

Integrability of Quadratic Non-autonomous Quantum Linear Systems

by

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ABSTRACT

The Quantum Harmonic Oscillator is one of the most important models in Quantum Mechanics. Analogous to the classical mass vibrating back and forth on a spring, the quantum oscillator system has attracted substantial attention over the years because of its importance in many advanced and difficult quantum problems. This dissertation deals with solving generalized models of the time-dependent Schrödinger equation which are called *generalized quantum harmonic oscillators*, and these are characterized by an arbitrary quadratic Hamiltonian of linear momentum and position operators. The primary challenge in this work is that most quantum models with time-dependence are not solvable explicitly, yet this challenge became the driving motivation for this work.

In this dissertation, the methods used to solve the time-dependent Schrödinger equation are the fundamental singularity (or Green's function) and the Fourier (eigenfunction expansion) methods. Certain Riccati- and Ermakov-type systems arise, and these systems are highlighted and investigated. The overall aims of this dissertation are to show that quadratic Hamiltonian systems are completely integrable systems, and to provide explicit approaches to solving the time-dependent Schrödinger equation governed by an arbitrary quadratic Hamiltonian operator. The methods and results established in the dissertation are not yet well recognized in the literature, yet hold for high promise for further future research.

Finally, the most recent results in the dissertation correspond to the harmonic oscillator group and its symmetries. A simple derivation of the maximum kinematical invariance groups of the free particle and quantum harmonic oscillator is constructed from the view point of the Riccati- and Ermakov-type systems, which shows an alternative to the traditional Lie Algebra approach. To conclude, a missing class of solutions of the time-dependent Schrödinger equation for the simple harmonic oscillator in one dimension is constructed. Probability distributions of the particle linear position and

momentum, are emphasized with `Mathematica` animations. The eigenfunctions qualitatively differ from the traditional standing waves of the one-dimensional Schrödinger equation. The physical relevance of these dynamic states is still questionable, and in order to investigate their physical meaning, animations could also be created for the *squeezed coherent states*. This will be addressed in future work.

A mis padres...

A Eloisa (1974-2001)...

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The printed pages of this dissertation hold far more than the mathematics and the culmination of years of study. They hold the invisible fear, tears, solitude and detachment from loved ones; they also reflect the relationships with many important, generous and inspiring people in my life. I want to express in this special space of the dissertation, my gratitude to all of you who have helped me, in one way or another, culminate this work. Accomplishing this dissertation has taken, not only mentors like the ones I have had, but also of an emotional balance that is only obtained with healthy surroundings. In these pages, I would like to give my sincere thanks to those individuals who have contributed to maintaining my spirit and my sanity, serving me as a kind of support, which without, it would have been for me impossible to arrive where I stand now. The list is long, yet I cherish each contribution to my personal growth and my development as a teacher and scholar.

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- 3.3 Figures (a)-(e) are a few *stills* taken from the mathematica movie animation [76]. Starting with (a) they denote the oscillating electron density (blue) of the first excited “dynamic harmonic state” of the time-dependent Schrödinger equation (3.1). These space oscillations complement (with the help of Mathematica) the corresponding “static” textbook solution (clear)[93]. (The color version of this figure is available only in the electronic version of the dissertation, and the actual video animation is available on the dissertation author’s collaborator’s website: [http://hahn.la.asu.edu/~suslov/.](http://hahn.la.asu.edu/~suslov/)) 48
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Chapter 1

INTRODUCTION

1.1 Motivation and Background

At the turn of the twentieth century, the unassailable field of classical mechanics in physics concerned with the set of physical laws mathematically describing the motion of macroscopic objects from projectiles to astronomical objects, [108, 111], was seriously challenged. In better words, physics was due for a major revision. The main reason was that it failed to explain adequately or even to approximate correctly the new phenomena observed at the atomic level. The best that classical mechanics could provide, were *ad-hoc* methods, and it became at one point obvious that the classical laws of physics needed to be reformulated. Problems which needed a theoretical explanation arose especially for phenomena involving “tiny” particles such as electrons and photons, and their interaction with electromagnetic fields [108].

Furthermore, historical literature explains that bold pioneers and scientists like Max Plank, Niels Bohr, Louis De Broglie, Paul Dirac, Werner Heisenberg, Max Born, Erwin Schrödinger among others soon established the theory, and became the father founders of the second major subfield of physics we know as Quantum Mechanics, one of the towering intellectual achievements of humankind. As soon as new experimental techniques were developed, their work turned out to show that classical physics fails miserably in providing the right explanation for atomic and subatomic phenomena [111]. Eventually this radical movement was formalized into a field of modern physics: Quantum Mechanics. This field that seemingly defied logic was able to accurately explain the rare occurrences related to very small particles such as electrons and photons. The mathematical equation used to predict these quantum effects is known as the Schrödinger Equation—a fundamental law of nature. Importantly, the fundamental framework for deeply understanding nature at the microscopical, infinitesimal level has opened the doors to new discoveries and many invaluable and fascinating prob-

lems in Engineering, Mathematical Physics, Chemistry and Biology. In fact, Quantum Mechanics is the founding basis of all modern physics (solid-state, molecular, atomic, nuclear, and particle physics, optics, thermodynamics, statistical mechanics, and so on), and is considered to be the foundation of chemistry and biology, according to [111].

The present dissertation contains the construction of exact solutions to the Schrödinger equation for variable quadratic time-dependent Hamiltonian systems (defined later). One main motivation for this work is that time-dependent Hamiltonians show up intrinsically in physical systems and yet not many models constructed from them have exact solutions. Adding a time dependence to the Hamiltonian is a natural way of incorporating an external potential force that depends on time. Importance of Hamiltonian dynamics is emphasized by the Banff International Research Station for Mathematical Innovation and Discovery: Hamiltonian systems should be studied because the principal equations of mathematical physics, whether it is Quantum Mechanics, Bose-Einstein condensates, molecular dynamics, ocean waves, the n -body problem of celestial mechanics, or Einstein's equations in general relativity, are in fact Hamiltonian dynamical systems when viewed in the proper coordinates [19, 27].

1.2 The Schrödinger Equation

The Schrödinger equation is a model which encompasses all principles of quantum physics. Its solution is called the wave function (not to be confused with the related concept of the Wave equation), and it is usually obtained explicitly and analytically only for simple cases. In its purest mathematical form, this law of Quantum Mechanics is:

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi + V(x) \psi = H \psi$$
$$\psi_0 = \psi(0, t)$$

where H is the so-called Hamiltonian operator and V is an arbitrary potential (energy) function. It was derived by Erwin Schrödinger in 1925-1926, and its fidelity to reality

earned him the Nobel Prize. In the standard interpretation of Quantum Mechanics, the so-called wave function (solution) represents the state of a particle. The quantum state or state vector, is the most complete description that can be given to a physical system. Solutions to Schrödinger’s equation describe not only molecular, atomic and subatomic systems, but also macroscopic systems (nowadays called Bose-Einstein Condensates).

A Hamiltonian H , represents the total energy of a physical quantum system (by analogy to classical mechanics, it represents the sum of kinetic and potential energy), and it is of fundamental importance in Quantum Mechanics. In general the Hamiltonian of the Schrödinger equation is an energy operator written with usual notation

$$H = \frac{p^2}{2m} + V(\mathbf{r}, t)$$

for a particle in \mathbb{R}^3 . The symbol $p = -i\hbar\nabla$ is Schrödinger’s momentum operator, ∇ is the gradient operator, \hbar is the reduced Plank’s constant ($\hbar = h/2\pi$) and i is the imaginary unit. Quantum Mechanics is intrinsically over the complex field (quantum mechanical formalism was born from the Hamilton-Jacobi Theory [15]), and the imaginary unit is necessary to ensure the Hermiticity of operators H and p . Plank’s constant is a physical constant relating the sizes of quanta—quantization is the procedure of constraining something from a continuous set of values to a discrete set. A “measurement” in Quantum Mechanics is defined thus, as an operator [81, 3], which acts on some wavefunction.

Time independence

The Schrödinger equation is as important in Quantum Mechanics as the fundamental laws of Newton are to classical mechanics [95, 104]. It is a postulate which equates the energy operator to the full energy of a particle or a system. If the Hamiltonian is not an explicit function of time, the equation is separable into its spatial and temporal parts. Hence the energy operator $E = i\hbar\partial/\partial t$ can then be replaced by the energy eigenvalue

E . In abstract form, it is an eigenvalue equation for the Hamiltonian H [95, 104]

$$E\psi = H\psi.$$

A solution of the time independent equation is called an energy eigenstate with energy E . [95, 104]. To find the time dependence of the state, consider starting the time-dependent equation with an initial condition $\psi(\mathbf{r})$. The time derivative at $t = 0$ is everywhere proportional to the value:

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) \Big|_{t=0} = H\psi(\mathbf{r}, t) \Big|_{t=0} = E\psi(\mathbf{r}, 0).$$

Initially the whole function just gets rescaled, and it maintains the property that its time derivative is proportional to itself, so for all times t ,

$$\psi(\mathbf{r}, t) = \tau(t) \psi(\mathbf{r})$$

substituting for ψ :

$$i\hbar \frac{\partial}{\partial t} \psi = -E\psi \rightarrow i\hbar \psi(\mathbf{r}) \frac{\partial \tau(t)}{\partial t} = -E\tau(t) \psi(\mathbf{r}) \psi(\mathbf{r})$$

where the $\psi(\mathbf{r})$ cancels, so solving this equation for $\tau(t)$ implies the solution of the time-dependent equation with this initial condition is:

$$\psi(\mathbf{r}, t) = \psi(t) e^{-iEt/\hbar} = \psi(\mathbf{r}) e^{-i\omega t}.$$

This case describes the standing wave solutions of the time-dependent equation, which are the states with definite energy (instead of a probability distribution of different energies). In physics, these standing waves are called “stationary states” or “energy eigenstates”; in chemistry they are called “atomic orbitals” or “molecular orbitals”. Superpositions of energy eigenstates change their properties according to the relative phases between the energy levels [10, 95, 104]. In **Chapter 3** of the dissertation we present an intriguing case of non-standing waves which complements the stationary states for the one dimensional Schrödinger equation.

The energy eigenvalues from this equation form a discrete spectrum of values, so mathematically energy must be quantized. More specifically, the energy Eigen states form a basis –any wavefunction may be written as a sum over the discrete energy states or an integral over continuous energy states, or more generally as an integral over a measure. This is the spectral theorem in mathematics, and in a finite state space it is just a statement of the completeness of the eigenvectors of a Hermitian matrix [10, 95, 104].

