.127}$$

which is precisely the result we found in the position basis, with only the labels of the

[6] If one does not count the $\nabla\alpha$ translation towards the vector potential transformation

variables and functions different.

3.3.6 On the Time transformation

There are some questions about the time transformation that we have not yet answered in this text. Do the γ transformations form a group? If we ignore the ambiguity about time being a parameter, not an operator, can we write a unitary operator for every γ transformation?

To answer the first question, we must check that the γ transformations satisfy all of the group axioms. Namely, the group product must satisfy closure, associativity, the existence of the identity element, and the existence of the inverse element [33]. Let us first consider two successive γ transformations: γ_1 and γ_2, and their corresponding group members $g(\gamma_1)$ and $g(\gamma_2)$. Since the group must close, there must be a third group member $g(\gamma_3)$ so that

$$g(\gamma_1)\cdot g(\gamma_2) = g(\gamma_3), \tag{3.128}$$

where this group member means to first apply γ_2 followed by the transformation γ_1. Under a γ transformation, the time coordinate undergoes the transformation

$$t \to \int_a^t \frac{d\tau}{\gamma^2(\tau)} = \Gamma(t), \tag{3.129}$$

where a is a real constant. We will denote the element of the group that corresponds to this transformation by the member $g(\gamma;a)$.

Then the total transformation due to two successive time transformations by $g(\gamma_2;b)$ followed by $g(\gamma_1;a)$ is

$$t \to \Gamma_3(t) = \Gamma_2(\Gamma_1(t)), \tag{3.130}$$

where Γ_n is the respective time transformation function (3.129) for γ_n. Since the Γ are at least once differentiable, we take the derivative of both sides of (3.129) with respect to time

to obtain

$$\gamma_3(t) = \pm\gamma_2(\Gamma_1(t))\gamma_1(t). \tag{3.131}$$

The square root introduces the $\pm$, however, this can be shown to be positive only since the position transformation is also a group and constrains it to be positive. Under the transformation $g(\gamma_3)$, the position changes as

$$x \xrightarrow[\gamma_2;b]{} \frac{x}{\gamma_2(t)} \xrightarrow[\gamma_1;a]{} \frac{x}{\gamma_2(\Gamma_1(t))\gamma_1(t)} = \frac{x}{\gamma_3(t)}, \tag{3.132}$$

which eliminates the negative case. Therefore, the group composition rule for a γ transformation is

$$g(\gamma_1;a)\cdot g(\gamma_2;b) = g[\gamma_2(\Gamma_1(t))\gamma_1;\Gamma_1^{-1}(b)], \tag{3.133}$$

and the group is therefore closed.

Now that we have verified closure, we must check that the group satisfies the additional group axioms, the first of which is the associative property. Associativity states that if $f,g,h \in G$ are elements of the group, then the composition rule must satisfy $(fg)h = f(gh)$. Then for the time transformations to be associative, we require

$$\Big(g(\gamma_1;a)\cdot g(\gamma_2;b)\Big)\cdot g(\gamma_3;c) = g(\gamma_1;a)\cdot\Big(g(\gamma_2;b)\cdot g(\gamma_3;c)\Big). \tag{3.134}$$

Using the composition rule we have already found, this is equivalent to the equality

$$g\left[\gamma_3(\Gamma_{12})\gamma_2(\Gamma_1)\gamma;\Gamma_{12}^{-1}(c)\right] = g\left[\gamma_3(\Gamma_2(\Gamma_1))\gamma_2(\Gamma_1)\gamma_1;\Gamma_1^{-1}(\Gamma_2^{-1}(c))\right]. \tag{3.135}$$

Where Γ_{12} is the time transformation of the resulting group member $g(\gamma_1;a)\cdot g(\gamma_2;b)$. But from the composition rule we know that $\Gamma_{12}(t) = \Gamma_2(\Gamma_1(t))$ and so both sides of (3.135) are equal, and the time transformations do satisfy associativity.

The next property the composition rule needs to satisfy is the existence of the identity

element. This is satisfied by the element $g(1;0)$, whose corresponding time transformation is the identity transformation $\Gamma_e(t) = t$, which is equal to its inverse function. Checking the identity on the left and right, we have

$$g(1;0) \cdot g(\gamma;a) = g(\gamma;a) \tag{3.136}$$

$$g(\gamma;a) \cdot g(1;0) = g(\gamma;\Gamma^{-1}(0)) \tag{3.137}$$

The second line contains the inverse term $\Gamma^{-1}(0)$. But since γ and Γ are arbitrary, the only time this is guaranteed to happen is when the beginning and end of the integral are the same. So if Γ is invertible, as we require, then the inverse at zero must be a. Thus, the element $g(1;0)$ is the identity on both the left and the right.

The last property the time transformations must satisfy to form a group is the existence of an inverse. Define the inverse element to be $g(1/\gamma(\Gamma^{-1}(t));\Gamma(0))$. According to the composition rule, the inverse element acting on the left and right of the group element $g(\gamma;a)$ yields

$$g(\gamma;a) \cdot g\left[\frac{1}{\gamma(\Gamma^{-1}(t))};\Gamma(0)\right] = g(1;0) = e \tag{3.138}$$

$$g\left[\frac{1}{\gamma(\Gamma^{-1}(t))};\Gamma(0)\right] \cdot g(\gamma;a) = g\left[\gamma(\Gamma_{inv}(t))\frac{1}{\gamma(\Gamma^{-1}(t))};\Gamma_{inv}^{-1}(a)\right], \tag{3.139}$$

where $\Gamma_{inv}(t)$ is the transformation

$$\begin{aligned}\Gamma_{inv}(t) &= \int_{\Gamma(0)}^{t} dt'\gamma^2(\Gamma^{-1}(t)). \text{ Let } u = \Gamma^{-1}(t), \\ &= \int_0^{\Gamma^{-1}(t)} du \\ &= \Gamma^{-1}(t),\end{aligned} \tag{3.140}$$

which is the inverse function of $\Gamma(t)$. So the inverse of the inverse is just itself, and $\Gamma(a)$ is

just zero. Thus (3.139) is just the identity, and the inverse of $g(\gamma;a)$ is

$$g^{-1}(\gamma;a) = g\left[\frac{1}{\gamma(\Gamma^{-1}(t))};\Gamma(0)\right]. \tag{3.141}$$

Therefore, since the composition rule we have defined for the time transformations satisfies associativity, the existence of an identity element, and an inverse, the time transformations do in fact form a group.

3.3.7 Lie Elements of the Time Transformation

There is a subset of the group of time transformations that can be represented as a Lie group. These members would be continuous and differentiable transformations of some parameter, as opposed to discrete elements such as the parity transformation $g(-1;0)$. Let α be some Lie parameter for some specific γ function that is representable as a Lie group. We can then Taylor expand Γ with respect to α around the identity

$$\Gamma(\alpha,t) \sim \Gamma(0,t) + \frac{\partial\Gamma}{\partial\alpha}\Big|_{\alpha=0}\alpha. \tag{3.142}$$

If we set $\alpha = 0$ to be the identity transformation, then we have

$$\Gamma(\alpha,t) \sim t + \alpha\zeta(t) \tag{3.143}$$

where $\zeta(t) = \partial_\alpha\Gamma|_{\alpha=0}$ is an arbitrary real function of time.

Taking $U = e^{i\alpha G/\hbar}$ to be a unitary transformation where G is a Hermitian operator, then we can write $\Gamma(t) = UtU^\dagger$. Expanding this to first order in α and equating to (3.143) yields the commutation relation

$$[G,t] = -i\hbar\zeta(t). \tag{3.144}$$

Since the resulting transformed Schrödinger operator cannot contain time derivatives higher

than first order, the only allowed form for G is

$$G = -i\hbar\zeta(t)\frac{\partial}{\partial t} + \Omega \tag{3.145}$$

where Ω is any Hermitian operator that commutes with time. The asymptotic expansion for γ then has to be

$$\gamma \sim 1 - \frac{\alpha}{2}\dot{\zeta}(t) \tag{3.146}$$

to agree with the asymptotic expansion for $\Gamma(t)$. So then the regular dilation operator that takes $\vec{x} \to \vec{x}/\gamma$ is $\exp(-i\ln\gamma D/\hbar) \sim \exp\left(\alpha\dot{\zeta}D/2\hbar\right)$. Thus, it is a reasonable assumption that the generator for the time transformation must be

$$G_\zeta = -i\hbar\zeta\partial_t + \frac{1}{2}\dot{\zeta}D. \tag{3.147}$$

Furthermore, for the transformed operators to exist, it is easy to see that $\zeta(t)$ must necessarily be infinitely differentiable or a C^∞ function $\zeta : \mathbb{R} \to \mathbb{R}$.

We may expand the time and space transformations to verify that the generator generates what we expect. The time transformation is

$$\Gamma(t) = e^{i\alpha G/\hbar} t e^{-i\alpha G/\hbar} = t + \alpha\zeta + \frac{\alpha^2}{2}\zeta\dot{\zeta} + \frac{\alpha^3}{3!}\zeta(\dot{\zeta}^2 + \zeta\ddot{\zeta}) + \ldots \tag{3.148}$$

And the spatial transformation is

$$\vec{X}' = e^{i\alpha G/\hbar}\vec{X}e^{-i\alpha G/\hbar} = \vec{X}\left[1 + \frac{\alpha}{2}\dot{\zeta} + \frac{\alpha^2}{4}\left(\zeta\ddot{\zeta} + \frac{1}{2}\dot{\zeta}^2\right) + \ldots\right]. \tag{3.149}$$

We can verify that this generate the correct transformation $(\vec{x},t) \to (\vec{x}/\gamma, \Gamma(t))$ by the fact that $\dot{\Gamma} = \gamma^{-2}$. Checking this in an asymptotic expansion for α, we have

$$\frac{1}{\gamma} = \sqrt{\dot{\Gamma}} \sim 1 + \frac{\alpha}{2}\dot{\zeta} + \frac{\alpha^2}{4}\left(\zeta\ddot{\zeta} + \frac{1}{2}\dot{\zeta}^2\right) + \ldots \tag{3.150}$$

which agrees with (3.149).

We do encounter some difficulties if we wish to include this into the rest of the form-preserving group. Earlier, we had assumed that time was a parameter; however, in order to execute the time transformations in an analogous unitary manner, we have essentially promoted it to an operator that itself is an element of the algebra. This means it no longer makes sense to use time-dependent parameters as they no longer commute with the entire algebra. Instead, if we wish to do this, the group will then encompass all $\eta(t) \times \{\vec{X}, \vec{P}, \vec{L}, D, Q, f(\vec{X})\}$ and G_ζ for all real C^∞ functions of time $\eta(t)$ and $\zeta(t)$. It is easy to convince yourself that the algebra will close.

There are other problems, however, for practical purposes. Given a function $\zeta(t)$, it is not guaranteed that you can find a closed form for γ and Γ except for a few elementary cases. In general, it is useful to avoid promoting the time transformations to part of the group, and instead let time remain a parameter only.

Lastly, we may compare the time transformation generator (3.147) to the expansion and dilation generators, A and D, of the Schrödinger algebra [12] in (3.45). These generators are elements of the form-preserving algebra, with $A = G[t^2] - mQ$ and (the Schrödinger algebra dilation generator) $D = G[2t]$. Indeed, this is also the case for the harmonic oscillator symmetry group in [17].

The corresponding generator for $\zeta(t) =$const, $\zeta(t) = t$ and $\zeta(t) = t^2$ cases are all handled within the Schrödinger symmetry group. The next simplest case one may consider is the cubic generator, $\zeta(t) = t^3$. This results in time transformation

$$\begin{aligned} \Gamma(t) &= t + \alpha[iG,t] + \frac{1}{2!}\alpha^2[iG,[iG,t]] + \dots \\ &= t + \alpha t^3 + \frac{3}{2}\alpha^2 t^5 + \frac{15}{3!}\alpha^3 t^7 + \dots \end{aligned} \tag{3.151}$$

By Taylor expansion about $\alpha = 0$, it is evident that this generates the time transformation

$$\Gamma(t) = \frac{t}{\sqrt{1-2\alpha t^2}}. \tag{3.152}$$

Comparing this to the $\zeta = t^2$ case, we see that there may be a simple pattern to the generators of the form $\zeta(t) = t^{n+1}$ for $n \neq 0$. In fact, one can show that these generate the time transformation

$$\Gamma(t) = \frac{t}{(1 - n\alpha t^n)^{1/n}}. \tag{3.153}$$

A diverse set of functions can be created by chaining together the transformations of this type. This means that we can use $\zeta = t^y$ where $y \in \mathbb{R}$ as a basis for the algebra. This will then span all ζ that are representable as a power series.

In the limit as $n \to 0$ we should expect this to become the regular dilation operator. Performing the limit, we have

$$\lim_{n\to 0} \frac{t}{(1 - n\alpha t^n)^{1/n}} = e^{\alpha} t, \tag{3.154}$$

which indeed does produce the expected dilation operation.

3.3.8 Spin-1/2 Particles

In this section, we will describe how spin is introduced into the three-dimensional FPT. A charged particle with spin has its time evolution determined by the Schrödinger -Pauli Hamiltonian [27]

$$H = \frac{[\vec{\sigma} \cdot (\vec{P} - \vec{A})]^2}{2m} + V \tag{3.155}$$

The Pauli spin matrices satisfy the identity $\sigma_i \sigma_j = \delta_{ij} + i\varepsilon_{ijk}\sigma_k$ [28]. Therefore, it follows that we can write $(\vec{\sigma} \cdot \vec{a})(\vec{\sigma} \cdot \vec{b}) = \vec{a} \cdot \vec{b} + i\vec{\sigma} \cdot (\vec{a} \times \vec{b})$. For the Hamiltonian, we can use this identity to show

$$[\vec{\sigma} \cdot (\vec{P} - \vec{A})]^2 = (\vec{P} - \vec{A})^2 + i\vec{\sigma} \cdot [(\vec{P} - \vec{A}) \times (\vec{P} - \vec{A})]. \tag{3.156}$$

The cross product between the kinetic momentum and itself would normally be zero if the kinetic momentum were an ordinary number. However, since its components do not

commute with the others, we instead have

$$\begin{aligned}[(\vec{P}-\vec{A})\times(\vec{P}-\vec{A})]_i &= \varepsilon_{ijk}(P_j-A_j)(P_k-A_k)\\ &= -\varepsilon_{ijk}[P_j,A_k]\\ &= i\hbar(\nabla\times\vec{A})_i.\end{aligned} \tag{3.157}$$

Therefore, the Hamiltonian is

$$H=\frac{(\vec{P}-\vec{A})^2}{2m}-\frac{\hbar}{2m}\vec{\sigma}\cdot\vec{B}+V. \tag{3.158}$$

where $\vec{B}=\nabla\times\vec{A}$ is the magnetic field. The interaction term of the spin of a charged particle with an external magnetic field evidently behaves as a magnetic dipole suspended in a magnetic field.

The spin of a particle is unaffected by translations, and since the electron has zero size in non-relativistic quantum mechanics, its spin cannot have dimensions that are affected by the scale transformations. Therefore, the only type of coordinate transformation that may interact with the spin is rotation.

Since the expectation value of spin is a vector in space, if we were to enter a rotated frame, the expectation value should rotate in the opposite direction. If $|\psi'\rangle = U|\psi\rangle$ is the state vector after a rotation, then the expectation value of the spin vector $\vec{S}=\hbar\vec{\sigma}/2$ in the rotated wave function should be

$$\langle\vec{S}\rangle' = R^T\langle\vec{S}\rangle. \tag{3.159}$$

Since the rotation matrix is just a c-number and the expectation value is linear, the transformed spin operator $\vec{S}'=U\vec{S}U^\dagger$ must be

$$U\vec{S}U^\dagger = R^T\vec{S}. \tag{3.160}$$

For small angles of rotation, this is

$$\vec{S}' \sim \vec{S} - \vec{\theta} \times \vec{S}. \tag{3.161}$$

If we denote the rotation operator by $e^{-i\vec{\theta}\cdot\vec{J}/\hbar}$, then the commutation relation between the rotation generator $\vec{\theta}\cdot\vec{J}$ and the spin operator must be

$$[J_a, S_b] = i\hbar\varepsilon_{abc}S_c, \tag{3.162}$$

which are the same commutation relations as quantum angular momentum ($\mathfrak{so}(3)$ and $\mathfrak{su}(2)$).