1.3 Some Quantum Mechanical Basics

In contrast with classical mechanics, it be incorrect to claim that there is an exact measure of the position and momentum simultaneously, because the position of a particle has an inherent uncertainty in it. The *Heisenberg Uncertainty Principle* due to German Theoretical Physicist Werner Heisenberg, states that both position and momentum are fuzzy and indeterminate quantities and cannot be ascribed with infinite precision simultaneously to the particle. Hence there exists a probability distribution assigned to both position and momentum [104, 81, 111]. Finding the corresponding wave function $\psi(\mathbf{r}, t)$ of a Schrödinger equation system gives us all physical quantities of an elementary particle, as stated previously. Yet the wave equation has no tangible statistical interpretation or meaning by itself. The interpretation turns out to be completely probabilistic.

To understand Schrödinger’s mechanics better, another architect of Quantum Mechanics, Max Born, suggested that in order to use the wave function $\psi(\mathbf{r}, t)$ for physical arguments, one must compute the positive quantity (complex modulus or complex norm)

$$|\psi|^2 = \psi^* \psi,$$

which he defined as a probability density function (ψ^* represents the complex conjugate of ψ). Born defined statistical and probabilistic interpretations for the wave mechanics, because the wavefunction has the property of being square-integrable (the integral of the square of the absolute value is finite). This later gave rise to statistical

mechanics. Therefore, the probability of detecting a particle anywhere in the interval $a \leq x \leq b$ (or space) at time t is defined by

$$P(a, b)(t) = \int_a^b |\psi(x, t)|^2 dx.$$

Naturally, the complete certainty or probability of finding the particle anywhere in an interval or space must be *unity*. Thus we must have

$$\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1.$$

An extension to three-dimensional space is easily done by considering triple integrals whenever necessary. In conclusion, although the Schrödinger equation is deterministic, the interpretation of the solution is completely probabilistic.

The quantum harmonic oscillator

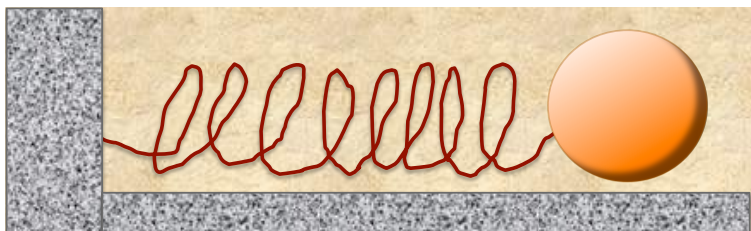


Figure 1.1: The artist's view of a classical harmonic oscillator (or vibrator) sketched for illustrative and motivational purposes. (The color version of this figure is available only in the electronic version of the dissertation.)

One of the most studied models in Quantum Mechanics is the equation of the simple harmonic oscillator (or vibrator). It is a dynamical system, and one of those few problems that are important to all branches of physics. The harmonic oscillator occurs naturally and frequently in nature, and its behavior describes many physical vibrational phenomena, found in classical mechanics, electrodynamics, statistical mechanics, solid-state, atomic, nuclear and particle physics [111]. In particular, the harmonic oscillator becomes more important at the microscopic level. It describes very well the behavior of jiggling particles. Many classifications of these harmonic oscillator systems exist, for example just a few types are the simple harmonic oscillator, the

damped harmonic oscillator, and the driven harmonic oscillator systems respectively (among others not discussed here). They are universal systems, with various frequencies of vibrations.



Figure 1.2: The artist's view of a classical harmonic oscillator (or vibrator) sketched for illustrative and motivational purposes. (The color version of this figure is available only in the electronic version of the dissertation.)

On the other hand, the harmonic oscillator assumes a privileged position in quantum mechanics and quantum field theory finding numerous and sometimes unexpected applications. It is constructed with the Schrödinger equation and it is one of the most important models in Quantum Mechanics. Quantum oscillator systems have attracted substantial attention over the years because of their importance in many advanced and difficult quantum problems. The quantum harmonic oscillator holds a unique importance in Quantum Mechanics because it is both one of the few problems that can be solved in closed form, and it is a very generally useful solution both in the approximation and in the exact solutions of various problems. Not to mention that it serves as an excellent pedagogical tool to introduce the concepts.

The quantum harmonic oscillator is characterized by the Hamiltonian

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2,$$

where m is the mass of the particle, ω is the angular frequency of the oscillator, $\hat{x} = x$ is the position operator and \hat{p} the momentum operator given by $\hat{p} = -i\hbar\partial_x$. The usual quantum problem is finding the energy eigenstates. To find these, one looks for solutions to the stationary energy-eigenvalue equation

$$\hat{H}\psi = E\psi$$

or we solve the time-dependent Schrödinger equation where

$$\hat{H}\psi = E\psi = i\hbar\partial_t\psi,$$

which looks simple, but it isn't actually the case. There are two ways of solving this equation, and the most elegant method is the *operator algebraic approach*, which is based on Ladder (creation and annihilation) operators. The creation and annihilation operators are used to climb up and down the energy ladder. The second way is by *analytically* (with eigenfunction expansion or separation of variables) finding the solution. This is more difficult and tedious without some numerical approach. The energy operators are defined by

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(x + i\frac{p}{m\omega} \right), \quad \hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(x - i\frac{p}{m\omega} \right).$$

or more simply as

$$\hat{a} = \frac{1}{\sqrt{2}}(x + ip), \quad \hat{a}^\dagger = \frac{1}{\sqrt{2}}(x - ip).$$

if we assume that the extra parameters $\hbar = \omega = m = 1$. In the algebraic operator approach, the eigenfunctions and energies are given by

$$\psi_n = \hat{a}^\dagger \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n \psi_0, \quad E_n = \left(n + \frac{1}{2} \right),$$

for quantum numbers $n = 1, 2, 3, \dots$ and $\{\psi_n | n = 0, 1, 2, 3, \dots\}$ where $n \in \mathbb{Z}_+$. The ground state ψ_0 is defined as the state with lowest energy, and the state with highest energy is called the excited state.

In the eigenfunction approach, in $\mathbb{R}_x \times \mathbb{R}_t$, it turns out that the harmonic oscillator wave functions are in fact shaped by *Hermite Polynomials*

$$\psi_n(x) = \sqrt{\frac{1}{2^n n!}} H_n(x) e^{-\frac{x^2}{2}}, \quad H_n = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2},$$

where $\frac{d^n}{dx^n} e^{-x^2}$ is the *Rodrigues Formula* corresponding to $n = 0, 1, 2, 3, \dots$ and $E_n = (n + \frac{1}{2})$ (see Figure (1.3)). This textbook result has been introduced because it helps

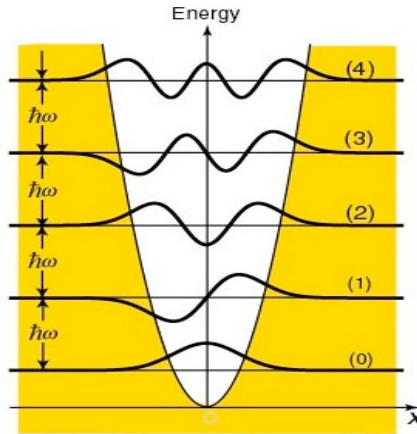


Figure 1.3: Wavefunction representations for the first five bound eigenstates, $n = 0$ to 4, where $\hbar\omega$ is the transition energy between energy levels. (The color version of this figure is available only in the electronic version of the dissertation.)

to understand the structure of the solution for more difficult and generalized problems which are solved by eigenfunction expansion. As time-dependence is incorporated in the Hamiltonian of the systems in the Schrödinger equation, the models become more complex and hence difficult to solve explicitly and analytically. This dissertation deals with solving generalized models of the time-dependent Schrödinger equation which are defined as the *generalized quantum harmonic oscillators*, where these are characterized by an arbitrary quadratic Hamiltonian operator of linear momentum and position operators.

1.4 Some Mathematical Methodologies

A popular method in mathematical physics is to use the method of propagators, or Green's functions. The mathematical method of choice in this work for the selected Schrödinger equation models is the application of Green's functions associated with initial value problems (IVPs). Green's functions always exist with IVPs when the coefficients of the differential equation in normal form are continuous. In contrast, boundary value problems do not always have unique solutions, and Green's functions fail to exist for this class of problems. Working with Green's functions allows us to deal not only with particular solutions; the solution has actual physical significance.

The Green's function has even more importance in this dissertation because in some contexts it has the physical interpretation of an impulse function (or propagator in the wave theory of electromagnetism), which is important in the interpretation of harmonic oscillator models.

Along with the method of Green's functions, a combination of asymptotic analysis is used. Our asymptotic estimates (approximations by "simple" functions which show how these quantities behave asymptotically when the arguments tend to zero or infinity) involve *Delta functions*. Finally, in our methods emerge special functions, such as the Rodrigues' formula, the Hermite polynomials and the most important Riccati and Ermakov equations, along with other integral transforms.

1.5 Method of Propagators or Green's Functions

Many of the problems in this dissertation and the study of time-dependent Schrödinger equations can be reduced to the initial value problem

$$i\hbar \frac{\partial \psi}{\partial t} = H(t)\psi, \quad (1.1)$$

$$\psi(x, t)|_{t=t_0} = \psi_0(x) \quad (1.2)$$

where ψ is a wave function satisfying the initial condition ψ_0 . Equation (1.1) is a partial differential equation called the Schrödinger equation. The Hamiltonian system above is in particular a Cauchy initial value problem due to the Cauchy condition $\psi_0(x)$. Cauchy conditions are values of the unknown wave function $\psi(x, t)$, $0 \leq t < \infty$, prescribed on the boundary $t = 0$ [5, 9]. A well behaved initial-value problem is one with a unique solution. To find the unique solution, the linear time-dependent Schrödinger equation is formulated as a Cauchy problem, but this dissertation we are mainly concerned with the continuous dependence of a solution on the initial data .

Whenever H is time independent, it is not difficult to see that the equation is separable, and that it has a recognizable exponential solution

$$\psi(t) = \psi_0 \exp\left(\frac{-iH}{\hbar}(t - t_0)\right)$$

The right hand-side has a very special significance. The exponential function is in fact an exponential operator. Many times it is referred to as a time evolution operator, or *propagator*, since it describes how the wave propagates from its initial configuration. Usually, more formally in functional analysis, it is appropriate to denote the propagator with the letter U , in that it stands for a *unitary* operator. Observe that when

$$U(t - t_0) = e^{-\frac{iH}{\hbar}(t-t_0)},$$

then

$$U(t - t_0)^\dagger = e^{\frac{iH^\dagger}{\hbar}(t-t_0)} = e^{\frac{iH}{\hbar}(t-t_0)} = U^{-1}(t - t_0),$$

where the complex operator satisfies the property that

$$UU^\dagger = U^\dagger U = 1,$$

with U^\dagger defined as the *Hermitian* adjoint of U (In finite dimensional matrix spaces, $U_n U_n^\dagger = U_n^\dagger U_n = I_n$). Yet in quantum physics, unitarity has an additional significance. It means that the sum of probabilities of all possible outcomes of any event is always 1. This property is necessary for the theory to be consistent, and has the implication that the operator which describes the progress of a physical system in time must be a unitary operator.

Solution to a Cauchy initial value problem

Time dependence of the Schrödinger equation most times suggests time-dependent Hamiltonians. Adding a time dependence to the Hamiltonian is a natural way of incorporating an external potential forcing term that depends on time. The generalized version of the Schrödinger equation motivated by the works in [21], is the time-dependent celebrated Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H(t) \psi.$$

In theory, the Schrödinger equation can be solved using a time evolution operator that has formally the following structure:

$$U(t, t_0) = T \left(\exp \left(-\frac{i}{\hbar} \int_{t_0}^t H(t') dt' \right) \right). \quad (1.3)$$

T is unitary, and it is also called the *time ordering operator*, which orders operators with larger times to the left. This unitary operator takes a state at time t_0 to a state at time t so it follows that the solution to the Schrödinger equation in general is given by

$$\psi(x, t) = U(t, t_0) \psi(x, t_0). \quad (1.4)$$

The model (1.1) seems trivial or perhaps too simple. One could mistakenly assume that the system can be solved in general, yet often $U(t, t_0)$ cannot be calculated for all systems explicitly, and thus the system cannot be solved in closed form (refer to [63]). However, we can look at special cases, and of course there exist other methods such as perturbation methods [64] and numerical schemes [13].

The structure of a Cauchy Initial Value Problem under consideration is given by the system

$$\begin{aligned} i \frac{\partial \psi}{\partial t} &= H(t) \psi, \\ \psi(x, t)|_{t=0} &= \psi_0(x), \end{aligned}$$

where the reduced Plank's constant \hbar is taken as unity. (It is customary to use natural units in solving problems in Quantum Mechanics for convenience and re-scaling purposes to avoid the mistakes in computation to a large extent [29].) It is possible to construct a time evolution operator explicitly in a general case of the one-dimensional Schrödinger equation when the Hamiltonian is an arbitrary quadratic form of the operators x and p (defined in the following paragraph). In quantum mechanics, every measurable quantity is associated with an operator. So the position operator happens to be “ x ” meaning, any given function will be multiplied by x .

Consider the quadratic Hamiltonian

$$H(x,t) = a(t)p^2 + b(t)x^2 + c(t)xp + d(t)px + f(t)x + g(t)p, \quad (1.5)$$

where $p = -i\partial/\partial x$ is the usual quantum linear momentum operator. Substituting the Hamiltonian into the equation (1.1) and after using the commutation relation this gives

$$i\frac{\partial\psi}{\partial t} = -a(t)\frac{\partial^2\psi}{\partial x^2} + b(t)x^2\psi - i\left(c(t)x\frac{\partial\psi}{\partial x} + d(t)\psi\right) - f(t)x\psi + ig(t)\frac{\partial\psi}{\partial x}, \quad (1.6)$$

where $a(t)$, $b(t)$, $c(t)$, $d(t)$, $f(t)$, and $g(t)$ are given real-valued functions of time t only. (For details on the resulting equations (1.5)–(1.6) and significance of $H(x,t)$ please see section 1.6.) The following polar Ansatz, represents the fundamental solution of (1.1)

$$\psi = Ae^{iS} = A(t)e^{iS(x,y,t)}, \quad A = A(t) = \frac{1}{\sqrt{2\pi i\mu(t)}},$$

where S is determined in the next pages. The functions $A(t)$ and $S(x,y,t)$ physically represent a time and space varying *amplitude* and *phase* of the wave function. The usefulness of the variable y will be apparent for the properties of the Green's function.

To prove that this is indeed a solution, we proceed by first expanding the left-hand side. This results in

$$\begin{aligned} i\psi_t &= (iA' - S'A)e^{iS} \\ &= \left(-i\frac{\mu'}{2\mu} - S_t\right)Ae^{iS}. \end{aligned} \quad (1.7)$$

The expression above can still be expanded and simplified with the following choice of S . By the method of moments for nonlinear Schrödinger equations [87], consider a general polynomial form of S

$$S(x, y, t) = \sum a_{nm}(t)x^n y^m.$$

More precisely with our own notation,

$$S(x,y,t) = \alpha_0(t)x^2 + \beta_0(t)xy + \gamma_0(t)y^2 + \delta_0(t)x + \varepsilon_0(t)y + \kappa_0(t),$$

where $\alpha_0(t)$, $\beta_0(t)$, $\gamma_0(t)$, $\delta_0(t)$, $\epsilon_0(t)$, and $\kappa_0(t)$ are differentiable real-valued functions of time t .

With this assumption of differentiability, indeed we can find the temporal and spatial derivatives $\frac{\partial S}{\partial t}$, $\frac{\partial S}{\partial x}$ which must be satisfied by the wavefunction. The first and second spatial partial derivatives of ψ are functions of S_x , S_{xx} , and the following expression must be satisfied:

$$\begin{aligned} -i\frac{\mu'}{2\mu}A - S_t A + a(t)(iS_{xx} - S_x^2)A + (f(t)x + g(t)S_x)A \\ = (b(t)x^2 + c(t)xS_x - id(t))A. \end{aligned} \quad (1.8)$$

Since $A(t)$ is certainly nonzero, collecting real and imaginary parts, we see that equation (1.8) is satisfied if and only if

$$S_t = -a(t)(S_x)^2 - b(t)x^2 + f(t)x + (g(t) - c(t)x)S_x \quad (1.9)$$

and

$$\frac{\mu'}{2\mu} = aS_{xx} + d = 2\alpha_0(t)a(t) + d(t). \quad (1.10)$$

These equations make it possible to find the coefficients that describe S . Expanding Equation (1.9) yields the polynomial relation

$$\begin{aligned} \alpha'_0(t)x^2 + \beta'_0(t)xy + \gamma'_0(t)y^2 + \delta'_0(t)x + \epsilon'_0(t)y + \kappa'_0(t) \\ = -a(t)(S_x)^2 - b(t)x^2 + f(t)x + (g(t) - c(t)x)S_x. \end{aligned} \quad (1.11)$$

Because we seek values of the coefficients, a necessary condition is that (1.11) vanishes when its coefficients are zero. Equating the coefficients of all admissible powers of $x^m y^n$ with $0 \leq m + n \leq 2$, gives the following coupled system of ordinary

differential equations

$$\frac{d\alpha_0}{dt} + b(t) + 2c(t)\alpha_0 + 4a(t)\alpha_0^2 = 0, \quad (1.12)$$

$$\frac{d\beta_0}{dt} + (c(t) + 4a(t)\alpha_0(t))\beta_0 = 0, \quad (1.13)$$

$$\frac{d\gamma_0}{dt} + a(t)\beta_0^2(t) = 0, \quad (1.14)$$

$$\frac{d\delta_0}{dt} + (c(t) + 4a(t)\alpha_0(t))\delta_0 = f(t) + 2\alpha_0(t)g(t), \quad (1.15)$$

$$\frac{d\varepsilon_0}{dt} = (g(t) - 2a(t)\delta_0(t))\beta_0(t), \quad (1.16)$$

$$\frac{d\kappa_0}{dt} = g(t)\delta_0(t) - a(t)\delta_0^2(t). \quad (1.17)$$

We first find a solution to (1.10) and use it to derive a second order linear differential equation to find the fundamental solution to the Schrödinger equation, in terms of propagators. The first equation (1.12) is the familiar Riccati nonlinear differential equation (see Methods of Solving Riccati equations [48, 105]). It should be evident that α' can be deduced from expression (1.10). Thus substituting Equation (1.10) into (1.12) results in the second order linear equation

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = 0, \quad (1.18)$$

where the time dependent coefficients σ and τ can be found explicitly by simple algebraic manipulations and they are given by

$$\tau(t) = \frac{a'}{a} - 2c + 4d, \quad \sigma(t) = ab - cd + d^2 + \frac{d}{2} \left(\frac{a'}{a} - \frac{d'}{d} \right).$$

We shall refer to equation (1.18) as the *characteristic equation* and its solution $\mu(t)$, as the *characteristic function*. The characteristic equation must be solved subject to the initial data

$$\mu(0) = 0, \quad \mu'(0) = 2a(0) \neq 0$$

in order to satisfy the initial condition for the corresponding Green's function. Thus, the Green's function (fundamental solution or propagator) is explicitly given in terms

of the characteristic function

$$\psi = G(x, y, t) = \frac{1}{\sqrt{2\pi i \mu(t)}} e^{i(\alpha_0(t)x^2 + \beta_0(t)xy + \gamma_0(t)y^2 + \delta_0(t)x + \varepsilon_0(t)y + \kappa_0(t))},$$

The time-dependent coefficients are explicitly given in the following Chapter (denoted as Riccati coefficients) and a corresponding asymptotic formula for the Green's function propagator is also approximated at $t = 0$ and explicitly given in **Chapter 2**. By the superposition principle, we obtain an explicit solution of the Cauchy initial value problem

$$i \frac{\partial \psi}{\partial t} = H(t) \psi, \quad \psi(x, t)|_{t=0} = \psi_0(x)$$

on the infinite interval $-\infty < x < \infty$ with the general quadratic Hamiltonian in the form

$$\psi(x, t) = \int_{-\infty}^{\infty} G(x, y, t) \psi_0(y) dy. \quad (1.19)$$

This yields the time evolution operator (1.3) explicitly as an integral operator.

This Green's function, which was constructed in terms of a Riccati System, as it will be seen later, represents the free particle solution to the Schrödinger equation. The constructed Green's function is a particular solution necessary to find the formal solution to the harmonic oscillator problem in **Chapter 2**.