Therefore, since $\vec{J}$ must also generate rotations of the position, we identify $\vec{J}$ with the total angular momentum operator

$$\vec{J} = \vec{L} + \vec{S}. \tag{3.163}$$

Since these have the same commutation relations as the original angular momentum algebra we used to rotate the spinless particles, it is easy to compute the time derivative of the spin-rotation generator just as before. Under the rotation $U = e^{-i\vec{\theta}\cdot\vec{J}/\hbar}$, the time-dependent rotation will introduce the term $i\hbar\dot{U}U^\dagger = \vec{\Omega}\cdot\vec{J}$, rather than the term $\vec{\Omega}\cdot\vec{L}$ from the spinless case (where $\vec{\Omega}$ is the rotated angular velocity of the rotation (D.42)). The total Hamiltonian can be shown to be

$$H = \frac{[\vec{\sigma}\cdot(\vec{P} - \vec{A}')]^2}{2m} + R\vec{A}(R^T\vec{X})\cdot(\vec{\Omega}\times\vec{X}) - \frac{m}{2}(\vec{\Omega}\times\vec{X})^2 + V(R^T\vec{X}) - \frac{1}{m}\vec{S}\cdot\vec{\Omega}, \tag{3.164}$$

where $\vec{A}' = R\vec{A}(R^T\vec{X}) - m\vec{\Omega}\times\vec{X}$ is the transformed vector potential. The only difference between this and the spinless case (3.109) is the addition of the spin-rotation interaction term $-\vec{S}\cdot\vec{\Omega}/m$.

The last thing we must consider is the transformation on the spinor itself. Since the spin and orbital angular momentum operators act on different spaces, they commute with

one another. This allows us to write $U = e^{-i\theta\cdot\vec{S}/\hbar}e^{-i\vec{\theta}\cdot\vec{L}}$. This is the usual rotation operator that rotates the position coordinate of the wave function, plus an extra rotation of the two components of the spinor. The formula for this rotation is well known, and can be found in texts such as [28, pg. 383]. The transformed spinor wave function that satisfies the Hamiltonian (3.164) is then just a rotation of the position coordinates and a rotation of the spinor components:

$$\psi'(\vec{x},t) = [\cos(\theta/2) + i\sin(\theta/2)\hat{\theta}\cdot\vec{\sigma}]\psi(R^T\vec{x},t). \tag{3.165}$$

Although straightforward, this argument used an entirely non-relativistic approach to include spin into the algebra. A full argument would look for symmetries in a radially symmetric scalar potential, which would identify the operator $\vec{L}+\vec{S}$ as the rotational symmetry generator [11]. Indeed, if one takes the rotation to be time-independent so that it does not introduce fictitious forces, the transformed Hamiltonian (3.164) is invariant if the potential is central.

Removing the Vector Potential of a Homogeneous Magnetic Field

Just as for the spinless case, we may use the FPT to completely remove the vector potential for a homogeneous magnetic field. However, due to spin-rotation coupling, we cannot completely remove all of the effects of the magnetic field, as will be apparent.

Let the state $|\psi(t)\rangle$ satisfy the Schrödinger -Pauli equation with the divergence-free vector potential $\vec{A} = \frac{1}{2}\vec{B}(t)\times\vec{x}$, and the central potential $V(r)$. The vector potential produces the homogeneous magnetic field $\vec{B}(t)$. Next, let us perform the unitary transformation $|\psi'(t)\rangle = U|\psi(t)\rangle$ where $U = e^{-i\vec{\theta}\cdot\vec{J}/\hbar}$ is a rotation. Then the transformed state will have time evolution according to the transformed Hamiltonian

$$H' = UHU^\dagger + i\hbar\dot{U}U^\dagger = \frac{[R^T\vec{P} - \vec{A}(R^T\vec{X})]^2}{2m} - \frac{\hbar}{2m}(R^T\vec{\sigma})\cdot\vec{B} + V + \vec{\omega}\cdot(R^T\vec{L}). \tag{3.166}$$

Remembering that $\vec{L} = \vec{X} \times \vec{P}$, and that $\vec{J} = \vec{L} + \frac{\hbar}{2}\vec{\sigma}$, we may rearrange the Hamiltonian to the simplified form

$$H' = \frac{[\vec{P} - R\vec{A}(R^T\vec{X}) + m(R\vec{\omega} \times \vec{X})]^2}{2m} - \frac{m}{2}(R\vec{\omega} \times \vec{X})^2 - \frac{\hbar}{2m}(R^T\vec{\sigma}) \cdot (\vec{B} - m\vec{\omega}) + V. \quad (3.167)$$

This has the effective, transformed vector potential

$$\vec{A}' = \frac{1}{2}[R(\vec{B} - 2m\vec{\omega})] \times \vec{X}. \quad (3.168)$$

Therefore, depending on our choice of $\vec{\omega}$, we may either eliminate the vector potential or the spin-coupling term, but not both. Choosing to remove the vector potential, we set $\vec{\omega}(t) = \vec{B}(t)/2m$. This results in the simplified Hamiltonian

$$H' = \frac{\vec{P}^2}{2m} + V - \frac{\hbar}{2m}\vec{\sigma} \cdot \vec{\Omega} - \frac{m}{2}(\vec{\Omega} \times \vec{X})^2. \quad (3.169)$$

Although the vector potential was removed, we have added a spin-rotation coupling term $-\vec{S} \cdot \vec{\Omega}/m$ and the Coriolis term $-m(\vec{\Omega} \times \vec{X})^2/2$ to the scalar potential.

Chapter 4

Form-Preservation in Phase Space

We have now examined the form-preserving transformation in terms of frame transformations in the position basis and as unitary transformations of the state vector. However, as we shall see, the FPT is a linear canonical transformation in phase space. Furthermore, the FPT has not been considered in the literature for phase space quantum mechanics (PSQM). Therefore, we should extend our analysis to phase space. In this chapter, we will briefly introduce some aspects of PSQM, followed by a discussion of canonical transformations in classical mechanics. We will then derive the form-preserving transformation in phase space for the case of no magnetic vector potentials and conclude with an analysis of the oscillator–free space equivalence in phase space.

4.1 Quantum Mechanics in Phase Space

PSQM is an alternative formulation of quantum mechanics in which all of NR quantum mechanics can be performed. It is fully self-consistent and equivalent to the Schrödinger formulation. In quantum mechanics, one usually performs computations in the position or momentum basis. However, in classical Hamiltonian mechanics, we use the phase space of conjugate variables (x, p) to describe the state and time evolution of particles. The position and the momentum of the particle are given equal importance to the time evolution of observables, which seems to be at odds with the usual approach to quantum mechanics. Phase space quantum mechanics aims to rectify the imbalance between position and momentum and give them equal footing in computations. However, there are fundamental limitations

to the accuracy of any prescription used to describe quantum mechanics in a phase space due to Heisenberg's uncertainty principle between conjugate variables. Therefore, unlike in classical mechanics, we cannot represent the state of a particle by a single point in the phase space. A single state must instead be distributed across phase space, representing the different possible measurements of (x, p) a particle may be observed in.

In the Schrödinger formulation of quantum mechanics, classical observables are quantized by replacing the classical c-numbers $\vec{x}$ and $\vec{p}$ with their non-commutative operator counterparts $\vec{X}$ and $\vec{P}$ (also called q-numbers). These operators obey the Heisenberg algebra

$$[X_a, P_b] = i\hbar\delta_{ab} \qquad [X_a, X_b] = 0 \qquad [P_a, P_b] = 0. \tag{4.1}$$

Unlike this approach, the phase space formulation of quantum mechanics does not replace the c-numbers with non-commutative q-numbers, but instead introduces a deformed product, usually called the *Moyal star product* "$\star$," which introduces the non-commutativity. The most common map between the quantum operators and the phase space observables is called the *Wigner map* [41], defined in N-dimensions as the inverse *Weyl transform*. The Wigner map of a quantum observable F is

$$f(\vec{x}, \vec{p}) = \mathcal{W}^{-1}\{f(\vec{X}, \vec{P})\} = 2^N \int \mathrm{d}^N y \, \langle \vec{x} + \vec{y} | F | \vec{x} - \vec{y} \rangle \, e^{-2i\vec{p}\cdot\vec{y}/\hbar}, \tag{4.2}$$

where $f(\vec{x}, \vec{p})$ is the corresponding c-number observable of the operator F, also called the symbol of F.

In general, the Wigner map of a function of the position operator is $\mathcal{W}^{-1}\{f(\vec{X}, \vec{P})\} \neq f(\vec{x}, \vec{p})$ since the Weyl transform of a phase space observable $\mathcal{W}\{f\} = F$ obeys the Weyl ordering. That is, since the position and momentum operators do not commute, when the classical observables are quantized to operators, we average over all distinct permutations of the operators. For example, the product $\vec{x} \cdot \vec{p}$ would be symmetrized to the operator $\frac{1}{2}(\vec{X} \cdot$

$\vec{P}+\vec{P}\cdot\vec{X}$). This also guarantees the Hermiticity of real observable operators constructed with $\vec{x}$ and $\vec{p}$.

Let F and G be two q-numbers in quantum mechanics, and $f(\vec{x},\vec{p})$ and $g(\vec{x},\vec{p})$ be their corresponding phase-space c-numbers. The Wigner map of the operator product is the Moyal star product

$$\mathcal{W}^{-1}\{FG\} = f(\vec{x},\vec{p})\star g(\vec{x},\vec{p}) \equiv f e^{\frac{i\hbar}{2}\overleftrightarrow{\mathscr{P}}} g \tag{4.3}$$

where $\star$ is the star product and $\mathscr{P}$ is the Poisson bracket. The exponential is understood to be a power series. The Poisson bracket can be defined as the pseudo bi-differential operator

$$\mathscr{P} = \overleftarrow{\partial}_{x_i}\overrightarrow{\partial}_{p_i} - \overleftarrow{\partial}_{p_i}\overrightarrow{\partial}_{x_i} \tag{4.4}$$

where the left and right arrows mean that the partial derivatives act only on the left and right of the Poisson operator $\mathscr{P}$, respectively. The summation over the indices i is implied. We will define the Moyal bracket, or the sine bracket, as

$$\{\{f,g\}\} = \frac{1}{i\hbar}[f,g]_\star = \frac{1}{i\hbar}(f\star g - g\star f) = f\frac{2}{\hbar}\sin\left(\frac{\hbar}{2}\overleftrightarrow{\mathscr{P}}\right) g. \tag{4.5}$$

It is also called a deformed Poisson bracket. This is because in the classical $\hbar\to 0$ limit, the Moyal bracket is the Poisson bracket

$$\lim_{\hbar\to 0}\{\{f,g\}\} = \{f,g\}, \tag{4.6}$$

assuming that f and g are independent of $\hbar$.

In QM the wave function contains all of the information of the state; all observable measurement probabilities can be computed from the wave function. The wave function can be further generalized to the density matrix ρ to include the classical mixing of probabilities. In PSQM the role of the density matrix is replaced by the Wigner quasi-probability distribution $W(\vec{x},\vec{p};t)$, from which all probabilities and expectation values can be computed, just

as with the wave function in the Schrödinger -Heisenberg-Dirac formulation of quantum mechanics (QM).

Though the Wigner function is always real, unlike the density matrix, it cannot be directly interpreted as a probability distribution as it is not ≥ 0 everywhere. There are regions that are negative, on the order of area $\Delta x \Delta p \approx \hbar$ (in one dimension)[7]. There exists other phase-space distributions that are always positive, but not without concessions [8].

In the absence of a magnetic vector potential[9], the Wigner function is defined as the Wigner map of the scaled density matrix $(\pi\hbar)^{-n}\rho$

$$W(\vec{x},\vec{p};t) = \mathcal{W}^{-1}\{(\pi\hbar)^{-N}\rho\} = \frac{1}{(\pi\hbar)^N}\int \mathrm{d}^N y \psi^*(\vec{x}+\vec{y})\psi(\vec{x}-\vec{y})e^{2i\vec{p}\cdot\vec{y}/\hbar} \tag{4.7}$$

for a pure state $\rho = |\psi\rangle\langle\psi|$. The expectation value of an observable $f(\vec{X},\vec{P})$ is then given by the phase space integral of the c-number observable as determined by the Wigner map:

$$\langle f\rangle = \int \mathrm{d}^N x \mathrm{d}^N p\, W(\vec{x},\vec{p};t) f(\vec{x},\vec{p};t) \tag{4.8}$$

The normalization in (4.7) is present so that the phase-space integral of the Wigner function is equal to the trace of the density matrix

$$\int \mathrm{d}^N x \mathrm{d}^N p\, W(x,p;t) = \mathrm{Tr}\,\rho(t). \tag{4.9}$$

The equation of motion for the Wigner function, called the *Moyal equation*, is determined by the Wigner transform of the von Neumann equation for the time evolution of the

[7] For an essay written about the concepts and implications of negative probabilities, see the essay R. Feynman, *Quantum implications* (Routledge, 1987) Chap. Negative Probabilities [42]

[8] Smearing out the Wigner function with a Gaussian convolution of size $> \hbar$ will always remove these negative regions and yield the positive Husimi distribution [43]. Despite being positive everywhere, it remains a quasiprobability distribution.

[9] See [44] for an attempt to create a gauge-invariant definition of the Wigner function.

density matrix. The Moyal equation [43] is then

$$\frac{\partial W}{\partial t} = -\{\{W, H\}\}. \tag{4.10}$$

The stationary states of the Wigner function occur when there is no time dependence, so that the Moyal bracket of the Wigner function with the Hamiltonian is zero, and the two star-commute. The Wigner transform of $H\rho = E\rho$ is the *stargenvalue equation*

$$H \star W = EW, \tag{4.11}$$

for which the Wigner function is an eigenfunction of the differential operator $H\star$ and E is a real eigenvalue, which is the energy of the stationary state.

4.2 Canonical Transformations

As we have seen in §3, the FPT can be entirely described by unitary transformations of the Schrödinger equation. Therefore, the transformations to the position and momentum operators are canonical in the sense that they preserve the Heisenberg algebra [38]. We then expect that the only transformations in phase space that preserve the Moyal equation (4.10) are linear and canonical. These are the only transformations that we could reasonably expect to preserve the Moyal equation since the star product itself is an infinite series of bi-differential operators (or, equivalently, can be represented by an integral kernel). Any general coordinate transformation that we perform on the star product will introduce arbitrary derivative terms to the series, of which we are not guaranteed to find any Hamiltonian that we can use to write a Moyal equation in the transformed coordinates. Therefore, it is reasonable to limit our consideration to transformations that preserve the Moyal bracket.

4.2.1 Classical Canonical Transformations

Canonical transformations are fundamental tools of classical mechanics. The reason that they are special is that canonical transformations preserve the form of Hamilton's equations, and the two conjugate variables will remain conjugate after the transformation. Thus, when examining a new physical system, it may be possible to use a canonical transformation to either simplify the equations of motion or transform them into ones that already have a known solution. This not only allows us to simplify the problem using the known symmetries of the system, but it also allows us to gain deeper physical insight into the physics involved.

Let f and g be two phase space observables. It is easy to check that Hamilton's equations are preserved for two conjugate variables if the Poisson bracket is preserved by the transformation. This is equivalent to the statement

$$\{f,g\}_{(x.p)} = \{f,g\}_{(Q,P)} \tag{4.12}$$

where the left-hand side is the Poisson bracket in the original coordinates and the right-hand side is the Poisson bracket in the transformed coordinate $(\vec{Q},\vec{P})$. The constraint (4.12) will be the main focus of canonical transformations in this section.

Since the Poisson bracket between conjugate coordinates is invariant, the fundamental Poisson brackets between any two conjugate variables $\vec{Q}$ and $\vec{P}$ are preserved

$$\{Q_i,P_j\} = \delta_{ij} \qquad \{Q_i,Q_j\} = 0 \qquad \{P_i,P_j\} = 0. \tag{4.13}$$

Thus, it is not important to write the particular coordinates that the Poisson bracket is being taken relative to. It remains invariant as long as any conjugate pair of variables satisfying the relations (4.13) is used to define the Poisson bracket.

We now follow [32, Chapter 9] to derive the constraints on canonical transformations.

The Poisson bracket with respect to the original coordinates can be written as

$$\{f,g\} = \frac{\partial f}{\partial x_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial x_i} = \nabla_x f \cdot \nabla_p g - \nabla_p f \cdot \nabla_x g, \tag{4.14}$$

where ∇_x and ∇_p are the gradient operators (as a column vector) with respect to either position or momentum, respectively. We define the coordinates η and the gradient ∇_η as the column vectors

$$\eta = \begin{pmatrix} \vec{x} \\ \vec{p} \end{pmatrix}, \quad \text{and} \quad \nabla_\eta = \begin{pmatrix} \nabla_x \\ \nabla_p \end{pmatrix}. \tag{4.15}$$

With the notation we just defined in (4.15), we can now conveniently rewrite the Poisson bracket using block matrices. Replacing the dot products the the product of a row and a column vector, we have

$$\{f,g\} = \begin{pmatrix} \nabla_x f \\ \nabla_p f \end{pmatrix}^T \begin{pmatrix} \nabla_p g \\ -\nabla_x g \end{pmatrix} = \nabla_\eta^T f J \nabla_\eta g \tag{4.16}$$

where the matrix J is the antisymmetric block matrix

$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \tag{4.17}$$

and I_N is the $N \times N$ identity matrix. Next, we consider a canonical transformation to the coordinates $\varepsilon = \binom{\vec{Q}}{\vec{P}}$ from η. Then by the chain rule, the gradient is $\nabla_\eta = S\nabla_\varepsilon$ where $S_{ij} = \partial_{\eta_i}\varepsilon_j$ is the Jacobian matrix.

Since canonical transformations must only swap the conjugate coordinates present in the Poisson bracket, we necessitate that

$$\{f,g\} = (S\nabla_\varepsilon)^T f J (S\nabla_\varepsilon) g = \nabla_\varepsilon^T f J \nabla_\varepsilon g. \tag{4.18}$$

Therefore, the Jacobian matrix S of the canonical transformation must satisfy the equation

$$S^T J S = J. \tag{4.19}$$

Matrices S that satisfy this equation are called *symplectic*, and together form a group of $2N \times 2N$ matrices.

If we let the symplectic matrix S be equal to the $\mathbb{R}^{2N\times 2N}$ block matrix

$$S = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{4.20}$$

where $A, B, C, D \in \mathbb{R}^{N\times N}$. Then the symplectic condition (4.19) reduces to the following three conditions on the matrices A, B, C, D:

$$\begin{aligned} A^T C - C^T A &= 0 \\ B^T D - D^T B &= 0 \\ A^T D - C^T B &= I. \end{aligned} \tag{4.21}$$

Taking the determinant of the symplectic condition (4.19), since the determinant J is nonzero, we immediately see that

$$\det S^2 \det J = \det J \implies \det S = \pm 1. \tag{4.22}$$

Therefore, the Jacobian determinant of our canonical transformation must either be plus or minus one. It is, however, worth noting that it is a well-known fact that the determinant of a symplectic matrix is always one. For a collection of proofs, see [45].

4.2.2 Canonical Transformations of the Time Coordinate

Until now, we have assumed that the canonical transformations do not transform the time coordinates. If we did allow transformations of the time coordinate $t \to t'$, this would introduce derivatives of the form $(\partial_{\eta_i} t')\partial_{t'}$ which needs to be zero to preserve the Poisson bracket and the canonical commutation relations, as will be shown in this section.

Let us perform the general coordinate transformation $(\vec{x}, \vec{p}) \to (\vec{Q}, \vec{P})$ and the time transformation $t \to t'$. The Poisson bracket between two functions f and g is then

$$\begin{aligned} \{f,g\} &= \left(S\nabla_\varepsilon f + \nabla_\eta t' \frac{\partial f}{\partial t'}\right)^T J \left(S\nabla_\varepsilon g + \nabla_\eta t' \frac{\partial g}{\partial t'}\right) \\ &= \nabla_\varepsilon^T f S^T J S \nabla_\varepsilon g + \frac{\partial f}{\partial t'}\{t', g\} + \{f, t'\}\frac{\partial g}{\partial t'} + \frac{\partial f}{\partial t'}\frac{\partial g}{\partial t'}\{t', t'\}. \end{aligned} \tag{4.23}$$

The last term is zero by the anti-symmetry of the Poisson bracket. Next, we are left with the transformed time derivative of f and g multiplied by the Poisson bracket of t' with the opposite function. Since we are looking exclusively for transformations that look like a Poisson bracket in the new coordinates, the coefficients of the time derivatives of f and g must be zero. Since f and g were arbitrary, this means that the only way to ensure this is to set

$$\frac{\partial t'}{\partial x_i} = 0, \quad \frac{\partial t'}{\partial p_i} = 0 \implies t' = t'(t), \tag{4.24}$$

so that the transformed time coordinate can only depend on time.

Thus, any time transformation that accompanies a time-dependent canonical transformation must only depend on time, and cannot depend on the position in phase space. Furthermore, the time transformation does not modify the requirements of the position and momentum transformation and thus satisfies the symplectic condition (4.19).

4.2.3 Canonical Transformations of the Star Product

Just as we would have assumed based on the work of previous chapters, the star product between two phase space observables $f(\vec{x}, \vec{p})$ and $g(\vec{x}, \vec{p})$ is invariant to linear canonical

transformations [43]. To see that this is the case, we will find it convenient to use the Fourier definition of the star product [46] generalized to higher dimensions:

$$f\star g=(\pi\hbar)^{-2N}\int \mathrm{d}^N x'\,\mathrm{d}^N p'\,\mathrm{d}^N x''\,\mathrm{d}^N p''\,f(\vec{x}+\vec{x}',\vec{p}+\vec{p}')g(\vec{x}+\vec{x}'',\vec{p}+\vec{p}'') \times\exp\left[\frac{2i}{\hbar}(\vec{x}'\cdot\vec{p}''-\vec{x}''\cdot\vec{p}')\right]. \quad (4.25)$$

From elementary calculus, the coordinate transformation $(\vec{x},\vec{p})\to(\vec{Q},\vec{P})$ will transform the phase space volume element [37] as

$$\mathrm{d}^N x\,\mathrm{d}^N p=|\det S|\,\mathrm{d}^N Q\,\mathrm{d}^N P, \quad (4.26)$$

where $\det S$ is the Jacobian determinant of the transformation

$$\det S=\begin{vmatrix}\frac{\partial\vec{Q}}{\partial\vec{x}} & \frac{\partial\vec{Q}}{\partial\vec{p}}\\ \frac{\partial\vec{P}}{\partial\vec{x}} & \frac{\partial\vec{P}}{\partial\vec{p}}\end{vmatrix}. \quad (4.27)$$

Canonical transformations will then preserve the phase-space volume element [47] since $|\det S|=1$ (see (4.22)). Therefore, the volume element in the integral star product (4.25) is preserved, and transforms as $\mathrm{d}^N x\mathrm{d}^N p=\mathrm{d}^N Q\mathrm{d}^N P$.

Let $\tilde{f}(\vec{Q},\vec{P})=f(\vec{x},\vec{p})$ and likewise for $\tilde{g}$. Since we have assumed the canonical transformations are linear, we necessarily have that $f(\vec{x}+\vec{x}',\vec{p}+\vec{p}')=\tilde{f}(\vec{Q}+\vec{Q}',\vec{P}+\vec{P}')$. So then the star product between the two phase space observables is

$$f\star g=(\pi\hbar)^{-2N}\int \mathrm{d}^N Q'\,\mathrm{d}^N P'\,\mathrm{d}^N Q''\,\mathrm{d}^N P''\,\tilde{f}(\vec{Q}+\vec{Q}',\vec{P}+\vec{P}')\tilde{g}(\vec{Q}+\vec{Q}'',\vec{P}+\vec{P}'') \times\exp\left[\frac{2i}{\hbar}(\vec{x}'\cdot\vec{p}''-\vec{x}''\cdot\vec{p}')\right]. \quad (4.28)$$

Since the canonical transformation is linear (and invertible, since $\det S\neq 0$), the inverse transformation is linear and symplectic [45] as well. Let us write the inverse canonical

transformation as the linear transformation

$$\begin{aligned}\vec{x}(\vec{Q},\vec{P}) &= A\vec{Q}+B\vec{P}\\ \vec{p}(\vec{Q},\vec{P}) &= C\vec{Q}+D\vec{P}\end{aligned} \tag{4.29}$$

where A,B,C,D are $\mathbb{R}^{N\times N}$ matrices that satisfy the symplectic condition for block matrices (4.21) so that this transformation is canonical. Then the product in the exponential (4.28) is

$$\begin{aligned}\vec{x}'\cdot\vec{p}''-\vec{x}''\cdot\vec{p}' = \vec{Q}'\cdot(A^TC-C^TA)\vec{Q}''+\vec{P}'\cdot(B^TD-D^TB)\vec{P}''\\ +\vec{Q}'\cdot(A^TD-C^TB)\vec{P}''-\vec{Q}''\cdot(A^TD-C^TB)\vec{P}'\end{aligned} \tag{4.30}$$

However, using the symplectic conditions (4.21) of the block matrices, this reduces to $\vec{Q}'\cdot\vec{P}''-\vec{Q}''\cdot\vec{P}'$. Thus, the star product becomes

$$\begin{aligned}f\star g = (\pi\hbar)^{-2N}\int \mathrm{d}^NQ'\,\mathrm{d}^NP'\,\mathrm{d}^NQ''\,\mathrm{d}^NP''\,\tilde{f}(\vec{Q}+\vec{Q}',\vec{P}+\vec{P}')\tilde{g}(\vec{Q}+\vec{Q}'',\vec{P}+\vec{P}'')\\ \times\exp\left[\frac{2i}{\hbar}(\vec{Q}'\cdot\vec{P}''-\vec{Q}''\cdot\vec{P}')\right] = \tilde{f}\star'\tilde{g},\end{aligned} \tag{4.31}$$

where $\star'$ is the star product with respect to the new canonical variables $\vec{Q}$ and $\vec{P}$. Since $f\star g=\tilde{f}\star'\tilde{g}$ for canonical transformations, the Moyal bracket is also conserved $\{\{f,g\}\}=\{\{\tilde{f},\tilde{g}\}\}'$. The star product is left invariant in the additional case of phase-space translations.

It is important to note that the Jacobian of the phase space coordinate transformation being one is not enough to preserve the star product in the new coordinates. In addition to a unit Jacobian, by requiring the exponential to be equal, we have identically enforced the symplectic condition. This argument only follows in general for linear canonical transformations, though it is not clear if there exists any non-linear transformations for which it is also true, and as authors before us [43], we do not claim there are no non-linear transformations for which the Moyal bracket or the star product are conserved.

4.3 Transforming the Moyal Equation

As in the Schrödinger -Heisenberg-Dirac formulation, we must be able to perform quantum mechanics in the transformed frame. Consequently, we are able to determine that the most general allowed coordinate transformation must be linear in position. We may also hold the same requirement for momentum, since the measured momentum must be the same in both coordinate frames. This leads to the ansatz for the wave function (2.21). Furthermore, since the transformed momentum must also be a linear function, the phase function $S(\vec{x},t)$ must be at most quadratic in position.

Denoting $\vec{x}' = R(\vec{x}/\gamma + \vec{\beta})$ and $\vec{p}\,' = R\left(\gamma\vec{p} - m\dot{\gamma}\vec{x} + m\gamma^2\dot{\vec{\beta}}\right)$, we may use the FPT (2.39) (restricting α to depend on time only) in the Wigner transform (4.7) to verify our ansatz for the Wigner function's transformation[10]. Doing this results in

$$W(\vec{x},\vec{p};t) = W'(\vec{x}',\vec{p}\,';t') \tag{4.32}$$

where W' satisfies the time evolution for a new Hamiltonian in the transformed coordinates, $H'(\vec{x}',\vec{p}\,',t')$:

$$\frac{\partial W'}{\partial t'} = -\{\{W',H'\}\}' \tag{4.33}$$

where $\{\{\cdot,\cdot\}\}'$ is the Moyal bracket with respect to the canonically transformed coordinates. Thus, it must obey the time evolution (4.33) with the same transformed Hamiltonian as the wave function. Therefore, we have shown that linear canonical transformations satisfy the desired ansatz we arrived at in the position basis.

According to (4.32), form preservation of the Wigner function should look very similar to form preservation of the wave function. The difference is the lack of a scale factor and phase. Although the Wigner function is a quasi-probability density, canonical transformations preserve the phase space volume element, and thus no scale factor is required to conserve expectation values and the norm of the state. In the wave function, the phase

[10] It is not necessary to use the exact FPT, the Wigner function ansatz can be derived directly from the wave function ansatz after restricting the phase factor to be quadratic.

normally carries the information about how the momentum transforms, but this has been moved to the arguments of the Wigner function.

With all of this information, we are ready to derive the allowable FPTs in phase space. We desire to perform the time-dependent coordinate transformation $(\vec{x},\vec{p}) \to (\vec{x}',\vec{p}')$ on the time evolution of the Wigner function (4.10) for the Hamiltonian $H(\vec{x},\vec{p},t) = \vec{p}^2/2m + V(\vec{x},t)$. Since we need to preserve the form of this equation, the Moyal bracket must transform to something that looks like another Moyal bracket. Any arbitrary coordinate transformation of the star product would introduce a complex series of derivatives into this equation. Therefore, it is a reasonable assumption that we need to limit the coordinate transformations to linear canonical transformations of the form

$$\begin{aligned} \vec{x}' &= A\vec{x} + B\vec{p} + \vec{x}_0 \\ \vec{p}' &= C\vec{x} + D\vec{p} + \vec{p}_0 \end{aligned} \tag{4.34}$$

where $A,B,C,D \in \mathbb{R}^{2N\times 2N}$ that satisfy the symplectic conditions for block matrices (4.21) and $\vec{x}_0, \vec{p}_0 : \mathbb{R} \to \mathbb{R}^N$ are real functions of time. The linear canonical transformation will leave the Moyal bracket invariant, as mentioned previously.

Expanding the time derivative in terms of the new coordinates, the Moyal equation (4.10) becomes

$$\left(\frac{\partial x_i'}{\partial t}\frac{\partial}{\partial x_i'} + \frac{\partial p_i'}{\partial t}\frac{\partial}{\partial p_i'} + \frac{\partial t'}{\partial t}\frac{\partial}{\partial t'}\right) W = -\{\{W,H\}\}. \tag{4.35}$$

However, the time transformation can only depend on the time coordinate and not on the position in phase space. This is because this would introduce $(\partial_{x_i} t')\partial_t'$ and $(\partial_{p_i} t')\partial_t'$ terms into the Poisson bracket, which cannot be cancelled, as was discussed in §4.2.2. After rearranging and subtracting (4.33), we obtain

$$\{\{W,H'\}\} = \left(\frac{\mathrm{d}t'}{\mathrm{d}t}\right)^{-1}\left(\{\{W,H\}\} + \frac{\partial x_i'}{\partial t}\frac{\partial W}{\partial x_i'} + \frac{\partial p_i'}{\partial t}\frac{\partial W}{\partial p_i'}\right), \tag{4.36}$$

since the Moyal bracket is invariant under linear canonical transformations.