1.6 Significance of the Generalized Quadratic Hamiltonian

Many authors have considered simple harmonic oscillators, but few have considered the driven type. In this work, the time dependent Hamiltonian is defined as

$$H = a_0 p^2 + b_0 x^2 + c_0 p x + d_0 x p + f_0 p + g_0 x.$$

The trivial commutation relation $[p, x] = -i$ gives us that $p x = x p - i$, $p = -i \partial_x$, so the Schrödinger equation is reduced into

$$i \frac{\partial \psi}{\partial t} = -a_0 \frac{\partial^2 \psi}{\partial x^2} + b_0 x^2 \psi - i(c_0 + d_0)x \frac{\partial \psi}{\partial x} - i c_0 \psi - i f_0 \frac{\partial \psi}{\partial x} + g_0 x \psi.$$

We rename coefficients and replace the Schrödinger equation by the coefficients

$$\begin{aligned} a_0 &= a & b_0 &= b & c_0 + d_0 &= c \\ c_0 &= d & f_0 &= -g & g_0 &= -f. \end{aligned} \quad (1.20)$$

In particular, choosing $-f_0 = g$ and $-g_0 = f$ gives the Hamiltonian a better physical interpretation with respect to Harmonic Oscillators. Replacing $-f_0 = g$ and $-g_0 = f$ in the Hamiltonian gives the external forcing, or an external potential forcing terms, typical of damped Harmonic Oscillators. This gives us the celebrated master equation

$$i \frac{\partial}{\partial t} \psi = -a(t) \frac{\partial^2 \psi}{\partial x^2} + bx^2 \psi - c(t)x \frac{\partial \psi}{\partial x} - id(t)\psi - f(t)x\psi + ig(t) \frac{\partial \psi}{\partial x}$$

that we use throughout this dissertation.

1.7 Plan of the dissertation

The organization of the dissertation goes as follows. In **Chapter 2** the time-dependent Schrödinger equation for the most general variable quadratic Hamiltonians is transformed into a standard autonomous equation. As a result of this transformation, exact eigenfunctions are determined, and the time-evolution of exact wave functions of generalized harmonic oscillators is determined by means of the solutions to certain Ermakov and Riccati-type systems. In addition, it is shown that the classical Arnold transformation is naturally connected with Ehrenfest's theorem for generalized harmonic oscillators. Combined in **Chapter 3**, the maximum kinematical invariance group of the quantum harmonic oscillator is discussed from a view point of the Ermakov-type system found already in **Chapter 2**. The invariance group of the generalized driven harmonic oscillator is shown to be isomorphic to the corresponding Schrödinger group of the free particle. Later, a six-parameter family of the square integrable wave functions is considered for the simple harmonic oscillator; this in fact cannot be obtained by the standard separation of variables. This family of parameters is determined by the action of the corresponding maximal kinematical invariance group on the standard solutions. In addition, the phase space oscillations of the electron position and linear momentum probability distributions are computer animated and some possible applications are briefly discussed and a visualization of the Heisenberg Uncertainty Principle is presented using the Mathematica library. Finally, **Chapter 4** discusses possible future works, and conclusions to the dissertation.

This dissertation is heavily based on the following published papers and manuscripts in preparation, and hence a great part of the text is extracted from them.

- Cordero-Soto, R., R. M. Lopez, E. Suazo and S. K. Suslov, *Propagator of a charged particle with a spin in uniform magnetic and perpendicular electric fields*, Lett. Math. Phys. **84** (2008) #2–3, 159–178.
- López, R. M. and S. K. Suslov, *The Cauchy problem for a forced harmonic oscillator*, Revista Mexicana de Física, **55** (2009) #2, 195–215; see also arXiv:0707.1902v8 [math-ph] 27 Dec 2007.
- Lanfear, N., R. M. Lopez and S. K. Suslov, *Exact wave functions for generalized harmonic oscillators*, Journal of Russian Laser Research **32** (2011) #4, 352–361; see also arXiv:11002.5119v2 [math-ph] 20 Jul 2011.
- López, R. M., S. K. Suslov and J. M. Vega-Guzmán, *On the harmonic oscillator group*, arXiv:1111.5569v2 [math-ph] Dec 2011.
- López, R. M., S. K. Suslov and J. M. Vega-Guzmán, *On a Hidden symmetry of Quantum Harmonic Oscillators*, arXiv:1112.2586 [math-ph] Dec 2011.

Chapter 2

EXACT WAVEFUNCTIONS FOR GENERALIZED QUANTUM HARMONIC OSCILLATORS

2.1 Introduction

Quantum systems with variable quadratic Hamiltonians are called the generalized harmonic oscillators [11, 23, 30, 32, 37, 41, 49, 69, 72, 77, 80, 107, 109, 112]. These systems have attracted substantial attention over the years because of their great importance in many advanced quantum problems. Examples are coherent states and uncertainty relations, Berry's phase, quantization of mechanical systems and Hamiltonian cosmology. More applications include, but are not limited to charged particle traps and motion in uniform magnetic fields, molecular spectroscopy and polyatomic molecules in varying external fields, crystals through which an electron is passing and exciting the oscillator modes, and other mode interactions with external fields. Quadratic Hamiltonians have particular applications in quantum electrodynamics because the electromagnetic field can be represented as a set of forced harmonic oscillators [41].

A goal of this chapter is to construct exact wave functions for generalized (driven) harmonic oscillators [11, 21, 49, 69, 72, 107, 109], in terms of Hermite polynomials by transforming the time-dependent Schrödinger equation into an autonomous form [112]. Resulting from the transformation are certain Ermakov and Riccati-type systems, and these are investigated in detail. There is a general sense that there is a lack of this type of analysis in the current, contemporary literature. Alternatively, a group theoretical approach to a similar class of partial differential equations is discussed in Refs. [1, 18, 26, 44, 82, 90, 98, 98]. Some applications to the nonlinear Schrödinger equation abound in the sources [28, 55, 56, 59, 62, 87, 97] and [100], for example.

2.2 Transforming Generalized Harmonic Oscillators into Autonomous Form

Again let us consider the one-dimensional time-dependent Schrödinger equation already discussed in **Chapter 1** :

$$i\frac{\partial\psi}{\partial t} = H\psi, \quad (2.1)$$

where the variable Hamiltonian $H = Q(p, x)$ is an arbitrary quadratic of two operators $p = -i\partial/\partial x$ and x , namely,

$$i\psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x - id(t)\psi - f(t)x\psi + ig(t)\psi_x, \quad (2.2)$$

(a, b, c, d, f and g are suitable real-valued functions of time only). These quantum systems shall be referred to as the *generalized (driven) harmonic oscillators*. Some examples, a general approach and known elementary solutions can be found in Refs. [21, 22, 23, 24, 30, 39, 40, 41, 72, 74, 79, 96, 107] and [109]. In addition, a case related to Airy functions is discussed in [67] and Ref. [25] deals with another special case of transcendental solutions.

The following is the first original result in the dissertation.

Lemma 2.2.1 *The substitution*

$$\psi = \frac{e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t))}}{\sqrt{\mu(t)}} \chi(\xi, \tau), \quad \xi = \beta(t)x + \varepsilon(t), \quad \tau = \gamma(t) \quad (2.3)$$

transforms the non-autonomous and inhomogeneous Schrödinger equation (2.2) into the autonomous form

$$-i\chi_\tau = -\chi_{\xi\xi} + c_0\xi^2\chi \quad (c_0 = 0, 1) \quad (2.4)$$

provided that

$$\frac{d\alpha}{dt} + b + 2c\alpha + 4a\alpha^2 = c_0a\beta^4, \quad (2.5)$$

$$\frac{d\beta}{dt} + (c + 4a\alpha)\beta = 0, \quad (2.6)$$

$$\frac{d\gamma}{dt} + a\beta^2 = 0 \quad (2.7)$$

and

$$\frac{d\delta}{dt} + (c + 4a\alpha)\delta = f + 2g\alpha + 2c_0a\beta^3\varepsilon, \quad (2.8)$$

$$\frac{d\varepsilon}{dt} = (g - 2a\delta)\beta, \quad (2.9)$$

$$\frac{d\kappa}{dt} = g\delta - a\delta^2 + c_0a\beta^2\varepsilon^2. \quad (2.10)$$

Here

$$\alpha = \frac{1}{4a} \frac{\mu'}{\mu} - \frac{d}{2a}. \quad (2.11)$$

Proof Differentiating $\psi = \mu^{-1/2}(t) e^{iS(x,t)} \chi(\xi, \tau)$ with $S = \alpha(t)x^2 + \delta(t)x + \kappa(t)$, $\xi = \beta(t)x + \varepsilon(t)$ and $\tau = \gamma(t)$ yields

$$ie^{-iS}\psi_t = \frac{1}{\sqrt{\mu}} \left[-(\alpha'x^2 + \delta'x + \kappa')\chi + i \left((\beta'x + \varepsilon')\chi_\xi + \gamma'\chi_\tau - \frac{\mu'}{2\mu}\chi \right) \right],$$

$$e^{-iS}\psi_x = \frac{1}{\sqrt{\mu}} [i(2\alpha x + \delta)\chi + \beta\chi_\xi]$$

and

$$e^{-iS}\psi_{xx} = \frac{1}{\sqrt{\mu}} \left[\left(2i\alpha - (2\alpha x + \delta)^2 \right) \chi + 2i(2\alpha x + \delta)\beta\chi_\xi + \beta^2\chi_{\xi\xi} \right].$$

Substituting into

$$i\psi_t = -a\psi_{xx} + (b - c_0a\beta^4)x^2\psi - icx\psi_x - id\psi$$

$$- (f + 2c_0a\beta^3\varepsilon)x\psi + ig\psi_x - c_0a\beta^2\varepsilon^2\psi + c_0a\beta^2\varepsilon^2\xi^2\psi$$

and using system (2.5)–(2.10), results in Eq. (2.4) \square

This transformation (2.3) provides a new interpretation to system (2.5)–(2.10) originally derived in Ref. [21] when $c_0 = 0$ by integrating the corresponding Schrödinger equation via the Green function method (see also [99] for an eigenfunction expansion). In this chapter, the case $c_0 \neq 0$ is discussed as its natural extension.