Since the Wigner function was arbitrary, the coefficients of the partial derivatives must be equal on both sides. Therefore, the first-order Poisson brackets must match (so the equation must be true to zeroth order $\hbar$). To satisfy the higher-order Poisson brackets, the additional terms in the Hamiltonian must be at most second order in $\vec{x}$ and $\vec{p}$. Looking at the first order equations and denoting the arbitrary derivative $\frac{dt'}{dt} = \gamma(t)^{-2}$, we have

$$\frac{\partial H'}{\partial p_i'} = \gamma^2 \left(\frac{\partial H}{\partial p_i'} + \frac{\partial x_i'}{\partial t} \right) \qquad \frac{\partial H'}{\partial x_i'} = \gamma^2 \left(\frac{\partial H}{\partial x_i'} - \frac{\partial p_i'}{\partial t} \right). \tag{4.37}$$

Assuming that the transformed Hamiltonian is of the form $H' = \vec{p}\,'^2/2m + V'(\vec{x}', t')$, the leftmost equation in (4.37) becomes

$$\frac{p_i'}{m} = \gamma^2 \left(\frac{\partial x_j}{\partial p_i'} \partial_j V + \frac{\partial p_j}{\partial p_i'} \frac{p_j}{m} + \frac{\partial x_i'}{\partial t} \right). \tag{4.38}$$

Since in general the derivative $\partial_j V$ will be greater than first order in position, we must have that $\partial_{p_i'} x_j = 0 \; \forall \; i, j$. Thus, the inverse canonical transformation must be $\vec{x} = A^{-1}\vec{x}' - \vec{x}_0$ and cannot depend on the transformed momentum. Consequently, B must be the zero matrix. Since $\vec{x}'$ does not depend on momentum anymore, we can perform the inverse transformation on the momentum to obtain the matrix $\partial_{p_i'} p_j = (D^{-1})_{ji}$. Now equation (4.38) becomes

$$\vec{p}\,' = \gamma^2 \left[(D^{-1})^T \vec{p} + m \frac{\partial \vec{x}'}{\partial t} \right]. \tag{4.39}$$

But comparing this to our canonical transformation (4.34), we see that the matrix $\gamma^2 (D^{-1})^T$ must be precisely D. Therefore, the matrix D must be

$$D = \gamma R \tag{4.40}$$

where R is an orthogonal matrix.

With $B = 0$, the symplectic condition $B^T D = D^T B$ is automatically satisfied, and the third condition becomes $A^T D = I$. Therefore $A = (D^{-1})^T = R/\gamma$. Now the total transfor-

mation of the momentum (4.38) becomes

$$p_i' = \gamma R_{ij} p_j + m(-\dot{\gamma} R_{ij} + \gamma \dot{R}_{ij}) x_j + m\gamma^2 \dot{x}_{0i}. \tag{4.41}$$

This equation allows us to read off the matrix $C = m(-\dot{\gamma}R + \gamma\dot{R})$ and the translation $\vec{p}_0 = m\gamma^2\dot{\vec{x}}_0$.

Next, we apply the symplectic condition $A^T C = C^T A$ which limits the time dependence of our orthogonal matrix, R, to

$$R^T \dot{R} = \dot{R}^T R. \tag{4.42}$$

But because the product $R^T\dot{R}$ is always antisymmetric for an orthogonal matrix R, the only way for the transformation to satisfy the symplectic condition (and therefore be canonical) is if $\dot{R} = 0$ and the rotation does not depend on time. This should not be surprising, as the time-dependent rotation must introduce a vector potential, as we have already seen.

Therefore, we have restricted the linear canonical transformations to

$$\begin{aligned} \vec{x}' &= R\left(\frac{\vec{x}}{\gamma} + \vec{\beta}\right) \\ \vec{p}' &= R\left(\gamma\vec{p} - m\dot{\gamma}\vec{x} + m\gamma^2\dot{\vec{\beta}}\right) \end{aligned} \tag{4.43}$$

where γ and $\vec{\beta} = R^T\vec{x}_0$ are real functions of time and R is a time-independent orthogonal matrix. Then the Jacobian matrix $S_{ij} = (\nabla_\eta)_j \varepsilon_i$ of the canonical transformation is

$$S = \begin{pmatrix} \frac{1}{\gamma}R & 0 \\ -m\dot{\gamma}R & \gamma R \end{pmatrix}. \tag{4.44}$$

This block matrix satisfies the symplectic condition (4.19). Therefore, the linear transformation $S\eta$ is canonical.

With this specific canonical transformation, the rightmost equation in (4.37) becomes

$$\frac{1}{\gamma^2}\nabla V' = \nabla V + m\frac{\ddot{\gamma}}{\gamma}\vec{x} - m(2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}). \tag{4.45}$$

After integrating, we have the transformed potential

$$\frac{1}{\gamma^2}V'(\vec{x}',t') = V(\vec{x},t) + \frac{m\dot{\gamma}}{2\gamma}\vec{x}^2 - m\vec{x}\cdot(2\dot{\gamma}\dot{\vec{\beta}} + \gamma\ddot{\vec{\beta}}) + \alpha(t) \tag{4.46}$$

where $\alpha(t)$ is an arbitrary real function of time. Since the corrections to the Hamiltonian are only second order in $\vec{x}'$ or $\vec{x}$, the higher order derivatives of the Moyal bracket in (4.36) are automatically satisfied. Thus, this represents the Hamiltonian we would obtain by performing this coordinate transformation entirely classically.

4.4 Oscillator–Free Equivalence

We will revisit the topic of the equivalence of the oscillator to the free particle in the phase space formalism. We will begin from where we left off in §2.5, where we set the primed coordinates to those of free space and the unprimed potential to the harmonic oscillator with frequency ω and the same mass. It is important to note that it does not matter which coordinates we call the primed and which we do not: the transformation is symmetric.

We already determined the parameters of the transformation in (2.88). Using the coordinate transformation (4.43) we have

$$\begin{aligned} x &= \frac{x' - v_0 t' - x_0}{\sqrt{1+(\omega t')^2}} \\ p &= (p' - mv_0)\sqrt{1+(\omega t')^2} - \frac{m\omega^2 t' x}{\sqrt{1+(\omega t')^2}}. \end{aligned} \tag{4.47}$$

The time evolution of the Wigner function is determined for both free space and the harmonic oscillator by the Moyal equation. But if the Hamiltonian is at most quadratic in

position and momentum, the Moyal bracket reduces to the Poisson bracket. This means that the Wigner function will obey the classical Liouville equation [32]

$$\frac{\partial W}{\partial t} = -\{W, H\}. \tag{4.48}$$

If we assume the ansatz that $W(x,p;t) = f(Q(x,p;t), P(x,p;t))$ where Q and P are conjugate variables that lie on the same level curve of the Hamiltonian as x and p, then Liouville's theorem [32] is solved for any f if Q and P evolve according to the anti-Hamiltonian flow

$$\frac{\partial Q_i}{\partial t} = -\frac{\partial H}{\partial P_i} \quad \frac{\partial P_i}{\partial t} = \frac{\partial H}{\partial Q_i}. \tag{4.49}$$

where $H(Q,P) = H(x,p)$. Therefore, the time-dependent solution to the Wigner function for free space should be

$$W(x',p';t') = f(x' - p't'/m - x_0, p' - p_0). \tag{4.50}$$

For a time-independent Wigner function where $\partial_t W = 0$, Liouville's equation is solved by setting $W(x,p) = f(H)$ where f is any arbitrary function of the Hamiltonian. Thus, our harmonic oscillator Wigner function is some function of the harmonic oscillator Hamiltonian

$$W(x,p) = f\left(\frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2\right). \tag{4.51}$$

So then the free space Wigner function $W'(x',p';t')$ is $f(H(x,p))$. However, the time dependence of the harmonic oscillator does not seem to match the free flow (4.50) upon first inspection.

Written in terms of the primed coordinates, the Hamiltonian for the harmonic oscillator

becomes

$$\begin{aligned}\frac{1}{2m}\left[(p'-mv_0)\sqrt{1+(\omega t')^2}-\frac{m\omega^2 t'x}{\sqrt{1+(\omega t')^2}}\right]^2+\frac{1}{2}m\omega^2\left(\frac{x'-v_0t'-x_0}{\sqrt{1+(\omega t')^2}}\right)^2\\ =\frac{1}{2m}\left(p'-mv_0\right)^2+\frac{1}{2}m\omega^2\left(x'-\frac{1}{m}p't'-x_0\right)^2\\ =H\left(x'-\frac{1}{m}p't'-x_0,p'-mv_0\right).\end{aligned}\tag{4.52}$$

This shows that this is the precise time evolution of the classical Hamiltonian in free space.

As we have already discussed, solutions to the free Schrödinger equation should not exhibit any momentum dispersion due to the lack of a potential. If we plot the dispersion of the level curves of the harmonic oscillator's Hamiltonian $H(x,p)=E=\text{const}$, then we can see the dispersion of the Wigner function of the stationary states as in figure 4.1. The level curves are parametrized by $\theta\in(-\pi,\pi)$ as

$$\begin{aligned}\frac{p}{p_0\sqrt{\varepsilon}}&=\sin\theta\\ \frac{x}{x_0\sqrt{\varepsilon}}&=\cos\theta+\omega t\sin\theta,\end{aligned}\tag{4.53}$$

where $\varepsilon=2E/\hbar\omega$ is the dimensionless energy and $x_0=\sqrt{\hbar/m\omega}$ and $p_0=\sqrt{m\hbar\omega}$ are the length and momentum scales of the oscillator. The limits of the momentum occur when the angle is $\pm\pi/2$, which have a corresponding momentum of $\pm p_0\sqrt{\varepsilon}$. The position extrema occur at $\pm\tan^{-1}\omega t$ with a corresponding extremum position of $\pm x_0\sqrt{\varepsilon}\sqrt{1+(\omega t)^2}$. Using the energy as the energy eigenvalues of the stationary states, $E_n=\hbar\omega(n+1/2)$, we see that the width of the positions and momentum of the eigenstates are on the order of

$$\Delta P\sim\frac{\sqrt{2}\hbar}{x_0}\sqrt{n+\frac{1}{2}}\qquad\Delta X\sim\sqrt{2}x_0\sqrt{\left[n+\frac{1}{2}\right][1+(\omega t)^2]},\tag{4.54}$$

which agree with the properly computed widths given in equation (2.93).

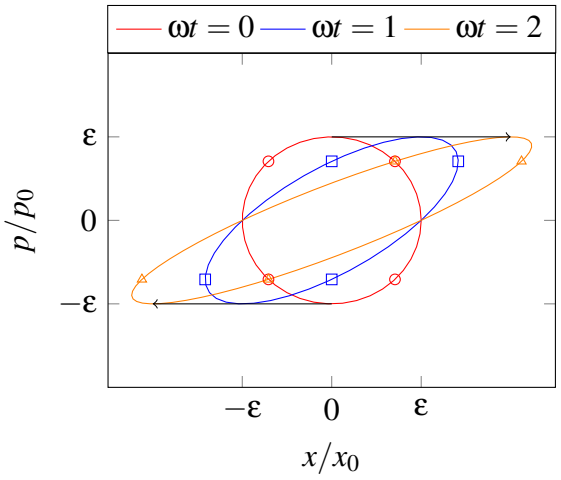

Figure 4.1: The free space evolution of level curves of the simple harmonic oscillator Wigner function in phase space. The dimensionless energy is $\varepsilon = 2E/\omega\hbar$.

4.5 Senitzky Coherent Excited States

Senitzky's coherent excited states [3] are a solution to the harmonic oscillator TDSE, which feature rigid rotation about the origin in phase space. The coherent excited states can be found by a FPT of the harmonic oscillator eigenstates. Specifically, it is an example of the harmonic oscillator symmetry group [17], which transforms an oscillator into another oscillator in different coordinates. Let $V' = \frac{1}{2}m\omega^2 x'^2$ and $V = \frac{1}{2}m\omega^2 x^2$ be the potentials in both coordinates, so that both are harmonic with the same frequency ω. Then the 1D case of the potential transformation (4.46) with $\gamma = 1$ is

$$\begin{aligned}\frac{1}{2}m\omega^2(x+\beta)^2 &= \frac{1}{2}m\omega^2 x^2 - mx\ddot{\beta} + \alpha \\ &= \frac{1}{2}m\omega^2\left(x - \omega^{-2}\ddot{\beta}\right)^2 - \frac{m}{2\omega^2}\ddot{\beta} + \alpha.\end{aligned} \tag{4.55}$$

Both sides of this equation can be made equal by setting $\alpha(t) = m\ddot{\beta}/2\omega^2$ and $\ddot{\beta} + \omega^2\beta = 0$. Thus $\beta = A\cos(\omega t + \phi)$ is harmonic.

Next, we solve the Wigner function in the case of time-independence for the transformed potential V'. The Wigner function W' then satisfies the stargenvalue equation

$EW' = H' \star W'$, for which we will employ the Bopp-shifts [48]:

$$\begin{aligned} EW'(x',p') &= H'(x',p') \star W'(x',p') \\ &= H'\left(x' + \frac{i\hbar}{2}\partial'_p, p' - \frac{i\hbar}{2}\partial'_x\right) W' \\ &= \left[\frac{1}{2m}\left(p'^2 - i\hbar p'\partial'_x - \frac{\hbar^2}{4}\partial'^2_x\right) + \frac{1}{2}m\omega^2\left(x' + i\hbar x'\partial'_p - \frac{\hbar^2}{4}\partial'^2_p\right)\right] W' \end{aligned} \tag{4.56}$$

Since the Wigner function is entirely real, we may separate this equation into two parts: the real and imaginary parts.

$$\left(\frac{p'^2}{2m} - \frac{\hbar^2}{8m}\partial'^2_x + \frac{1}{2}m\omega^2 x'^2 - \frac{m\omega^2\hbar^2}{8}\partial'^2_p - E\right) W' = 0 \tag{4.57}$$

$$\left(-\frac{p'}{m}\partial'_x + m\omega^2 x'\partial'_p\right) W' = 0. \tag{4.58}$$

The potential is quadratic, so the second of these equations (4.58) is satisfied by setting the Wigner function to be a function of a single variable $W'(x',p') = W'(u)$ where u is proportional to the harmonic Hamiltonian.

Let u be the dimensionless variable $u = 4H'/\hbar\omega$. Then the real part of the stargenvalue equation becomes

$$\left(\frac{u}{4} - \frac{E}{\hbar\omega} - \frac{\mathrm{d}}{\mathrm{d}u} - u\frac{\mathrm{d}^2}{\mathrm{d}u^2}\right) W' = 0. \tag{4.59}$$

Substituting $W' = L(u)e^{-u/2}$ yields

$$\left(u\frac{\mathrm{d}^2}{\mathrm{d}u^2} + (1-u)\frac{\mathrm{d}}{\mathrm{d}u} + \frac{E}{\hbar\omega} - \frac{1}{2}\right) L(u) = 0. \tag{4.60}$$

This equation is known as Laguerre's differential equation, and are solved by the Laguerre polynomials $L_n(u)$ (see [37, Chapter 18.7]) when $E/\omega\hbar - 1/2 = n$ is a natural number. Then the Wigner function for the nth energy state $E_n = \hbar\omega(n + \frac{1}{2})$ is $W_n = C_n L_n(u)e^{-u/2}$, where C_n is a normalization constant.

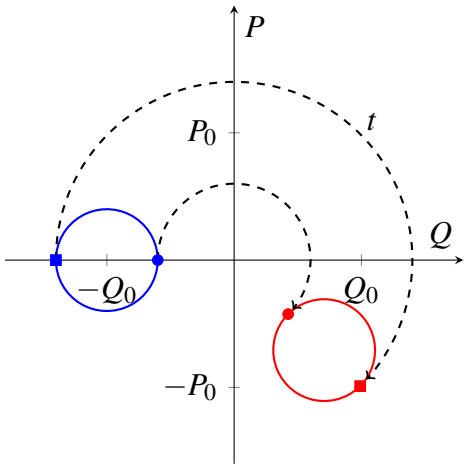

Figure 4.2: Phase space rotation of the level curves of the CES Wigner function with dimensionless axes.

The CES are then the time-dependent solution to the Moyal equation

$$W(x,p;t) = W_n\{u[x + A\cos(\omega t + \phi), p - m\omega A\sin(\omega t + \phi)]\}. \tag{4.61}$$

Therefore, a solution to the time-dependent harmonic oscillator is a harmonic oscillator eigenfunction that rotates about the origin clockwise (for $A > 0$) in the dimensionless phase space $(x\sqrt{m\omega/\hbar}, p/\sqrt{m\hbar\omega})$. The level curves of the Wigner function are circles in the dimensionless phase space that rotate around the origin. The time evolution of the level curves is depicted in Figure 4.2.

4.6 Berry-Balazs Airy Beam

The Airy beam [5] is a solution for the free TDSE that has an accelerating wave front, seemingly in violation the Ehrenfest theorem [27, 28]. This is however not the case, since the Airy function in not square-integrable and thus the state is non-normalizable.

The Airy function itself is the energy eigenstate of a constant force, suggesting that the Airy beam is produced by an FPT from the free particle $V = 0$ to the constant force potential $V' = ax'$. We will use the FPT in phase space to solve for the Wigner function of the Airy beam directly using the stargenvalue equation (4.11). Using the potential relation (4.46),

we have

$$\ddot{\beta} = -\frac{a}{m} \implies \beta(t) = -\frac{a}{2m}t^2 + v_0 t + x_0 \tag{4.62}$$

where v_0 and x_0 are real constants of integration.

Like the CES, to solve the free space Wigner function, we must now solve the time-independent stargenvalue equation for the constant force potential, $V = ax$. Again, using Bopp shifts, the stargenvalue equation becomes

$$\begin{aligned} EW'(x',p') &= H'(x',p') \star W'(x',p') \\ &= H\left(x' + \frac{i\hbar}{2}\partial'_p, p' - \frac{i\hbar}{2}\partial'_x\right) W' \\ &= \left[\frac{1}{2m}\left(p'^2 - i\hbar p'\partial'_x - \frac{\hbar^2}{4}\partial'^2_x\right) + a\left(x' + \frac{i\hbar}{2}\partial'_p\right)\right] W' \end{aligned} \tag{4.63}$$

Separating this equation into the real and imaginary parts yields the two equations:

$$\left(\frac{p'^2}{2m} - \frac{\hbar^2}{8m}\partial'^2_x + ax' - E\right) W' = 0 \tag{4.64}$$

$$\left(\frac{p'}{m}\partial'_x - a\partial'_p +\right) W' = 0. \tag{4.65}$$

The second of these equations (4.65) is again satisfied by setting the Wigner function to be a function of a single variable $W'(x',p') = W'(u)$ where u is proportional to the constant-force Hamiltonian.

Let $u = 8mH'/a^2\hbar^2$. Then, through a change of variables, the real part (4.64) becomes the Airy equation

$$\frac{\mathrm{d}^2 W'}{\mathrm{d}u^2} - uW' = 0, \tag{4.66}$$

for which the solution is the Airy function $W' = C\,\mathrm{Ai}(u)$, where C is an arbitrary constant.

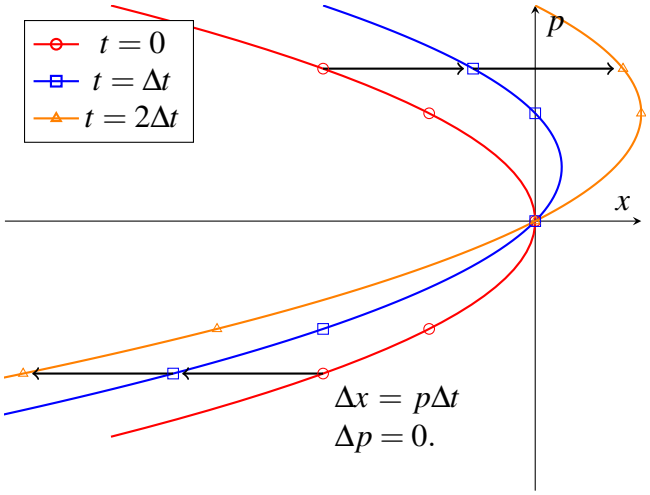

Figure 4.3: Time evolution of the level curves of the Airy beam Wigner function.

Therefore, a solution to the free TDSE is the Wigner function[11]

$$W(x,p;t) = C\,\mathrm{Ai}\left\{\left(\frac{8m}{a^2\hbar^2}\right)^{1/3}\left[\frac{1}{2m}(p-at+mv_0)^2 + a\left(x-\frac{a}{2m}t^2+mv_0+x_0\right)-E\right]\right\}. \tag{4.67}$$

The level curves of the Wigner function again do not appear to obey the free time-evolution, but one can show that it does indeed obey the free Hamiltonian flow

$$\text{const} = \frac{(p+mv_0)^2}{2m} + a(x-\frac{pt}{m}+x_0). \tag{4.68}$$

The rigidly translating parabolic level curves of the Wigner function are depicted in Figure 4.3.

[11] In [5], they use $B^3 = 2m/a^2$.

Conclusion

While form-preserving transformations may be applied to any differential equation, they highlight some important and surprising properties of fundamental quantum mechanics. Namely, the ability of quantum mechanics to deal with linear transformations into non-inertial reference frames. FPTs then provide a framework for performing these transformations and quickly determining the Hamiltonian that results from the transformation. They also explain several remarkable time-dependent solutions of the Schrödinger equation, such as the Coherent Excited States [3], the Airy beam [5], and Yan's time-dependent oscillator [26]. However, in some ways, the FPT also highlights a limitation of quantum mechanics in its inability to describe generalized nonlinear coordinate transformations. The FPT may then give us insight into the fundamental nature of quantum mechanics or may hint at some deeper phenomenon.

FPTs also represent an important method for determining solutions to the Schrödinger equation, one that should be more well-known. Their primary utility is that they allow one to create new solutions to problems in terms of potentials that have already been solved, or to use strategic coordinate transformations to simplify the problem. This forms equivalence classes between different potentials, such as the equivalence between the harmonic oscillator and free potentials that has been discussed previously. These equivalence classes then show how seemingly unrelated systems can share physical properties; however, they are limited to system whose potentials differ at most by second order in position.

In this work, we began by expanding on the work of [9], generalizing the FPT to N dimensions for the spinless Schrödinger -Pauli equation. We show that the most general coordinate transformations allowed by the FPT are of the form (2.28). This results in the

transformed wave function (2.39), which satisfies the Schrödinger -Pauli equation with a vector potential (2.40) and a scalar potential (2.41). In §3.3.8, this was further generalized in three dimensions for spin-1/2 particles.

We showed that the FPT can be directly interpreted as being the transformation between two wave functions of the same particle: one wave function belonging to one set of coordinates and the other belonging to the transformed coordinates. The ansatz for the FPT wave function (2.21) follows from this assumption as a consequence of elementary arguments of probability and the uniqueness of experimental outcome. Then, under the requirement that expectation values of position correspond to the same point in space for both coordinate systems, we showed that quantum mechanics fundamentally restricts the coordinate transformations to be linear. Without this requirement, we would not be able to transfer the results of experiments from one reference frame to another, an obvious problem for the theory. Furthermore, these facts follow without an explicit form for a Hamiltonian and are instead a direct consequence of the linearity of quantum mechanics. To our knowledge, this argument appears to be new.

The operator representation of the FPT was covered in Chapter 3. We showed that FPTs of the Schrödinger equation form a continuous *quasi-symmetry* group if one lets time be a parameter rather than an operator[12]. The Lie algebra of the form-preserving group is shown in equations (3.91) and (3.93). The transformations present in the FPT are then generated by elements of the algebra. We then proceeded to show the exact transformations that each of the generators creates in §3.3.5 and that the most general unitary transformation (3.125) reproduces the form-preserving transformation identically.

The time transformations are the least well-understood part of the FPT. The current literature fails to answer several questions. In §3.3.6, we analyze the properties of the time transformation in more detail. We show, for the first time to our knowledge, that the time transformations $t \to t'(t)$ satisfy all the properties of a group; we determined the composi-

[12]In the literature, such as in [10, 12, 17], the quantum mechanical treatment of the Galilean and Schrödinger groups often include time in the Lie algebra.

tion rules and inverse elements. Then, for continuous elements of the time transformation, we construct a Lie algebra and describe one possible basis for generating the transformation. It is an open question whether the entire group is a Lie group or if there exists discrete elements which are not differentiable.

Lastly, in Chapter 4 we cover the FPT in PSQM in the case of no magnetic fields. We show that the FPT is the linear canonical transformation (4.43). Therefore, the Poisson bracket and the star product are invariant under FPTs. This allows the form of the Moyal bracket to be preserved. The transformed Wigner function obeys the ansatz (4.32) and satisfies the transformed Moyal equation (4.33) with the transformed potential (4.46). To our knowledge, there is no existing work in the literature on the FPT in the phase-space formalism.

Although we covered many different aspects of the FPT in this work, there are still a few open questions and generalizations to be performed. The extension to particles with spin is not complete; we do not describe particles of arbitrary spin-s. Furthermore, our treatment of the spin-1/2 particle was done only for three dimensions. A fully general treatment of the NR FPT would describe particles with arbitrary spin and any number of dimensions. We also did not consider how boundary conditions are affected by the FPT, nor did we show which types of boundary conditions remain valid after an FPT.

Future work may expand the FPT to relativistic quantum mechanics, doing analogous work for the Klein-Gordon equation and the Dirac equation. Since these equations are relativistic, we expect that they will treat the space and time coordinates symmetrically. The FPT for the TDSE is not symmetric about time and space, instead it scales the position by γ^{-1} but the time by γ^{-2}. It would be expected that the FPT should be obtainable by the non-relativistic limit of its relativistic counterparts.

More work may be done in the future to show whether the entire group of time transformations is a Lie group. It is also an open question whether linear canonical transformations are the only possible transformations that we can perform in phase space. This question

remains unanswered in the literature on canonical transformations in the phase-space formalism.

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Appendix A

Electromagnetism in Quantum Mechanics

Electromagnetism is the most ubiquitous force in quantum mechanics, and is responsible for all of chemistry. It is the primary fundamental force that the Schrödinger equation is able to model, and the only force we deal with in this work. In this appendix we will show how the non-relativistic Hamiltonian of a charged particle is derived from classical electromagnetism, which is the only Hamiltonian we use. The classical theory of electromagnetism is a relativistic theory, so we will get the Hamiltonian of the system by first finding the Lagrangian of a charged particle, and taking the non-relativistic limit. Then we perform a Legendre transform to get the classical Hamiltonian, which then may be quantized to obtain the quantum one. We then examine the force on the quantum particle within an electromagnetic field to determine the quantized Lorentz force law, which we use in several places in the main body of this work.

A.1 Classical Electromagnetism

The Lagrangian density for electromagnetism is

$$\mathscr{L} = j_\mu A^\mu + \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \tag{A.1}$$

where j_μ is the 4-vector current density $j^\mu = (c\rho, \vec{J})$, A^μ is the 4-vector potential $A^\mu = (\phi/c, \vec{A})$ and $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field tensor [29].

We will introduce a single charged particle to the Lagrangian. The non-relativistic charge density is then $\rho(\vec{x},t) = q\delta^3(\vec{x} - \vec{x}_0(t))$ where $\vec{x}_0(t)$ is the location of the particle. Likewise, the non-relativistic current density is $\vec{J}(\vec{x},t) = q\vec{v}\delta^3(\vec{x} - \vec{x}_0(t))$. The simplest generalization to special relativity is to replace the velocity with the 4-velocity $v^\mu/\gamma = (c, \vec{v})$ where $\gamma(v)$ is the Lorentz factor and τ is the proper time. We also generalize the delta function to the 4-dimensional version. Therefore, this quantity is the 4-density, instead of just the space density. Thus, we integrate over the proper time of the particle τ to obtain

$$j^\mu = cq \int d\tau \frac{1}{\gamma} u^\mu(\tau) \delta^4(x - x_0(\tau)). \tag{A.2}$$

We will assume that the single charge creates negligible changes in the potential A^μ,

and thus also has no effect on the electromagnetic tensor $F_{\mu\nu}$. We will drop these from the Lagrangian since they will not affect the Euler-Lagrange equations. The Lagrangian is computed as the integral over space of the Lagrangian density, or

$$\begin{aligned} L(x_0,u_0,t) &= \int \mathrm{d}^3x\mathscr{L} = cq\int \mathrm{d}^3xA_\mu(x)\int \mathrm{d}\tau\frac{1}{\gamma}u^\mu(\tau)\delta^4(x-x_0) \\ &= \frac{q}{\gamma}A_\mu(x_0)u^\mu(\tau) \end{aligned} \tag{A.3}$$

This is the interaction Lagrangian for the particle and the electromagnetic field.

In special relativity, the action of a particle is the negative of the length of its world line multiplied by mc to obtain the proper units

$$S = -mc\int \mathrm{d}s, \tag{A.4}$$

where $\mathrm{d}s^2 = \eta_{\mu\nu}\mathrm{d}x^\mu\mathrm{d}x^\nu$. The principle of least action then chooses the path through spacetime that minimizes the length of a particles world line. Diving both sides by the infinitesimal time interval, $\mathrm{d}t$ and taking the square root, we have $\mathrm{d}s/\mathrm{d}t = \sqrt{\dot{x}_\mu\dot{x}^\mu}$ where $\dot{x}^\mu$ is the total time derivative of x^μ, as opposed to the 4-velocity. With a metric signature of $(-,+,+,+)$, we then introduce a minus sign into the square root so that the action is real. This gives the Lagrangian of a relativistic free particle as

$$L_{\text{free}} = -mc\sqrt{-\dot{x}_\mu\dot{x}^\mu} = -\frac{mc}{\gamma}. \tag{A.5}$$

Adding this to the interaction Lagrangian, we obtain the total Lagrangian of a charged particle in a electromagnetic field:

$$L = -mc\sqrt{-\dot{x}_\mu\dot{x}^\mu} + q\frac{1}{\gamma}A_\mu\dot{u}^\mu = -mc\sqrt{-\dot{x}_\mu\dot{x}^\mu} + qA_\mu\dot{x}^\mu. \tag{A.6}$$

Next, we wish to find the equations of motion for the particle. To do this, we take the Euler-Lagrange equation for the position of the particle at the spacetime position x^μ

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{x}^\mu} - \frac{\partial L}{\partial x^\mu} = 0. \tag{A.7}$$

This gives the result

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{mc\dot{x}_\mu}{\sqrt{-\dot{x}_\nu\dot{x}^\nu}} + qA^\mu\right) - q\dot{x}_\nu\partial^\mu A^\nu = 0. \tag{A.8}$$

Next, the total derivative on A^μ of time can be written by the chain rule as $\dot{x}_\nu\partial^\nu$, and the total time derivative can be replaced by the proper time derivative $dt = \gamma d\tau$. The result is that the 4-force F_μ on the particle is

$$\frac{\mathrm{d}p_\mu}{\mathrm{d}\tau} = qF_{\mu\nu}u^\nu. \tag{A.9}$$

From the definition of the electromagnetic tensor, $F_{i0} = E_i/c$ and $F_{ij} = \varepsilon_{ijk}B^k$ where $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields. Thus, it follows that the Lorentz force on a particle $d\vec{p}/dt$ is

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = q(\vec{E} + \vec{v} \times \vec{B}), \tag{A.10}$$

where $\vec{p} = \gamma m\vec{v}$ is the relativistic momentum. In the non-relativistic limit, this matches the classical Lorentz force.

Next we wish to quantize the non-relativistic Hamiltonian to describe a spinless charged particle in quantum mechanics. In the non-relativistic limit, the Lagrangian becomes $L = \frac{m}{2}v^2 - q\Phi + q\vec{A}\cdot\vec{v}$, and the canonical momentum $\vec{p} = \partial_{\vec{v}}L$ is $m\vec{v} + q\vec{A}$. The Hamiltonian is defined as the Legendre transform of the Lagrangian $H = \vec{p}\cdot\vec{v} - L$, where $\vec{p}$ is the canonical momentum obtained from the Lagrangian. This gives us the Hamiltonian in terms of the velocity:

$$H = \vec{v}\cdot(m\vec{v} + q\vec{A}) - \frac{m}{2}\vec{v}^2 + q\Phi - q\vec{v}\cdot\vec{A} = \frac{m}{2}\vec{v}^2 + q\Phi. \tag{A.11}$$

Replacing the velocity with the momentum $\vec{p} = m\vec{v} + q\vec{A}$, we arrive at the classical Hamiltonian for a charged particle in an electromagnetic field

$$H(\vec{x},\vec{p}) = \frac{(\vec{p} - q\vec{A})^2}{2m} + q\Phi. \tag{A.12}$$

In the case of a spin-$1/2$ particle such as an electron, we take $\vec{p} - q\vec{A} \to \vec{\sigma}\cdot(\vec{p} - q\vec{A})$ where σ_i are the Pauli spin matrices. The matrices $\frac{\hbar}{2}\sigma_i$ form the spin-$1/2$ representation of the $\mathfrak{su}(2)$ Lie algebra.