The substitution (2.11), which has been already used in [21], appears here from a new “transformation perspective”. It now reduces the inhomogeneous equation (2.5) to the second order ordinary differential equation

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = c_0(2a)^2\beta^4\mu, \quad (2.12)$$

that has the familiar time-varying coefficients

$$\tau(t) = \frac{a'}{a} - 2c + 4d, \quad \sigma(t) = ab - cd + d^2 + \frac{d}{2} \left(\frac{a'}{a} - \frac{d'}{d} \right). \quad (2.13)$$

(This derivation is straightforward and given in the following subsection.)

For terminology purposes, when $c_0 = 0$, equation (2.5) is called the *Riccati nonlinear differential equation* [105, 106]; consequently, the system (2.5)–(2.10) shall be referred to as a *Riccati-type system*. (Similar terminology is used in [98] for the corresponding parabolic equation.) Now if $c_0 = 1$, equation (2.12) is disguised as an equation which results abundantly in the analysis of harmonic oscillators. The equation (2.12) can be reduced to a generalized version of the *Ermakov nonlinear differential equation* (2.50) (see, for example, [23, 36, 70, 99] and references therein regarding Ermakov’s equation) and naturally, we shall refer to the corresponding system (2.5)–(2.10) with $c_0 \neq 0$ as an *Ermakov-type system*.

Derivation of the second order inhomogeneous ode

The substitution (2.11) below

$$\alpha = \frac{1}{4a} \frac{\mu'}{\mu} - \frac{d}{2a},$$

(which has already been used in [21]) is treated as a new “transform perspective”. It follows that equation (2.11) reduces the inhomogeneous differential equation

$$\frac{d\alpha}{dt} + b + 2c\alpha + 4a\alpha^2 = c_0 a \beta^4 \quad (2.14)$$

to a second-order ordinary differential equation. By differentiating the expression

$$4a\alpha = \frac{\mu'}{\mu} - 2d,$$

gives us

$$4a\alpha' = \frac{\mu''}{\mu} - \left(\frac{\mu'}{\mu} \right)^2 - 2d' - \frac{a'}{a} \frac{\mu'}{\mu} + 2\frac{a'}{a} d. \quad (2.15)$$

By multiplying (2.14) by $4a$ on both sides, we find the expression

$$4a\alpha' = -4ab - 8ac\alpha - (4a\alpha)^2 + c_0 a \beta^4. \quad (2.16)$$

Equating (2.15) and (2.16) and simplifying the result, gives us

$$\frac{\mu''}{\mu} - \left(\frac{a'}{a} - 2c + 4d \right) \frac{\mu'}{\mu} + 4 \left(ab - cd + d^2 + \frac{d}{2} \left(\frac{a'}{a} - \frac{d'}{d} \right) \right) = 4c_0 a^2 \beta^4.$$

A final multiplication by μ on both sides gives us the second order differential equation

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = 4c_0 a^2 \beta^4 \mu,$$

which has the familiar time-varying coefficients (2.13).

2.3 Green's Function and Wavefunctions

Two particular solutions of the time-dependent Schrödinger equation (2.2) are useful in physical applications. Using standard oscillator wave functions for equation (2.4) when $c_0 = 1$ (for example, [42, 65] and/or [81]) results in the solution

$$\psi_n(x, t) = \frac{e^{i(\alpha x^2 + \delta x + \kappa) + i(2n+1)\gamma}}{\sqrt{2^n n! \mu \sqrt{\pi}}} e^{-(\beta x + \varepsilon)^2 / 2} H_n(\beta x + \varepsilon), \quad (2.17)$$

where $H_n(x)$ are the Hermite polynomials [86], corresponding to quantum numbers $n = 0, 1, 2, 3, \dots$, provided that the solution of the Ermakov-type system (2.5)–(2.10) is available. Here, the Hermite polynomials control the shape of the oscillator wavefunctions.

The Green's function of generalized harmonic oscillators has been constructed in the following fashion in Ref. [21]:

$$G(x, y, t) = \frac{1}{\sqrt{2\pi i \mu_0(t)}} \exp \left[i \left(\alpha_0(t) x^2 + \beta_0(t) xy + \gamma_0(t) y^2 + \delta_0(t) x + \varepsilon_0(t) y + \kappa_0(t) \right) \right]. \quad (2.18)$$

The time-dependent coefficients $\alpha_0, \beta_0, \gamma_0, \delta_0, \varepsilon_0, \kappa_0$ satisfy the Riccati-type system (2.5)–(2.10) ($c_0 = 0$) and are given as follows [21, 96, 99]:

$$\alpha_0(t) = \frac{1}{4a(t)} \frac{\mu_0'(t)}{\mu_0(t)} - \frac{d(t)}{2a(t)}, \quad (2.19)$$

$$\beta_0(t) = -\frac{\lambda(t)}{\mu_0(t)}, \quad \lambda(t) = \exp \left(- \int_0^t (c(s) - 2d(s)) ds \right), \quad (2.20)$$

$$\gamma_0(t) = \frac{1}{2\mu_1(0)} \frac{\mu_1(t)}{\mu_0(t)} + \frac{d(0)}{2a(0)} \quad (2.21)$$

and

$$\delta_0(t) = \frac{\lambda(t)}{\mu_0(t)} \int_0^t \left[\left(f(s) - \frac{d(s)}{a(s)} g(s) \right) \mu_0(s) + \frac{g(s)}{2a(s)} \mu_0'(s) \right] \frac{ds}{\lambda(s)}, \quad (2.22)$$

$$\begin{aligned} \varepsilon_0(t) = & -\frac{2a(t)\lambda(t)}{\mu_0'(t)} \delta_0(t) + 8 \int_0^t \frac{a(s)\sigma(s)\lambda(s)}{(\mu_0'(s))^2} (\mu_0(s)\delta_0(s)) ds \quad (2.23) \\ & + 2 \int_0^t \frac{a(s)\lambda(s)}{\mu_0'(s)} \left(f(s) - \frac{d(s)}{a(s)} g(s) \right) ds, \end{aligned}$$

$$\begin{aligned} \kappa_0(t) = & \frac{a(t)\mu_0(t)}{\mu_0'(t)} \delta_0^2(t) - 4 \int_0^t \frac{a(s)\sigma(s)}{(\mu_0'(s))^2} (\mu_0(s)\delta_0(s))^2 ds \quad (2.24) \\ & - 2 \int_0^t \frac{a(s)}{\mu_0'(s)} (\mu_0(s)\delta_0(s)) \left(f(s) - \frac{d(s)}{a(s)} g(s) \right) ds \end{aligned}$$

($\delta_0(0) = -\varepsilon_0(0) = g(0)/(2a(0))$ and $\kappa_0(0) = 0$) provided that μ_0 and μ_1 are standard solutions of equation (2.12) with $c_0 = 0$ corresponding to the initial conditions $\mu_0(0) = 0$, $\mu_0'(0) = 2a(0) \neq 0$ and $\mu_1(0) \neq 0$, $\mu_1'(0) = 0$. (Proofs of these facts are outlined in Refs. [21], [25] and [96]. See also important previous works [32, 77, 107, 109, 112] and references therein for more details.)

Hence, the corresponding Cauchy initial value problem can be solved (formally) by the superposition principle¹. That is,

$$\psi(x,t) = \int_{-\infty}^{\infty} G(x,y,t) \psi(y,0) dy \quad (2.25)$$

for some suitable initial data $\psi(x,0) = \varphi(x)$ (see Refs. [21, 96] and [99] for further details).

In particular, using the wave functions (2.17) we get the integral

$$\psi_n(x,t) = \int_{-\infty}^{\infty} G(x,y,t) \psi_n(y,0) dy, \quad (2.26)$$

¹Because physical systems are generally only approximately linear, the Superposition Principle is only an approximation of the true physical behavior; it provides insight for typical operational regions for these systems. The Superposition Principle is very much used in Green's function analysis. The stimulus is written as the superposition of infinitely many impulse functions, and the response is then a superposition of impulse responses.

and this can be evaluated by the Hermite Gaussian transform

$$\begin{aligned} & \int_{-\infty}^{\infty} e^{-\lambda^2(x-y)^2} H_n(ay) dy \\ &= \frac{\sqrt{\pi}}{\lambda^{n+1}} (\lambda^2 - a^2)^{n/2} H_n \left(\frac{\lambda ax}{(\lambda^2 - a^2)^{1/2}} \right), \quad \text{Re } \lambda^2 > 0, \end{aligned} \quad (2.27)$$

which is an integral transform in terms of elementary functions equivalent to Eq. (30) on page 195 of Vol. 2 of Ref. [34] (the Gauss transform of Hermite polynomials), or Eq. (17) on page 290 of Vol. 2 of Ref. [35].

2.4 Solution to the Ermakov-type System

As shown in the previous section, the time evolution of the wave functions (2.17) is determined in terms of the solution to the initial value problem for the Ermakov-type system. In this section, formulas (2.17)–(2.18) and (2.26)–(2.27) shall be used in order to solve the general system (2.5)–(2.10) when $c_0 \neq 0$ along with the uniqueness property of the Cauchy initial value problem. At this point, we must remind the reader how to handle the special case $c_0 = 0$ considered in [96].

Lemma 2.4.1 *The solution of the Riccati-type system (2.5)–(2.10) ($c_0 = 0$) is given by*

$$\mu(t) = 2\mu(0)\mu_0(t)(\alpha(0) + \gamma_0(t)), \quad (2.28)$$

$$\alpha(t) = \alpha_0(t) - \frac{\beta_0^2(t)}{4(\alpha(0) + \gamma_0(t))}, \quad (2.29)$$

$$\beta(t) = -\frac{\beta(0)\beta_0(t)}{2(\alpha(0) + \gamma_0(t))} = \frac{\beta(0)\mu(0)}{\mu(t)}\lambda(t), \quad (2.30)$$

$$\gamma(t) = \gamma(0) - \frac{\beta^2(0)}{4(\alpha(0) + \gamma_0(t))} \quad (2.31)$$

and

$$\delta(t) = \delta_0(t) - \frac{\beta_0(t)(\delta(0) + \varepsilon_0(t))}{2(\alpha(0) + \gamma_0(t))}, \quad (2.32)$$

$$\varepsilon(t) = \varepsilon(0) - \frac{\beta(0)(\delta(0) + \varepsilon_0(t))}{2(\alpha(0) + \gamma_0(t))}, \quad (2.33)$$

$$\kappa(t) = \kappa(0) + \kappa_0(t) - \frac{(\delta(0) + \varepsilon_0(t))^2}{4(\alpha(0) + \gamma_0(t))} \quad (2.34)$$

in terms of the fundamental solution (2.19)–(2.24) subject to the arbitrary initial data $\mu(0), \alpha(0), \beta(0) \neq 0, \gamma(0), \delta(0), \varepsilon(0), \kappa(0)$.