The result is the modified Hamiltonian for a spin-$1/2$ particle

$$H = \frac{1}{2m}\left[(\vec{p} - q\vec{A})^2 - q\hbar\vec{\sigma}\cdot\vec{B}\right] + q\Phi. \tag{A.13}$$

Let the spin angular momentum operator be $\vec{S} = \hbar\vec{\sigma}/2$. Then we can write the interaction potential of spin with the magnetic field as $-\frac{q}{m}\vec{S}\cdot\vec{B}$. Comparing this to the potential energy of a magnetic dipole $U = -\vec{\mu}\cdot\vec{B}$, we see that we can interpret this interaction term as the interaction of a magnetic field with the magnetic dipole moment of a spin-1/2 particle, $q\vec{S}/m$. The magnetic dipole moment of a charge with angular momentum $\vec{L}$ is $\vec{\mu} = q\vec{L}/2m$. Thus, the quantum dipole moment of a spin-1/2 particle is twice the classical result. This factor of two is called the g factor. The Schrödinger-Pauli equation (and the Dirac equation) predicts that the g-factor is precisely 2. Quantum field theory predicts corrections in quantum electrodynamics from the self-interaction of electrons with the electromagnetic field that increases the g factor by about .2% for the electron.

The Schrödinger-Pauli equation can be derived as the non-relativistic limit of the Dirac equation for the electron. But since spin has no classical analog, it cannot be derived from quantizing classical theories. See [28, Chapter 20] for a derivation from the Dirac equation.

A.2 Lorentz Force in Quantum Mechanics

The equations of motion for expectation values of an observable Ω in the Schrödinger picture are given by the Ehrenfest theorem [28]

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Omega\rangle = \left\langle\frac{\partial\Omega}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle[\Omega,H]\rangle\,, \tag{A.14}$$

where H is the Hamiltonian, given that the state is normalizable. The velocity of the state is the time derivative of position [27], which for a particle in an electric and magnetic field is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{X}\rangle = \frac{1}{2im\hbar}\left\langle\left[\vec{X},(\vec{P}-q\vec{A})^2\right]\right\rangle = \frac{1}{m}\left\langle\vec{P}-q\vec{A}\right\rangle. \tag{A.15}$$

Let us define the velocity operator $m\vec{V} = \vec{P}-q\vec{A}$. Next, the force on the particle is the mass m times the time derivative of position, which is

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{V}\rangle = \left\langle -q\frac{\partial\vec{A}}{\partial t}\right\rangle + \frac{1}{i\hbar}\left\langle\left[\vec{P}-q\vec{A},\frac{(\vec{P}-q\vec{A})^2}{2m}+q\Phi\right]\right\rangle \tag{A.16}$$

The commutator $[\vec{P},q\Phi]$ is just the gradient of the scalar potential $-i\hbar q\Phi$, and since the vector potential and the scalar potentials are functions of position and time only, they commute. Since the electric field is defined as $-\nabla\Phi-\partial_t\vec{A}$, we now have the force

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{V}\rangle = \langle q\vec{E}\rangle + \frac{1}{2im\hbar}\left\langle\left[\vec{P}-q\vec{A},(\vec{P}-q\vec{A})^2\right]\right\rangle. \tag{A.17}$$

Next, the ith component of the remaining commutator yields

$$-qV_j\left(\left[A_i,P_j\right]+\left[P_i,A_j\right]\right) - q\left(\left[A_i,P_j\right]+\left[P_i,A_j\right]\right)V_j. \tag{A.18}$$

The inside of the parentheses is $i\hbar\partial_j A_i - i\hbar\partial_i A_j = -i\hbar F_{ij}$ where F is the electromagnetic tensor. In three-dimensions we can write this as $-i\hbar\varepsilon_{ijk}\varepsilon_{abk}\partial_a A_b$ using the identity (B.5). Since the magnetic field is the curl of the vector potential, $\varepsilon_{abk}\partial_a A_b = B_k$. Thus, we have

$$\left[P_i-qA_i,(\vec{P}-q\vec{A})^2\right] = qi\hbar\varepsilon_{ijk}V_jB_k + qi\hbar\varepsilon_{ijk}B_kV_j = qi\hbar(\vec{V}\times\vec{B}-\vec{B}\times\vec{V})_i. \tag{A.19}$$

Therefore, the total Lorentz force is

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle\vec{V}\rangle = q\left\langle\vec{E}+\frac{1}{2}(\vec{V}\times\vec{B}-\vec{B}\times\vec{V})\right\rangle. \tag{A.20}$$

This is the Weyl ordering[13] of the classical Lorentz force, where the two orderings of the cross product $\vec{V}\times\vec{B}$ and $-\vec{B}\times\vec{V}$ are averaged over. This ordering guarantees that the

[13]The Weyl ordering is the sum of all distinct permutations of operators, divided by the total number of permutations. For example, the Weyl ordering of x^2p is $\frac{1}{3}(x^2p+xpx+px^2)$

resulting operator is Hermitian. For higher dimensions, this is given by:

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle V_i\rangle = q\left\langle E_i + \frac{1}{2}(V_j F_{ij} + F_{ij}V_j)\right\rangle. \tag{A.21}$$

Appendix B

Levi-Civita Symbol

The Levi-Civita symbol ε in 3-dimensions has the components

$$\varepsilon_{ijk} = \begin{cases} +1 & (i,j,k) = \text{cyclic permutation of } (1,2,3) \\ -1 & (i,j,k) = \text{cyclic permutation of } (3,2,1) \\ 0 & \text{otherwise.} \end{cases} \tag{B.1}$$

It is completely antisymmetric, so swapping any two indices introduces a minus sign, eg. $\varepsilon_{jik} = -\varepsilon_{ijk}$.

The Levi-Civita symbol can be used to define several mathematical operations such as the cross product of two vectors

$$(\vec{a} \times \vec{b})_i = \varepsilon_{ijk} a_j b_k, \tag{B.2}$$

and the determinant of a 3×3 matrix

$$\det \mathbf{A} = \varepsilon_{ijk} A_{1i} A_{2j} A_{3k}. \tag{B.3}$$

The Levi-Civita symbol has the following useful identities

$$\varepsilon_{ijk}\varepsilon_{ijl} = 2\delta_{kl} \tag{B.4}$$

$$\varepsilon_{ijk}\varepsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}, \tag{B.5}$$

which are often used for proving mathematical identities in vector calculus, and are used many times in this work.

The Levi-Civita symbol may be extended to any number of dimensions. If N is the number of dimensions, then we may define the Levi-Civita symbol as

$$\varepsilon_{i_1 i_2 \ldots i_N} = \begin{cases} 1 & i_1, i_2, \ldots i_N \text{ is an even permutation of } 1,2,\ldots N \\ -1 & i_1, i_2, \ldots i_N \text{ is an odd permutation of } 1,2,\ldots N \\ 0 & \text{otherwise.} \end{cases} \tag{B.6}$$

It is totally antisymmetric, so swapping any two indices results in the introduction of a minus sign. For example,

$$\varepsilon_{i_1 i_2 \ldots i_N} = -\varepsilon_{i_2 i_1 \ldots i_N}. \tag{B.7}$$

Appendix C

Groups

A group is a set of elements with a defined product or operation that combines two elements into a new one. Let g_1, g_2, g_3 be elements of the group G. Denoting the group product by "$\cdot$," the group and its product must satisfy the following properties:

1. Closure: $g_1 \cdot g_2 = g_3 \in G$.
2. Associativity: $g_1 \cdot (g_2 \cdot g_3) = (g_1 \cdot g_2) \cdot g_3$.
3. Existence of an identity element e: $e \cdot g = g \cdot e = g$.
4. Existence of an inverse element g^{-1}: $g \cdot g^{-1} = g^{-1} \cdot g = e$.

If the set of objects and its product operator "$\cdot$" satisfies these properties, then G is a group.

Groups are very important in the analysis of symmetries since symmetries form a group. For example, consider the group of transformations that keeps the orientation of an equilateral triangle invariant (called D_3). Doing two of these operations in a row will still preserve the orientation and shape of the triangle and, therefore, the closure property is automatically preserved. This is the case in general, since if two operations preserve some symmetry, then performing the two operations in sequence will still be a symmetry, irrespective of the symmetry in question.

C.1 Special Linear Group

The special linear group $SL(2,\mathbb{R})$ is the group of 2×2 linear transformations with real entries and that are special, or have determinant 1. As with most matrix groups, they multiply by ordinary matrix multiplication. In other words, the group $SL(2,\mathbb{R})$ is the group that is equivalent to the two-dimensional representation

$$R(g) \in \left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} : a,b,c,d \in \mathbb{R} \text{ and } ad - cd = 1 \right\}. \tag{C.1}$$

Here R is the representation and $g \in SL(2,\mathbb{R})$. The constraint leaves 3 free parameters to define an element of $SL(2,\mathbb{R})$, such as the numbers (a,b,c), with $d = (1+cd)/a$. The group of two-dimensional rotations, $SO(2)$, is a subgroup of $SL(2,\mathbb{R})$. The main difference between this group and $SO(2)$ is that these matrices are not all orthogonal, so they do

not preserve the angles and distances between vectors. However, since both of their determinants are still unity, they preserve the area of shapes. The additional constraint is why $SO(2)$ is a 2-parameter group while $SL(2,\mathbb{R})$ has 3 parameters.

$SL(2,\mathbb{R})$ is a continuous group with three degrees of freedom. It will not be shown here, but $SL(2,\mathbb{R})$ is smooth and differentiable, and thus it is a Lie group. Let the matrix $M = e^{\varepsilon A}$ be an element of $SL(2,\mathbb{R})$, where A is a 2×2 real matrix. Then the matrix M must have unit determinant. Using Jacobi's formula, $1 = \det M = e^{\mathrm{Tr}(\varepsilon A)}$. Therefore, the matrix A must have zero trace for $\varepsilon \neq 0$. We choose the traceless basis

$$h = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad e = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad f = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{C.2}$$

so that $A \in \mathrm{span}(\{e,f,h\})$. The span of this basis completely covers the vector space of all traceless 2×2 real matrices.

In this basis, the matrices form the closed Lie algebra

$$[h,e] = 2e \qquad [h,f] = -2f \qquad [e,f] = h. \tag{C.3}$$

Any collection of 3 operators $\{e,f,h\}$ that satisfy the commutation relations (C.3) is called an sl_2-triplet. The group the set of operators generates is then isomorphic to $SL(2,\mathbb{R})$ when using real parameters, and $SL(2,\mathbb{C})$ if the space is spanned with complex parameters.

Appendix D

Orthogonal Transformations and SO(N)

The orthogonal group in three dimensions, $O(3)$, is defined as the set of $\mathbb{R}^{3\times 3}$ matrices whose transpose is equal to its inverse:

$$RR^T = R^T R = I, \tag{D.1}$$

where the group product is the matrix product. The reader is encouraged to verify that this definition satisfies all of the axioms for a group, namely closure, associativity, the existence of the identity element, and the existence of an inverse.

The property (D.1) is very important because linear transformations by such matrices leave the inner product of two vectors invariant. Let $\vec{u}$ and $\vec{v}$ be vectors in $\mathbb{R}^3$. Let $\vec{u}' = R\vec{u}$ and $\vec{v}' = R\vec{v}$ be the transformed vectors under an orthogonal linear transformation. Then the inner product between the two transformed vectors is

$$\begin{aligned} \vec{u}' \cdot \vec{v}' &= (R\vec{u}) \cdot (R\vec{v}) \\ &= \vec{u}^T R^T R \vec{v} \\ &= \vec{u}^T \vec{v} \\ &= \vec{u} \cdot \vec{v}, \end{aligned} \tag{D.2}$$

the inner product of the two original vectors. Therefore, orthogonal transformations preserve both angles and distances between vectors.

There are two types of orthogonal matrices, classified by their determinant. Taking the determinant of $R^T R = I$, we see that the determinant of an orthogonal matrix is $\det R = \pm 1$. The orthogonal matrices with determinant $+1$ are called proper rotations, and make up the group of *special* orthogonal matrices, $SO(3)$. Orthogonal matrices with determinant -1 are called improper rotations, as they contain a reflection as well as a rotation. As a consequence, they change the handedness of coordinate systems.

Rotation matrices in $SO(3)$ have the property that they preserve cross products, since they preserve the handedness of coordinates as well as angles and distances. As a consequence, rotating the resulting cross product of two vectors is the same as taking the cross product of two rotated vectors:

$$R(\vec{u} \times \vec{v}) = (R\vec{u}) \times (R\vec{v}). \tag{D.3}$$

For an orthogonal matrix with determinant -1, the right-hand side picks up an additional

minus sign.

To show this is the case, begin with the i-th component of the cross product

$$[(R\vec{u}) \times (R\vec{v})]_i = \varepsilon_{ijk} R_{jq} R_{ks} u_q v_s \tag{D.4}$$

$$= \varepsilon_{\ell jk} \delta_{i\ell} R_{jq} R_{ks} u_q v_s. \tag{D.5}$$

But since the R matrices are orthogonal, we can rewrite the Kronecker delta as the product of R with its transpose. Thus we have

$$[(R\vec{u}) \times (R\vec{v})]_i = \varepsilon_{\ell jk} R_{ip} R_{\ell p} R_{jq} R_{ks} u_q v_s. \tag{D.6}$$

But we can define the determinant of any 3×3 matrix [31] as $\varepsilon_{ijk} R_{ip} R_{jq} R_{ks} = \varepsilon_{pqs} \det R$, and it is clear that the Levi-Civita symbol is an invariant tensor under $SO(3)$ transformations (for which the determinant is one). With this identity, we can write the cross product between the two rotated vectors as

$$[(R\vec{u}) \times (R\vec{v})]_i = \det(R) R_{ip} \varepsilon_{pqs} u_q v_s = \det(R) [R(\vec{u} \times \vec{v})]_i \tag{D.7}$$

which is equivalent to (D.3).

D.1 Lie Algebra so(3)

Rotation matrices are smooth and differentiable. For example, consider the rotation in 2 dimensions

$$R = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \tag{D.8}$$

that is parametrized by the angle $\theta \in [0, 2\pi)$. This familiar matrix is differentiable with respect to the continuous parameter θ. Since the group is smooth and differentiable, it is a called a *Lie group*. The parameters serve as the coordinates of the group element on the group manifold.

The *Lie algebra* of a Lie group is the tangent space at the identity element and the algebra of the tangent space: the commutation relations between all elements of the tangent space. The algebra must be closed (otherwise we wouldn't get closure of the group elements), so the commutator between two elements of the Lie algebra must itself be an element of the algebra. The structure of the entire Lie group can be recovered only from its Lie algebra and the exponential map.

Since $SO(3)$ is orthogonal, we may define $R = e^{-i\lambda J}$ where the matrix J is a 3×3 antisymmetric matrix and λ is a real parameter. To find the tangent of the matrix R with respect to the parameter λ, we take its derivative and set the parameter to zero: $\frac{\mathrm{d}}{\mathrm{d}\lambda} R\big|_{\lambda=0} = -iJ$. Consequently, the matrix $-iJ$ is an element of the tangent space of $SO(3)$ matrices.

The reason we can recover the entire rotation group and its manifold structure only from its Lie algebra and the exponential map is a consequence of the group being differentiable. Consider, for example, n successive infinitesimal rotations by the angle $\Delta\theta = \theta/n$, which will approximate a rotation by the angle θ. Each infinitesimal rotation may be described by the matrix $R(\Delta\theta) \sim 1 - i\Delta\theta J$, and the full rotation by $[R(\Delta\theta)]^n$. Since the infinitesimal rotation is caused by the matrix J, we sometimes call this a *generator* of $SO(3)$. As we

increase n, the approximation will become successively better until it becomes identical to the full rotation in the limit as n grows to infinity. Performing this explicitly, we obtain

$$R(\theta) = \lim_{n\to\infty}\left(1 - \frac{i\theta J}{n}\right)^n = \lim_{n\to\infty}\sum_{k=0}^{n}\binom{n}{k}\left(\frac{-i\theta J}{n}\right)^k = \exp(-i\theta J) \tag{D.9}$$

since $\lim_{n\to\infty}\binom{n}{k}n^{-j} = 1/k!$. For this reason the exponential function is sometimes called the exponential map, since it maps an element of the Lie algebra to its Lie group.

To see why J must be antisymmetric, we expand $R^T R = 1$ to first order in λ, obtaining

$$R^T R = 1 + i\lambda J^T + i\lambda J + O(\lambda^2). \tag{D.10}$$

Equating this to the identity, we see that the matrix R with by orthogonal if

$$J^T = -J, \tag{D.11}$$

or that the elements of the Lie algebra are antisymmetric matrices. The most general way to write an antisymmetric matrix in three dimensions is with the Levi-Civita symbol $J_{ij} = i\varepsilon_{ikj}\theta_k$ where θ_k are real numbers. The imaginary number i keeps the generator Hermitian. Using these as a basis gives the adjoint representation of $\mathfrak{so}(3)$:

$$J^{(a)}_{ij} = i\varepsilon_{iaj}, \tag{D.12}$$

which represents the infinitesimal generator of rotations for the $a = (x,y,z)$ axis, according to the right hand rule.

The Lie algebra $\mathfrak{so}(3)$ can then be directly determined from the properties of the Levi-Civita symbol by

$$\begin{aligned}
[J^{(a)}, J^{(b)}]_{ik} &= J^{(a)}_{ic}J^{(b)}_{ck} - J^{(b)}_{ic}J^{(a)}_{ck} \\
&= -(\varepsilon_{iac}\varepsilon_{cbk} - \varepsilon_{ibc}\varepsilon_{cak}) \\
&= -[(\delta_{ib}\delta_{ak} - \delta_{ik}\delta_{ab}) - (\delta_{ia}\delta_{bk} - \delta_{ik}\delta_{ab})] \\
&= -(\delta_{ib}\delta_{ka} - \delta_{ia}\delta_{kb}) \\
&= -\varepsilon_{ikc}\varepsilon_{bac}
\end{aligned} \tag{D.13}$$

Rearranging the indices in the Levi-Civita symbols, it is easy to obtain

$$[J^{(a)}, J^{(b)}] = i\varepsilon_{abc}J^{(c)}. \tag{D.14}$$

The most general generator is then the antisymmetric matrix $-i\vec{\theta}\cdot\vec{J} = [\vec{\theta}]_\times$ where the matrix $[\vec{\theta}]_\times$ has the effect of taking a cross product of a vector: $[\vec{\theta}]_\times\vec{v} = \vec{\theta}\times\vec{v}$. This allows us to explicitly compute the rotation matrix from the generators by the exponential map

$$R(\vec{\theta}) = e^{-i\vec{\theta}\cdot\vec{J}} = e^{[\vec{\theta}]_\times} = \sum_{n=0}^{\infty}\frac{1}{n!}[\vec{\theta}]^n_\times. \tag{D.15}$$

As a side note, from this equation it is obvious that the inverse rotation $R^T(\vec{\theta}) = R(-\vec{\theta})$ is simply an equal and opposite rotation.

The exponential map may be computed exactly by exploiting the recursion relation for the powers of cross products. By the vector triple product, we have $[\vec{\theta}]_\times^2 \vec{a} = \vec{\theta}(\vec{\theta}\cdot\vec{a}) - \theta^2\vec{a}$, which means that the cube is $[\vec{\theta}]_\times^3 = -\theta^2[\vec{\theta}]_\times$. By mathematical induction, it follows that

$$\begin{aligned} [\vec{\theta}]_\times^{2n+1} &= (-\vec{\theta}^2)^n[\vec{\theta}]_\times \quad n \geq 0 \\ [\vec{\theta}]_\times^{2n} &= (-\vec{\theta}^2)^{n-1}[\vec{\theta}]_\times^2 \quad n \geq 1. \end{aligned} \tag{D.16}$$

Let $\hat{n}$ denote the direction of $\vec{\theta}$, or the axis of rotation. Then by breaking the exponential into even and odd terms, it is easy to see that

$$\begin{aligned} R(\vec{\theta}) &= I + \sin\theta[\hat{n}]_\times + (1-\cos\theta)[\hat{n}]_\times^2 \\ &= \cos\theta I + \sin\theta[\hat{n}]_\times + (1-\cos\theta)(\hat{n}\otimes\hat{n}), \end{aligned} \tag{D.17}$$

where $(\hat{n}\otimes\hat{n})_{ij} = n_i n_j$ is the outer product. This formula for calculating rotations explicitly is usually called Rodrigues' rotation formula.

D.2 Rotations in Higher Dimensions and so(N)

In three dimensions, we are safe to label rotations by the singular vector that is orthogonal to the plane of rotation. This is only possible in three dimensions, and for higher ones, there is no longer one unique vector that is orthogonal to a given plane of rotation. Thus, in higher dimensions, it becomes more convenient to label rotations by the plane of rotation, which can be done by specifying the two basis vectors that span the plane. Let the rotation generator be the antisymmetric matrix $J^{(ab)}$ where the labels run from $a,b = 1,2,\ldots N$ where N is the number of dimensions. We will give these antisymmetric matrices components

$$J_{ij}^{(ab)} = -i(\delta_{ai}\delta_{bj} - \delta_{aj}\delta_{bi}). \tag{D.18}$$

These generators will then generate infinitesimal rotations from the coordinate axis a into b. For example, in three dimensions, the rotation generator for rotations about the z axis is simply $J^{(z)} = J^{(12)}$. It can be checked that this antisymmetric basis has the commutation relations

$$[J^{(ij)}, J^{(ab)}] = i(\delta_{jb}J^{(ia)} + \delta_{ia}J^{(jb)} - \delta_{ja}J^{(ib)} - \delta_{ib}J^{(ja)}). \tag{D.19}$$

There are $N(N-1)/2$ basis matrices that span the vector space of antisymmetric matrices. We may write a general antisymmetric matrix in this basis as $\frac{i}{2}S_{ij}J^{(ij)} = S$ where S_{ij} is itself another real, antisymmetric matrix. Since this also has $N(N-1)/2$ free parameters, this is not an issue. Each entry of S_{ab} tells you the angle that axis a is rotated into axis b. Then in total, the rotation matrix is

$$R = e^{\frac{i}{2}S_{ij}J^{(ij)}} = e^S. \tag{D.20}$$

D.3 The Orbital Angular Momentum Tensor Operator

We may define a rotation generator operator, or the orbital angular momentum tensor

$$L_{ij} = X_i P_j - X_j P_i. \tag{D.21}$$

This will satisfy the (scaled) commutation relation for generators of rotations along the i and j axes as

$$[L_{ij}, L_{ab}] = i\hbar(\delta_{jb}L_{ia} + \delta_{ia}L_{jb} - \delta_{ja}L_{ib} - \delta_{ib}L_{ja}). \tag{D.22}$$

Physically, these angular momenta are the angular momentum in the plane spanned by the i and j axes. In three dimensions, the angular momentum vector is related to the angular momentum tensor by $L_a = \frac{1}{2}\varepsilon_{abc}L_{bc}$.

If an operator V_a transforms as a vector, such as the position or momentum operators, then it will have the commutation relation[14]

$$[V_a, L_{bc}] = i\hbar(\delta_{ac}V_b - \delta_{ab}V_c). \tag{D.23}$$

Defining the rotation generator $G = -\frac{1}{2}S_{ij}L_{ij}$ for the real antisymmetric matrix S_{ij}, we have

$$[iG/\hbar, V_a] = S_{ab}V_b. \tag{D.24}$$

That is, the action of an infinitesimal rotation is to take $\vec{V} \to \vec{V} - S\vec{V}$. It then follows that the operator will transform as

$$\vec{V}' = U\vec{V}U^\dagger = e^S\vec{V} = R\vec{V} \tag{D.25}$$

We may apply this to the angular momentum tensor. Let $L'_{ij} = UL_{ij}U^\dagger$, then

$$\begin{aligned} L'_{ij} &= X'_i P'_j - X'_j P'_i \\ &= R_{ir}R_{js}X_r P_s - R_{js}R_{ri}X_s P_r \\ &= R_{ir}R_{js}L_{rs}. \end{aligned} \tag{D.26}$$

And so the angular momentum tensor does indeed transform as a tensor under rotations.

D.4 Time Derivative of Rotations

Taking the time derivative of (D.1), we get that $\dot{R}^T R + R^T\dot{R} = 0$. Rearranging this equation, it becomes

$$(R^T\dot{R})^T = -R^T\dot{R}. \tag{D.27}$$

Therefore, the matrix $R^T\dot{R}$ is antisymmetric. In three dimensions, we can write this as

$$(R^T\dot{R})_{ij} = ([\vec{\omega}]_\times)_{ij} = \varepsilon_{i\ell j}\omega_\ell \tag{D.28}$$

[14] Tensor operators, such as L_{ij}, will have each index transform in this same manner, as is consistent with (D.22).

where $[\vec{\omega}]_\times \vec{a} = \vec{\omega} \times \vec{a}$ is the cross product matrix and $\vec{\omega}$ is some real vector. Since the Levi-Civita symbol is completely antisymmetric, this satisfies (D.27) and $[\vec{\omega}]_\times$ spans all antisymmetric matrices in $\mathbb{R}^{3\times 3}$. Therefore, the time derivative of an $SO(3)$ matrix can be written as

$$\dot{R} = R[\vec{\omega}]_\times \tag{D.29}$$

for some as-yet undetermined $\vec{\omega}$.

For a constant axis of rotation, consider an unmoving point $\vec{x}$ being observed after a time-dependent rotation $R(\theta(t)\hat{n})$. The time velocity of this point in the rotating frame is

$$\vec{v} = R(\vec{\omega} \times \vec{x}) = \vec{\omega} \times (R\vec{x}), \tag{D.30}$$

since $\vec{\omega}$ is parallel to the axis of rotation and is left invariant under the rotation. That this is just the velocity of regular rotational motion means that $\vec{\omega}$ must just be the angular velocity in this case.

For the general case of a time-dependent axis of rotation, this is no longer true. Since $\vec{\theta}$ is left unchanged by rotations, we may take the derivative of $R\vec{\theta} = \vec{\theta}$ to yield $\dot{R}\vec{\theta} + R\dot{\vec{\theta}} = \dot{\vec{\theta}}$. Rearranging, we obtain

$$R^T \dot{R}\vec{\theta} = \vec{\omega} \times \vec{\theta} = (R^T - I)\dot{\vec{\theta}}. \tag{D.31}$$

Solving this equation yields

$$\vec{\omega} = a\hat{n} + \sin\theta\dot{\hat{n}} + (\cos\theta - 1)\hat{n} \times \dot{\hat{n}}, \tag{D.32}$$

where a is an arbitrary real constant with dimensions of inverse time. The only scalar quantity with these dimensions that could be a is $\dot{\theta}$. However, we will show this more rigorously in the subsequent section.

D.5 Time Derivative of the Rotation Operators

We will show how the time derivative of the rotation generators is derived; first in 3-dimensions and then for any number of dimensions. The total derivative of the exponential map e^X with respect to the parameter t is given by [1, theorem 5, sec. 1.2]

$$\frac{\mathrm{d}}{\mathrm{d}t}e^X = e^X \frac{1 - e^{-\mathrm{ad}_X}}{\mathrm{ad}_X}\frac{\mathrm{d}X}{\mathrm{d}t} = e^X \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!}\mathrm{ad}_X^n \frac{\mathrm{d}X}{\mathrm{d}t}. \tag{D.33}$$

Using the derivative (D.33), we can compute the time derivative of the rotation $U = \exp\left(-i\vec{\theta}\cdot\vec{L}/\hbar\right)$. This is

$$\dot{U} = \frac{-i}{\hbar} U \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!}\mathrm{ad}^n_{-i\vec{\theta}\cdot\vec{L}/\hbar}\dot{\vec{\theta}}\cdot\vec{L}. \tag{D.34}$$

Next, the first-order commutator is easily shown to be

$$\frac{-i}{\hbar}[\theta_a L_a, \dot{\theta}_b L_b] = \varepsilon_{abc}\theta_a\dot{\theta}_b L_c = (\vec{\theta} \times \dot{\vec{\theta}})\cdot\vec{L}. \tag{D.35}$$

Since $\dot{\vec{\theta}}$ was arbitrary, this means that the action of the adjoint operator $\mathrm{ad}_{-i\vec{\theta}\cdot\vec{L}/\hbar}$ on the operator $\vec{a}\cdot\vec{L}$, for some vector $\vec{a}$, is to take $\vec{a}\to\vec{\theta}\times\vec{a}$. Therefore, after repeating this n times, the nth order adjoint is just

$$\mathrm{ad}^n_{-i\vec{\theta}\cdot\vec{L}/\hbar}\dot{\vec{\theta}}\cdot L=([\vec{\theta}]^n_\times\dot{\vec{\theta}})\cdot\vec{L} \tag{D.36}$$

where $[\vec{\theta}]_\times$ is the anti-symmetric cross product matrix with $[\vec{\theta}]_\times\vec{a}=\vec{\theta}\times\vec{a}$.

We can write an explicit formula for the vector $\vec{\omega}$ by exploiting the recursion relations for powers of $[\vec{\theta}]_\times$. We have the vector triple product identity $[\vec{\theta}]^2_\times\vec{a}=\vec{\theta}\times(\vec{\theta}\times\vec{a})=(\vec{\theta}\cdot\vec{a})\vec{\theta}-\vec{\theta}^2\vec{a}$, which means that $[\vec{\theta}]^3_\times=-\vec{\theta}^2[\vec{\theta}]_\times$. By mathematical induction, it follows that

$$\begin{aligned}[\vec{\theta}]^{2k+1}_\times&=(-\vec{\theta}^2)^k[\vec{\theta}]_\times\quad k\geq 0,\\ [\vec{\theta}]^{2k}_\times&=(-\vec{\theta}^2)^{k-1}[\vec{\theta}]^2_\times\quad k\geq 1.\end{aligned} \tag{D.37}$$

Let $\hat{n}$ denote the direction of $\vec{\theta}$, or the axis of rotation. Then by breaking the exponential into even and odd terms power of $[\vec{\theta}]_\times$, we have

$$\begin{aligned}\vec{\omega}&=\left(1-\sum_{k=0}^{\infty}\frac{(-1)^k}{(2k+2)!}\theta^{2k}[\hat{n}]_\times-\sum_{k=1}^{\infty}\frac{(-1)^k}{(2k+1)!}\theta^{2k}[\hat{n}]^2_\times\right)\dot{\vec{\theta}}\\&=\left(1+\frac{\cos\theta-1}{\theta}[\hat{n}]_\times+\frac{\theta-\sin\theta}{\theta}[\hat{n}]^2_\times\right)\dot{\vec{\theta}}.\end{aligned} \tag{D.38}$$

Where $\dot{U}=\frac{1}{i\hbar}U\vec{\omega}\cdot\vec{L}$. Using the vector triple product identity, we may simplify this further to

$$\vec{\omega}=\frac{1}{\theta}\left\{\sin\theta+(\cos\theta-1)[\hat{n}]_\times+(\theta-\sin\theta)\hat{n}\otimes\hat{n}\right\}\dot{\vec{\theta}} \tag{D.39}$$

where the outer product between two vectors $\vec{a}\otimes\vec{b}$ is defined as the matrix with components $(\vec{a}\otimes\vec{b})_{ij}=a_ib_j$.