The verification of this lemma can be done so by direct substitution and/or by an integral evaluation very similar to the Gauss transform of Hermite polynomials. This result in *Lemma 2.4.1* can be proposed as a nonlinear superposition principle for the Riccati-type system where the continuity to initial data always holds [96]. From equations (2.28)–(2.34) one is also able to extract expressions which lead to necessary asymptotics to approximate the fundamental solution to the Cauchy problem.

Next, we do a Taylor expansion in the vicinity of the branch point, and this procedure yields the following asymptotic relations for our fundamental solution. In the limiting case $t \rightarrow 0$, the Green's function approaches a Delta function, sensitive to an excitation point $x = y$. So by making use of *Lemma 2.4.1*, and linearizing to first order gives us the following asymptotic relations established in [96]:

$$\alpha_0(t) = \frac{1}{4a(0)t} - \frac{c(0)}{4a(0)} - \frac{a'(0)}{8a^2(0)} + O(t), \quad (2.35)$$

$$\beta_0(t) = -\frac{1}{2a(0)t} + \frac{a'(0)}{4a^2(0)} + O(t), \quad (2.36)$$

$$\gamma_0(t) = \frac{1}{4a(0)t} + \frac{c(0)}{4a(0)} - \frac{a'(0)}{8a^2(0)} + O(t), \quad (2.37)$$

$$\delta_0(t) = \frac{g(0)}{2a(0)} + O(t), \quad (2.38)$$

$$\varepsilon_0(t) = -\frac{g(0)}{2a(0)} + O(t), \quad (2.39)$$

$$\kappa_0(t) = O(t) \quad (2.40)$$

as $t \rightarrow 0$ for sufficiently smooth (infinitely differentiable in the small vicinity of t). Neglecting the higher order terms $O(t)$ as t reaches asymptotic level, we then have

coefficients of the original Schrödinger equation (2.2). Therefore,

$$G(x, y, t) \sim \frac{1}{\sqrt{2\pi i a(0)t}} \exp \left[i \frac{(x-y)^2}{4a(0)t} \right] \quad (2.41)$$

$$\times \exp \left[-i \left(\frac{a'(0)}{8a^2(0)} (x-y)^2 + \frac{c(0)}{4a(0)} (x^2 - y^2) - \frac{g(0)}{2a(0)} (x-y) \right) \right]$$

as $t \rightarrow 0$, where

$$f \sim g \quad \text{as } t \rightarrow 0, \quad \text{if } \lim_{t \rightarrow 0} \frac{f}{g} = 1.$$

This result corrects an errata in Ref. [21].

Finally, we present the extension to a general case when $c_0 \neq 0$. Our main result is the following lemma.

Lemma 2.4.2 *The solution of the Ermakov-type system (2.5)–(2.10) when $c_0 = 1 (\neq 0)$ is given by*

$$\mu = \mu(0) \mu_0 \sqrt{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}, \quad (2.42)$$

$$\alpha = \alpha_0 - \beta_0^2 \frac{\alpha(0) + \gamma_0}{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}, \quad (2.43)$$

$$\beta = -\frac{\beta(0) \beta_0}{\sqrt{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}} = \frac{\beta(0) \mu(0)}{\mu(t)} \lambda(t), \quad (2.44)$$

$$\gamma = \gamma(0) - \frac{1}{2} \arctan \frac{\beta^2(0)}{2(\alpha(0) + \gamma_0)}, \quad a(0) > 0 \quad (2.45)$$

and

$$\delta = \delta_0 - \beta_0 \frac{\varepsilon(0) \beta^3(0) + 2(\alpha(0) + \gamma_0)(\delta(0) + \varepsilon_0)}{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}, \quad (2.46)$$

$$\varepsilon = \frac{2\varepsilon(0)(\alpha(0) + \gamma_0) - \beta(0)(\delta(0) + \varepsilon_0)}{\sqrt{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}}, \quad (2.47)$$

$$\kappa = \kappa(0) + \kappa_0 - \varepsilon(0) \beta^3(0) \frac{\delta(0) + \varepsilon_0}{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2} \quad (2.48)$$

$$+ (\alpha(0) + \gamma_0) \frac{\varepsilon^2(0) \beta^2(0) - (\delta(0) + \varepsilon_0)^2}{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}$$

in terms of the fundamental solution (2.19)–(2.24) subject to the arbitrary initial data $\mu(0), \alpha(0), \beta(0) \neq 0, \gamma(0), \delta(0), \varepsilon(0), \kappa(0)$.

Proof By evaluating the integral (2.26) with the use of (2.27) by completing the square, gives us the Ermakov and Riccati-type systems along with the uniqueness property of the Cauchy initial value problem. One can also verify our solution by a direct substitution into the system (2.5)–(2.10) when $c_0 = 1$. (The computer algebra system *Mathematica* has been used in this proof because although elementary, they are rather tedious calculations, and Appendix A contains more details on the exact steps of the derivation.) \square

Furthermore, the asymptotics (2.35)–(2.40) together (2.42)–(2.48) give us the continuity with respect to initial data. These results in:

$$\lim_{t \rightarrow 0^+} \mu(t) = \mu(0), \quad \lim_{t \rightarrow 0^+} \alpha(t) = \alpha(0), \quad \text{etc.} \quad (2.49)$$

Thus the transformation property (2.42)–(2.48) makes it possible to find a solution of the initial value problem in terms of the fundamental solution (2.19)–(2.24) and it may be referred to as a *nonlinear superposition principle* for the Ermakov-type system.

Solution of the ermakov-type equation

In this section we emphasize the reason for the chosen terminology in the case $c_0 = 1$. More than a century ago Ermakov [89] has introduced an equation, which appears in many branches of modern physics [70, 47]. In quantum mechanics the Ermakov equation comes out in the case of a harmonic oscillator [83, 94], and the evolution of this equation is given by the Schrödinger equation in general. Below we derive the Ermakov-type equation and its explicit solution. Starting from (2.12)–(2.13) when $c_0 = 1$, and using (2.44) (this explains the nonlinearity on the right hand side) we arrive at

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = (2a)^2(\beta(0)\mu(0)\lambda)^4\mu^{-3},$$

which is a familiar Ermakov-type equation (see [16, 23, 36, 70, 99, 112] and references therein). Then our formula (2.42) leads to the representation

$$\left(\frac{\mu(t)}{\mu(0)}\right)^2 = \beta^4(0)\mu_0^2(t) + \left(\frac{\mu_1(t)}{\mu_1(0)} + \frac{\mu'(0)}{2\mu(0)}\frac{\mu_0(t)}{a(0)}\right)^2 \quad (2.50)$$

given in terms of standard solutions μ_0 and μ_1 of the linear characteristic equation (2.12) when $c_0 = 0$. Historically, the original solution to the Ermakov equation, is called the Pinney equation and it represents a nonlinear superposition principle [58, 92]. By *Lemma 2.4.2*, equation (2.50) is represented as

$$\mu = \mu(0)\mu_0\sqrt{\beta^4(0) + 4(\alpha(0) + \gamma_0)^2}. \quad (2.51)$$

It follows that equation (2.51) is referred to as the Pinney-type in our context. Further details on this Pinney-type solution and the corresponding Ermakov-type invariant are given in [16] and [99].

2.5 Ehrenfest's Theorem Transformations

Ehrenfest's theorem relates the time derivative of expectation value for a quantum mechanical operator to the commutator of that operator with the Hamiltonian of the system, and it is defined as the following relation (Appendix B contains more details about Ehrenfest's theorems)

$$\frac{d}{dt}\langle A \rangle = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i\hbar}\langle AH - H^\dagger A \rangle,$$

where $A(x, p, t)$ is some operator, and $H(x, p, t)$ is the hamiltonian governing the system. This theorem only holds for expectation values (averages of the measurements) and not the eigenvalues themselves. In this section we propose a transformation which derives Ehrenfest's Theorem for the harmonic oscillator. We will find that expectation values of displacement and momentum obey time evolution equations which are analogous to those of classical mechanics. Essentially, Ehrenfest's theorem is a bridge from quantum to classical mechanics because it relates the quantum-mechanical Hamiltonian to the classical equations of motion via expectation values.

By introducing expectation values of the coordinate and momentum operators in the following form

$$\bar{x} = \frac{\langle x \rangle}{\langle 1 \rangle} = \frac{\langle \Psi, x \Psi \rangle}{\langle \Psi, \Psi \rangle}, \quad \bar{p} = \frac{\langle p \rangle}{\langle 1 \rangle} = \frac{\langle \Psi, p \Psi \rangle}{\langle \Psi, \Psi \rangle},$$

one can derive Ehrenfest's theorem for the generalized (driven) harmonic oscillators (see, for example, [22] and [23]). Then

$$\frac{d\bar{x}}{dt} = 2a\bar{p} + c\bar{x} - g, \quad \frac{d\bar{p}}{dt} = -2b\bar{x} - c\bar{p} + f$$

and the following classical equation of motion of the parametric driven oscillator holds

$$\frac{d^2\bar{x}}{dt^2} - \frac{a'}{a} \frac{d\bar{x}}{dt} + \left(4ab - c^2 + c \frac{a'}{a} - c' \right) \bar{x} = 2af - g' + g \frac{a'}{a} - cg. \quad (2.52)$$

(Derivation of a similar equation for \bar{p} is quite similar.)

The transformation of the expectation values

$$\bar{\xi} = \beta \bar{x} + \varepsilon, \quad \bar{\xi} = \langle \chi, \xi \chi \rangle \quad \text{with} \quad \langle \chi, \chi \rangle = 1,$$

corresponding to *Lemma 2.2.1*, converts (2.52) into the simplest equation of motion of the free particle and/or harmonic oscillator:

$$\frac{d^2\bar{\xi}}{d\tau^2} + 4c_0\bar{\xi} = 0 \quad (c_0 = 0, 1).$$

(This can be verified by a direct calculation.) All details of derivations and examples are given in Appendix B.