We may at this point use the fact that the time derivative of the rotation vector is $\dot{\vec{\theta}}=\dot{\theta}\hat{n}+\theta\dot{\hat{n}}$. This gives the resulting angular velocity vector $\dot{\theta}\hat{n}+\sin\theta\dot{\hat{n}}+(\cos\theta-1)\hat{n}\times\dot{\hat{n}}$

$$\boxed{\vec{\omega}=\frac{\mathrm{d}\vec{\theta}}{\mathrm{d}t}+(\sin\theta-\theta)\dot{\hat{n}}+(\cos\theta-1)\hat{n}\times\dot{\hat{n}}} \tag{D.40}$$

where we have used $\hat{n}\cdot\dot{\hat{n}}=0$ since $\dot{\hat{n}}$ must be orthogonal to $\hat{n}$. If this were not the case, then the length of $\hat{n}$ would change, which by definition must be held constant at one. For a small time step $\Delta t=t-t_0\ll 1$, the length of the unit vector is

$$|\hat{n}(t)|^2\sim|\hat{n}(t_0)+\Delta t\dot{\hat{n}}(t_0)|^2\sim 1+2\Delta t\hat{n}\cdot\dot{\hat{n}}. \tag{D.41}$$

Since it must be constant, $\dot{\hat{n}}$ must be orthogonal to the unit vector. The vectors $\{\hat{n},\dot{\hat{n}},\hat{n}\times\dot{\hat{n}}\}$ then form an orthogonal set of basis vectors, as seen in Figure D.1.

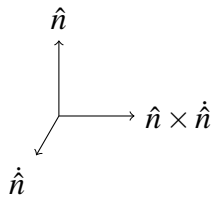

Figure D.1: Orthogonal basis created by the axis of rotation and its time derivative.

Another relevant quantity is the rotated angular velocity $R\vec{\omega} = \vec{\Omega}$. Using (D.40), it is

$$\vec{\Omega} = \frac{\mathrm{d}\vec{\theta}}{\mathrm{d}t} + (\sin\theta - \theta)\dot{\hat{n}} - (\cos\theta - 1)\hat{n} \times \dot{\hat{n}}. \tag{D.42}$$

The quantity relevant to the transformed Hamiltonian in the FPT is

$$i\hbar \dot{U} U^{\dagger} = \vec{\Omega} \cdot L = (\dot{R} R^T \vec{X}) \cdot \vec{P} \tag{D.43}$$

We mentioned that this must be related to the time derivative of the rotation matrix $R(\vec{\theta}) = \exp\left(-i\vec{\theta} \cdot \vec{J}\right)$ where $-i\vec{\theta} \cdot \vec{J} = [\vec{\theta}]_{\times}$ is the usual coordinate basis for the Lie algebra $\mathfrak{so}(3)$. This is easy to show using the same derivative formula (D.33)

$$\dot{R} = R \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \mathrm{ad}^n_{-i\vec{\theta}\cdot J}(-i\dot{\vec{\theta}} \cdot \vec{J}). \tag{D.44}$$

Using the $\mathfrak{so}(3)$ commutation relation $[J^{(a)}, J^{(b)}] = i\varepsilon_{abc} J^{(c)}$, it is clear that the adjoint is related to the previous case $\mathrm{ad}^n_{-i\vec{\theta}\cdot\vec{J}} \dot{\vec{\theta}} \cdot \vec{J} = ([\vec{\theta}]^n_{\times} \dot{\vec{\theta}}) \cdot \vec{J}$. Thus, the time derivative of the rotation matrix is

$$\dot{R} = -iR\vec{\omega} \cdot \vec{J} = R[\vec{\omega}]_{\times}, \tag{D.45}$$

where $\vec{\omega}$ is the same vector in (D.40).

Time Derivatives in Higher Dimensions

Next for higher dimensions, we will find the time derivative of the exponential map of the angular momentum tensor, $U = \exp\left(\frac{i}{2\hbar} S_{ij} L_{ij}\right)$. We will relate this to the time derivative of the rotation matrix $R = \exp\left(\frac{i}{2} S_{ij} J^{(ij)}\right)$. Beginning in the same manner as before, the time derivatives of the unitary rotation operator and the real rotation matrix are

$$\begin{aligned} \dot{U} &= \frac{i}{2\hbar} U \dot{S}_{ab} \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \mathrm{ad}^n_{\frac{i}{2\hbar} S_{ij} L_{ij}} L_{ab} \\ \dot{R} &= \frac{i}{2} R \dot{S}_{ab} \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} \mathrm{ad}^n_{\frac{i}{2} S_{ij} J^{(ij)}} J^{(ab)}. \end{aligned} \tag{D.46}$$

Since the algebras for the angular momentum tensor and the rotation generators is the same (up to a factor of $\hbar$, the adjoint of the operators $\frac{i}{2\hbar} S_{ij} L_{ij}$ and $\frac{i}{2} S_{ij} J^{(ij)}$ with L_{ab} and $J^{(ab)}$ respectively, will transform each into the same linear combination of themselves. The adjoint

will be $(S_{ia}\delta_{jb}+S_{jb}\delta_{ia})L_{ij}$ for the angular momentum tensor and $(S_{ia}\delta_{jb}+S_{jb}\delta_{ia})J^{(ij)}$. Let $T_{abij}=S_{ia}\delta_{jb}+S_{jb}\delta_{ia}$, and $T^n_{abij}=T_{abi_1j_1}T_{i_1j_1i_2j_2}\cdots T_{i_{n-1}j_{n-1}ij}$. Then we can rewrite the time derivatives (D.46) as

$$\begin{aligned}\dot{U}&=\frac{i}{2\hbar}U\dot{S}_{ab}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}T^n_{abij}L_{ij}=\frac{i}{\hbar}U\dot{S}_{ab}A_{abij}L_{ij}\\ \dot{R}&=\frac{i}{2}R\dot{S}_{ab}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}T^n_{abij}J^{(ij)}=iR\dot{S}_{ab}A_{abij}J^{(ij)}.\end{aligned}\tag{D.47}$$

where the components A_{abij} are the real numbers

$$A_{abij}=\frac{1}{2}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)!}T^n_{abij}.\tag{D.48}$$

From (D.47), without having an explicit formula for the object A, we can see that $\dot{U}$ is related to the time derivative of the rotation matrix.

Using the components of the rotations generators (D.18), we can show that the components of the antisymmetric matrix $R^T\dot{R}$ are

$$(R^T\dot{R})_{ij}=\dot{S}_{ab}(A_{abij}-A_{abji}).\tag{D.49}$$

Using the asymmetry of the angular momentum tensor, we can then write $\dot{U}$ as

$$\dot{U}=\frac{i}{2\hbar}U\dot{S}_{ab}(A_{abij}-A_{abji})L_{ij}=\frac{i}{2\hbar}U(R^T\dot{R})_{ij}L_{ij}.\tag{D.50}$$

The term relevant to the Hamiltonian in the FPT for time-dependent rotations is $i\hbar\dot{U}U^\dagger$. Then using (D.26), this evaluates to

$$\begin{aligned}i\hbar\dot{U}U^\dagger&=-\frac{1}{2}R_{ki}\dot{R}_{kj}R_{ai}R_{bj}L_{ab}\\&=\frac{1}{2}\dot{R}_{ai}R_{bj}L_{ba}\\&=(\dot{R}R^T\vec{X})\cdot\vec{P}\end{aligned}\tag{D.51}$$

Therefore, for general N dimensions this becomes

$$i\hbar\dot{U}U^\dagger=(\dot{R}R^T\vec{X})\cdot\vec{P}=\begin{cases}\vec{\Omega}\cdot\vec{L} & N=3,\\ -\frac{1}{2}\dot{R}_{ai}R_{bj}L_{ab} & N\neq 3.\end{cases}\tag{D.52}$$

Appendix E

Free Dispersion of the SHO Stationary States

In this appendix, we calculate the expectation values of X, P, X^2, and P^2 for the free dispersion of the wave functions (2.90), which are the SHO stationary states at $t = 0$. Let $a(t) = a_0\sqrt{1+(\omega t)^2}$ where $a_0 = \sqrt{\hbar/m\omega}$ is the length scale of the oscillator. Then the expectation value of the position of the state is

$$\begin{aligned}\langle X\rangle &= \frac{1}{2^n n! a(t)\sqrt{\pi}}\int_{-\infty}^{\infty} dx\, x \exp\left[\frac{-(x-\beta)^2}{a^2(t)}\right] \mathrm{H}_n^2\left(\frac{x'-\beta}{a(t)}\right) \\ &= \frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} du\,[a(t)u+\beta]\, e^{-u^2}\,\mathrm{H}_n^2(u).\end{aligned}$$

The integrand $u\mathrm{H}_n^2(u)e^-u^2$ is an odd function, and therefore it integrates to zero. Using the orthogonality condition $\int \mathrm{H}_n(u)\,\mathrm{H}_m(u)e^{-u^2}\,du = \sqrt{\pi}2^n n!\delta_{nm}$ (see [37, Chapter 18.9] for properties of the Hermite polynomials) results in the expectation value of position

$$\langle X\rangle = \beta. \tag{E.1}$$

The expectation value of the position-squared is

$$\begin{aligned}\langle X^2\rangle &= \frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} du\,(a(t)u+\beta)^2\, e^{-u^2}\,\mathrm{H}_n^2(u) \\ &= \frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} du\left(a^2(t)u^2+2a(t)u\beta+\beta^2\right) e^{-u^2}\,\mathrm{H}_n^2(u).\end{aligned}$$

The constant term will integrate according to the orthogonality condition, and the linear term will again be zero. For the term that is quadratic in u, we use the the recursion relation

$$\mathrm{H}_{n+1}(u) = 2u\,\mathrm{H}_n(u) + 2n\,\mathrm{H}_{n-1}(u), \tag{E.2}$$

so that

$$\begin{aligned}\left\langle X^2\right\rangle &= \beta^2 + \frac{a^2(t)}{2^{n+2}n!\sqrt{\pi}}\int_{-\infty}^{\infty} \mathrm{d}u\left(\mathrm{H}_{n+1}^2 - 4n\,\mathrm{H}_{n+1}\,\mathrm{H}_{n-1} + 4n^2\,\mathrm{H}_{n-1}^2\right)e^{-u^2} \\ &= \beta^2 + \frac{a^2(t)}{2^{n+2}n!\sqrt{\pi}}\left[\sqrt{\pi}2^{n+1}(n+1)! + 4n^2\sqrt{\pi}2^{n-1}(n-1)!\right].\end{aligned} \tag{E.3}$$

This finally gives the result for all $n \geq 0$ that

$$\left\langle X^2\right\rangle = \beta^2 + a^2(t)(n+1/2). \tag{E.4}$$

With the two position expectation values, we can calculate the width of the distribution

$$\Delta X = \sqrt{\langle X^2\rangle - \langle X\rangle^2} = a(t)\sqrt{n+1/2} = a_0\sqrt{(n+1/2)(1+\omega^2 t^2)}. \tag{E.5}$$

The expectation value of momentum can be calculated by the Ehrenfest theorem $\langle P\rangle = m\langle\dot{X}\rangle = mv_0$. One may also compute it directly:

$$\begin{aligned}\langle P\rangle &= \frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} -i\hbar\left[\left(\frac{(\beta-x)(1-i\omega t)}{a^2(t)} + \frac{imv_0}{\hbar}\right)\mathrm{H}_n + \frac{\mathrm{H}_n'}{a(t)}\right]e^{-(x-\beta)^2/a^2(t)}\,\mathrm{H}_n\,\mathrm{d}x \\ &= \frac{1}{2^n n!\sqrt{\pi}}\int_{-\infty}^{\infty} -i\hbar\left[\left(\frac{-u(1-i\omega t)}{a(t)} + \frac{imv_0}{\hbar}\right)\mathrm{H}_n + \frac{\mathrm{H}_n'}{a(t)}\right]e^{-u^2}\,\mathrm{H}_n\,\mathrm{d}u\end{aligned} \tag{E.6}$$

The derivative of a Hermite polynomial is $\mathrm{H}_n' = 2n\,\mathrm{H}_{n-1}$, so this will integrate to zero due to orthogonality. Likewise, the term linear in u will integrate to zero, leaving only the constant coefficient of $\mathrm{H}_n^2 e^{-u^2}$ to integrate, which leaves us with

$$\langle P\rangle = \frac{1}{2^n n!\sqrt{\pi}} mv_0\sqrt{\pi}2^n n! = mv_0. \tag{E.7}$$

Lastly, the momentum-squared operator has the expectation value

$$\begin{aligned}\left\langle P^2\right\rangle = \frac{-\hbar^2}{2^n n! a(t)\sqrt{\pi}}\int_{-\infty}^{\infty}\Bigg\{ &-\frac{1-i\omega t}{a^2(t)}\,\mathrm{H}_n + 2\left[\frac{(\beta-x)(1-i\omega t)}{a^2(t)} + \frac{imv_0}{\hbar}\right]\frac{\mathrm{H}_n'}{a(t)} \\ &+ \left[\frac{(\beta-x)(1-i\omega t)}{a^2(t)} + \frac{imv_0}{\hbar}\right]^2 \mathrm{H}_n + \frac{\mathrm{H}_n''}{a^2(t)}\Bigg\}\,\mathrm{H}_n\,e^{-(x-\beta)^2/a^2(t)}\,\mathrm{d}x.\end{aligned} \tag{E.8}$$

The H_n'' term will integrate to zero, as will the constant coefficient of H_n'. After making the

usual substition $u = (x-\beta)/a(t)$

$$\left\langle P^2 \right\rangle = \frac{\hbar^2(1-i\omega t)}{a^2(t)} + \frac{\hbar^2}{2^n n!\sqrt{\pi}} \int_{-\infty}^{\infty} \left\{ +2\left[\frac{u(1-i\omega t)}{a^2(t)}\right] \mathrm{H}_n' \right. \\ \left. - \left[\frac{u(1-i\omega t)}{a(t)} - \frac{imv_0}{\hbar}\right]^2 \mathrm{H}_n \right\} \mathrm{H}_n e^{-u^2}\,\mathrm{d}u \quad \text{(E.9)}$$

For the derivative term, $u\mathrm{H}_n' = 2un\,\mathrm{H}_{n-1} = n[\mathrm{H}_n - 2(n-1)H_{n-1}]$ as per the recurrence relation used earlier. The $n-1$ Hermite polynomial will integrate to zero, and the n term that is linear in u

$$\begin{aligned}
\left\langle P^2 \right\rangle &= \frac{\hbar^2(1-i\omega t)}{a^2(t)} + \frac{\hbar^2}{2^n n!\sqrt{\pi}} \int_{-\infty}^{\infty} \left\{ 2n\frac{(1-i\omega t)}{a^2(t)} - \frac{u^2(1-i\omega t)^2}{a(t)^2} + \frac{m^2v_0^2}{\hbar^2} \right\} \mathrm{H}_n^2 e^{-u^2}\,\mathrm{d}u \\
&= \frac{\hbar^2(1-i\omega t)(1+2n)}{a^2(t)} + \frac{\hbar^2}{2^n n!\sqrt{\pi}} \int_{-\infty}^{\infty} \left\{ \frac{m^2v_0^2}{\hbar^2} - \frac{u^2(1-i\omega t)^2}{a(t)^2} \right\} \mathrm{H}_n^2 e^{-u^2}\,\mathrm{d}u \\
&= m^2v_0^2 + \frac{\hbar^2(1-i\omega t)(1+2n)}{a^2(t)} - \frac{\hbar^2}{2^n n!\sqrt{\pi}} \frac{m^2v_0^2}{\hbar^2} \frac{(1-i\omega t)^2}{a(t)^2} \\
&\qquad \times \frac{1}{4}\left[\sqrt{\pi}2^{n+1}(n+1)! + 4n^2\sqrt{\pi}2^{n-1}(n-1)!\right]
\end{aligned} \quad \text{(E.10)}$$

This then simplifies to the result

$$\left\langle P^2 \right\rangle = (mv_0)^2 + \hbar^2 \frac{n+1/2}{a_0^2}. \quad \text{(E.11)}$$

Therefore the width of the momentum distribution is

$$\Delta P = \frac{\hbar}{a_0}\sqrt{n+1/2}, \quad \text{(E.12)}$$

and product of the width of position and momentum is

$$\boxed{\Delta X \Delta P = \hbar \frac{n+1/2}{\sqrt{1+(\omega t)^2}} = \frac{E_n/\omega}{\sqrt{1+(\omega t)^2}},}. \quad \text{(E.13)}$$