Summary

In [66], we were able to develop a mathematical framework to find solutions to two of the most studied problems from Quantum Mechanics: The Free particle (defined by $c_0 = 0$) and the harmonic oscillator problem (defined by $c_0 = 1$). The physical interpretation of our framework could be viewed as the switching on and off of a harmonic potential, such that a particle is free or trapped by electromagnetic forces. We have determined the time evolution of the wave functions of generalized (driven) harmonic

oscillators (2.17), known for their great importance in many advanced quantum problems [41], in terms of the solution to the Ermakov-type system (2.5)–(2.10) by means of a variant of the nonlinear superposition principle (2.42)–(2.48). (In our approach, the standard solutions of equation (2.12) with $c_0 = 0$ should be found analytically or numerically for any given variable quadratic Hamiltonian.) We have established in general that

1. The Green's function propagator, corresponds to the free particle solution, where its evolution is given by a Riccati-type system
2. The Harmonic oscillator solutions are given by exact wavefunctions, where their evolution is determined by an Ermakov-type system.

2.6 Special Cases of *Lemma 2.2.1*

First observation: Some authors in [4] have considered similar transformations as the first general result in this dissertation. A special case of *Lemma 2.2.1* is the *Quantum Arnold Transformation* or QAT. With this important example we are able to illustrate the importance of the transformation and the second order linear *ordinary differential equation* (denoted as the characteristic equation in the homogeneous case of the Riccati-type system). Similar to our case, the authors in [4] consider

$$\ddot{x} + \dot{f}\dot{x} + \omega^2 x = 0 \quad (= \Lambda). \quad (2.53)$$

using Newtonian notation from physics. Here, the coefficients are all functions of time $f(t)$, $\omega(t)$ and $\lambda(t)$. The solutions u_1 , u_2 (u_p) to equation (2.53) are linearly independent solutions (where u_p is the particular solution of equation (2.53) such that $W(t) \neq 0$). Their transformation, resembles that of lemma 2.2.1 and it is extremely useful for computing objects such as wave functions, quantum propagator or the evolution operator (which otherwise would require difficult laborious calculations). The complete Quan-

tum Arnold transformation as follows,

$$\left\{ \begin{array}{l} \tau = \frac{u_1(t)}{u_2(t)} \\ \kappa = \frac{x}{u_2(t)} \quad \ddot{\kappa} = 0 \text{ (classical equation)} \longleftrightarrow \ddot{x} + \dot{f}\dot{x} + \omega^2 x = 0 \\ \varphi = \phi \sqrt{u_2(t)} \exp\left(-i \frac{m}{2\hbar} \frac{1}{W(t)} \frac{u_2(t)}{u_2(t)} x^2\right) \end{array} \right.$$

is a special case of Lemma 2.2.1. From section 2.2

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = 0 \quad (= 4c_0 a^2 \beta^4 \mu)$$

$$\tau = \frac{a'}{a} - 2c + 4d \quad \sigma = ab - cd + d^2 + \frac{d}{2} \left(\frac{a'}{a} - \frac{d'}{d} \right)$$

we choose linearly independent fundamental solutions μ_0, μ_1 , which satisfy the conditions $\mu_1(0) = 0, \mu_1'(0) = 1, \mu_2(0) = 0, \mu_2'(0) = 0$, of the homogeneous characteristic equation. Translating the QAT to our terms, we have

$$\left\{ \begin{array}{l} \tau = \gamma(t) \\ \xi = \beta(t)x + \varepsilon(t) \quad \mu'' = 0 \text{ (classical equation)} \longleftrightarrow \mu'' - \tau(t)\mu' + 4\sigma(t)\mu = 0 \\ \psi = \frac{\chi(\xi, \tau)}{\sqrt{\mu(t)}} \exp(i(\alpha(t)x^2 + \delta(t)x + \kappa(t))). \end{array} \right.$$

Second observation: The authors have proposed the Schrödinger equation

$$i\hbar\phi_t = -\frac{\hbar^2}{2m} e^{-f(t)} \phi_{xx} + \frac{1}{2} m \omega^2 e^{f(t)} x^2 \phi - m \Lambda e^{f(t)} x \phi, \quad \Lambda \neq 0 \quad (2.54)$$

and we see that this is just a special case of our *master* quadratic Schrödinger equation (2.2)

$$i\hbar\psi_t = -a(t)\psi_{xx} + b(t)x^2\psi - ic(t)x\psi_x - id(t)\psi - f(t)x\psi + ig(t)\psi_x, \quad \hbar = 1.$$

Observe that equation (2.54) can be re-written as

$$i\phi_t = -a(t)\phi_{xx} + b(t)x^2\phi - f(t)x\phi.$$

The time-dependent coefficients can be extracted easily and they are explicitly

$$a(t) = \frac{\hbar}{2m} e^{-f(t)}, \quad b(t) = \frac{m\omega^2}{2\hbar} e^{f(t)}, \quad f(t) = \frac{m\Lambda}{\hbar} e^{f(t)}, \quad c(t) = d(t) = g(t) = 0.$$

Thus, the characteristic equation can be constructed and defined by,

$$\mu'' + f'\mu' + \omega^2\mu = 0 \quad \tau = -f', \quad \sigma = \omega^2/4.$$

Therefore, the QAT in terms of our lemma is given below:

$$\left\{ \begin{array}{l} i\frac{\partial \psi}{\partial t} = H\psi \\ \psi = \frac{e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t))}}{\sqrt{\mu(t)}} \chi(\xi, \tau) \\ \mu'' - \tau\mu' + \sigma\mu = 0 \end{array} \right. \quad \begin{array}{l} \longmapsto i\chi = -\chi_{\xi\xi} \\ \\ \longmapsto \mu_{\tau\tau} \end{array}$$

which solves the free particle problem.

Chapter 3

ON A HIDDEN SYMMETRY OF QUANTUM HARMONIC OSCILLATORS

3.1 Introduction

In this chapter, a (hidden revealing symmetry) connection with certain Ermakov-type system is established; it makes it possible to bypass certain complexities of the traditional Lie algebra approach [75] (see [36, 70] and the references therein regarding the Ermakov equation). A general procedure of obtaining new solutions by acting on any set of given ones by enveloping algebra of generators of the Heisenberg–Weyl group is described in [32]. In addition, the maximal invariance group of the generalized driven harmonic oscillators is shown to be isomorphic to the Schrödinger group of the free particle and the simple harmonic oscillator [75, 84, 85].

The goal is to elaborate on a “missing” class of solutions to the time-dependent Schrödinger equation for the simple harmonic oscillator in one dimension. The most exciting result in the dissertation has to do with computer-animated solutions. This research on finding explicit solutions for the first time provides an interesting feature of these solutions not seen before for the one dimensional case: the phase space oscillations of the electron density and the corresponding probability distribution of the particle linear momentum. As a result, a dynamic visualization of the fundamental Heisenberg Uncertainty Principle [52] is also provided [76, 102]. The next section discusses the harmonic oscillator group and its special cases.

3.2 The Schrödinger Group for Simple Harmonic Oscillators

Symmetry considerations are very important in quantum theory. Known already by Niederer [84], the Schrödinger equation is also represented in group theory as the *Schrödinger group* Sch_1 . It is defined as the (maximal) group of symmetry transformations [103, 14] of the free one-dimensional Schrödinger equation $i\partial_t\psi = -\frac{1}{2}\partial_{xx}\psi$. A year later Niederer [85] again studied the maximal symmetry group of the Schrödinger equation $i\partial_t\psi = -\frac{1}{2}\partial_{xx}\psi + \frac{1}{2}x^2\psi$ with a harmonic potential, and he found that this equation ad-

mits an invariance group which is isomorphic to Sch_1 [103]. Our aim in this part of the dissertation is to reconstruct the symmetric properties of the Schrödinger group, as a humble contribution to Niederer's work. So we revisit the time-dependent Schrödinger equation for the simple harmonic oscillator,

$$2i\psi_t + \psi_{xx} - x^2\psi = 0, \quad (3.1)$$

and find a six-parameter family of square integrable solutions as follows

$$\psi_n(x, t) = \frac{e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t)) + i(2n+1)\gamma(t)}}{\sqrt{2^n n! \mu(t)} \sqrt{\pi}} e^{-(\beta(t)x + \varepsilon(t))^2/2} H_n(\beta(t)x + \varepsilon(t)), \quad (3.2)$$

where $H_n(x)$ are the Hermite polynomials [86] and

$$\mu(t) = \mu_0 \sqrt{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}, \quad (3.3)$$

$$\alpha(t) = \frac{\alpha_0 \cos 2t + \sin 2t (\beta_0^4 + 4\alpha_0^2 - 1)/4}{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}, \quad (3.4)$$

$$\beta(t) = \frac{\beta_0}{\sqrt{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}}, \quad (3.5)$$

$$\gamma(t) = \gamma_0 - \frac{1}{2} \arctan \frac{\beta_0^2 \sin t}{2\alpha_0 \sin t + \cos t}, \quad (3.6)$$

$$\delta(t) = \frac{\delta_0 (2\alpha_0 \sin t + \cos t) + \varepsilon_0 \beta_0^3 \sin t}{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}, \quad (3.7)$$

$$\varepsilon(t) = \frac{\varepsilon_0 (2\alpha_0 \sin t + \cos t) - \beta_0 \delta_0 \sin t}{\sqrt{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}}, \quad (3.8)$$

$$\begin{aligned} \kappa(t) = & \kappa_0 + \sin^2 t \frac{\varepsilon_0 \beta_0^2 (\alpha_0 \varepsilon_0 - \beta_0 \delta_0) - \alpha_0 \delta_0^2}{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2} \\ & + \frac{1}{4} \sin 2t \frac{\varepsilon_0^2 \beta_0^2 - \delta_0^2}{\beta_0^4 \sin^2 t + (2\alpha_0 \sin t + \cos t)^2}. \end{aligned} \quad (3.9)$$

Here, $\mu_0 > 0$, $\alpha_0, \beta_0 \neq 0$, $\gamma_0, \delta_0, \varepsilon_0, \kappa_0$ are real initial data. These “missing” solutions can be derived analytically in a unified approach to generalized harmonic oscillators (see similar derivations in Ref. [21, 23, 66] and the references therein). They can also be verified by a direct substitution with the aid of Mathematica computer algebra system [60, 76, 102]. In addition, the simplest special case given by $\mu_0 = \beta_0 = 1$

and $\alpha_0 = \gamma_0 = \delta_0 = \varepsilon_0 = \kappa_0 = 0$ reproduces the textbook solution obtained by the separation of variables (note the following references: [42, 45, 65, 81] and the original Schrödinger paper [93]); and the shape-preserving oscillator evolutions occur when $\alpha_0 = 0$ and $\beta_0 = 1$. More details on the derivation of these formulas can be found in Refs. [75] and [85] and other sources within.

3.3 The Maximal Kinematical Invariance Group of the Generalized Driven Harmonic Oscillators

The transformation (2.3) from Lemma 2.2.1 admits an inversion when the coefficient $a(t)$ does not change sign (see (2.7) for the monotonicity and local time inversion). As a result, the invariance group of generalized driven harmonic oscillator is isomorphic to the Schrödinger group of the free particle,

$$T = S^{-1}T_0S, \quad (3.10)$$

thus extending the result of [85] to the corresponding nonautonomous systems (in the classical case, see (3.16) and (3.24) for possible operators S and S^{-1} and the operator T_0 is defined by (3.11) in general). The structure of the Schrödinger group of operators T_0 in two-dimensional space-time as a semidirect product of $SL(2, \mathbb{R})$ and Weyl $W(1)$ groups is discussed, for example, in Refs. [14, 57] and [82]. The key ingredients for the maximum kinematical invariance groups of the free particle and harmonic oscillator have been introduced in [6, 7, 50, 54, 84] and [85] (see also [14, 57, 82, 90, 98, 98, 103] and the references therein). The following diagram gives a general visual representation of this isomorphism maps. Examples follow in the next subsection.

3.4 Special Cases

We have discovered that the following substitution

$$\psi(x, t) = \frac{e^{i(\alpha(t)x^2 + \delta(t)x + \kappa(t))}}{\sqrt{\mu(t)}} \chi(\xi, \tau),$$

where relations (3.3)–(3.9) hold, transforms the time-dependent Schrödinger equation (3.1) into itself with respect to the new variables $\xi = \beta(t)x + \varepsilon(t)$ and $\tau = -\gamma(t)$ [85]

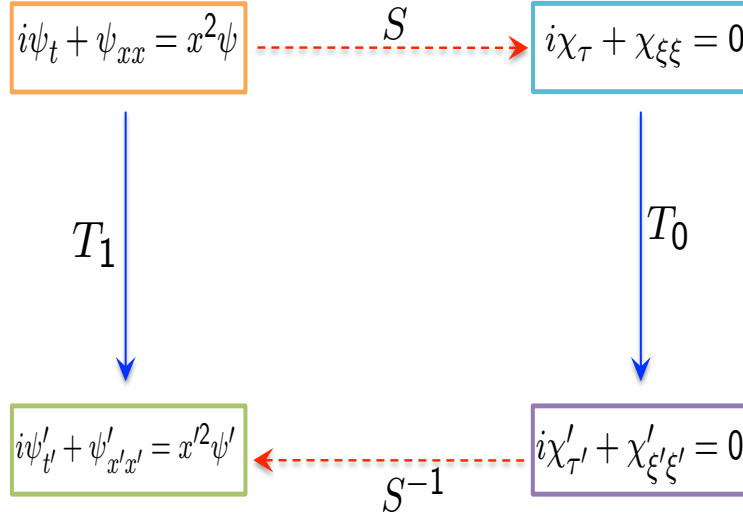


Figure 3.1: A visual representation of a commutative diagram of the Free and Schrödinger groups approached from the view point of a Riccati- and Ermakov-type systems, for $\tau = -\gamma$.

(see also [75] and the references therein). The `Mathematica` verification can be found in auxiliary References [60] and [102].

The maximal kinematic invariance groups of the free Schrödinger equation [84] and the harmonic oscillator [85] and their isomorphism are special cases of the transformation (2.3). In this section, we apply these general results to the maximum kinematical invariance groups of the free Schrödinger equation and of the harmonic oscillator [84, 85].

Transformation from the free particle to the free particle

In the simplest case $a = 1, b = c = d = f = g = c_0 = 0$, one finds $\mu_0 = 2t, \mu_1 = 1$ and $\alpha_0 = -\beta_0/2 = \gamma_0 = 1/(4t), \delta_0 = \varepsilon_0 = \kappa_0 = 0$. The general solution of the corresponding Riccati-type system is given by

$$\mu(t) = \mu(0)(1 + 4\alpha(0)t),$$

and

$$\begin{aligned}
\alpha(t) &= \frac{\alpha(0)}{1+4\alpha(0)t}, & \beta(t) &= \frac{\beta(0)}{1+4\alpha(0)t}, \\
\gamma(t) &= \gamma(0) - \frac{\beta^2(0)t}{1+4\alpha(0)t}, & \delta(t) &= \frac{\delta(0)}{1+4\alpha(0)t}, \\
\varepsilon(t) &= \varepsilon(0) - \frac{2\beta(0)\delta(0)t}{1+4\alpha(0)t}, & \kappa(t) &= \kappa(0) - \frac{\delta^2(0)t}{1+4\alpha(0)t}.
\end{aligned}$$

The Ansatz (2.3) together with these formulas determine the Schrödinger group, namely, the maximum kinematical invariance group of the free Schrödinger equation, as follows [84]:

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{\mu(0)(1+4\alpha(0)t)}} \exp \left[i \left(\frac{\alpha(0)x^2 + \delta(0)x - \delta^2(0)t}{1+4\alpha(0)t} + \kappa(0) \right) \right] \\
&\times \chi \left(\frac{\beta(0)x - 2\beta(0)\delta(0)t}{1+4\alpha(0)t} + \varepsilon(0), \frac{\beta^2(0)t}{1+4\alpha(0)t} - \gamma(0) \right) \quad (3.11)
\end{aligned}$$

We have established a connection of the Schrödinger group with the Riccati-type system (see also [14, 44, 57, 82, 85, 103]).

Special cases include the familiar *Galilei transformations*:

$$\psi(x,t) = \exp \left[i \left(\frac{V}{2}x - \frac{V^2}{4}t \right) \right] \chi(x - Vt + x_0, t - t_0), \quad (3.12)$$

when $\alpha(0) = \kappa(0) = 0$, $\beta(0) = \mu(0) = 1$, $\gamma(0) = t_0$, $\varepsilon(0) = x_0$ and $\delta(0) = V/2$; supplemented by *dilatations*:

$$\psi(x,t) = \chi(lx, l^2t) \quad (3.13)$$

with $\alpha(0) = \gamma(0) = \delta(0) = \varepsilon(0) = \kappa(0) = 0$, $\mu(0) = 1$ and $\beta(0) = l$; and *expansions*:

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{1+mt}} \exp \left(i \frac{mx^2}{4(1+mt)} \right) \chi \left(\frac{x}{1+mt}, \frac{t}{1+mt} \right) \quad (3.14) \\
&(\mu(0) = 1 (\neq 0), \quad \mu'(0) = m),
\end{aligned}$$

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2t}} \exp \left(i \frac{x^2}{4t} \right) \chi \left(-\frac{x}{2t}, -\frac{1}{4t} \right) \quad (3.15) \\
&(\mu(0) = 0, \quad \mu'(0) = 2 (\neq 0))
\end{aligned}$$

with $\beta(0) = 1$, $\delta(0) = \varepsilon(0) = \kappa(0) = 0$. The symmetry group of the corresponding diffusion equation is discussed in [57, 82, 90] and [98].

Transformations from the harmonic oscillator to the free particle

In the case $a = b = 1$, $c = d = f = g = c_0 = 0$, the corresponding characteristic equation, $\mu'' + 4\mu = 0$, has two standard solutions $\mu_0 = \sin 2t$, $\mu_1 = \cos 2t$ and

$$\alpha_0 = -\frac{1}{2}\beta_0 = \gamma_0 = \frac{\cos 2t}{2 \sin 2t}, \quad \delta_0 = \varepsilon_0 = \kappa_0 = 0,$$

$$\mu = \mu(0) (2\alpha(0) \sin 2t + \cos 2t).$$

The general solution of the corresponding Riccati-type system takes the form

$$\alpha(t) = \frac{2\alpha(0) \cos 2t - \sin 2t}{2(2\alpha(0) \sin 2t + \cos 2t)},$$

$$\beta(t) = \frac{\beta(0)}{2\alpha(0) \sin 2t + \cos 2t},$$

$$\gamma(t) = \gamma(0) - \frac{\beta^2(0) \sin 2t}{2(2\alpha(0) \sin 2t + \cos 2t)},$$

$$\delta(t) = \frac{\delta(0)}{2\alpha(0) \sin 2t + \cos 2t},$$

$$\varepsilon(t) = \varepsilon(0) - \frac{2\beta(0) \delta(0) \sin 2t}{2\alpha(0) \sin 2t + \cos 2t},$$

$$\kappa(t) = \kappa(0) - \frac{\delta^2(0) \sin 2t}{2(2\alpha(0) \sin 2t + \cos 2t)}.$$

Letting $\mu(0) = \beta(0) = 1$ and $\alpha(0) = \gamma(0) = \delta(0) = \varepsilon(0) = \kappa(0) = 0$, we arrive at the simple substitution [85]:

$$\psi(x, t) = \frac{e^{-i(1/2)x^2 \tan 2t}}{\sqrt{\cos 2t}} \chi\left(\frac{x}{\cos 2t}, \frac{\tan 2t}{2}\right) \quad (3.16)$$

(see also [44, 46, 82, 100]).

Transformation from the free particle to the harmonic oscillator

In the simplest case $a = c_0 = 1$, $b = c = d = f = g = 0$, the general solution of the corresponding Ermakov-type system is given by

$$\mu(t) = \mu(0) \sqrt{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}, \quad (3.17)$$

$$\alpha(t) = \frac{\beta^4(0)t + \alpha(0)(4\alpha(0)t + 1)}{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}, \quad (3.18)$$

$$\beta(t) = \frac{\beta(0)}{\sqrt{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}}, \quad (3.19)$$

$$\gamma(t) = \gamma(0) - \frac{1}{2} \arctan \frac{2\beta^2(0)t}{4\alpha(0)t + 1}, \quad (3.20)$$

$$\delta(t) = \frac{2\varepsilon(0)\beta^3(0)t + \delta(0)(4\alpha(0)t + 1)}{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}, \quad (3.21)$$

$$\varepsilon(t) = \frac{\varepsilon(0)(4\alpha(0)t + 1) - 2\beta(0)\delta(0)t}{\sqrt{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}}, \quad (3.22)$$

$$\begin{aligned} \kappa(t) = \kappa(0) + t & \frac{(4\alpha(0)t + 1)(\varepsilon^2(0)\beta^2(0) - \delta^2(0))}{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2} \\ & - t^2 \frac{4\varepsilon(0)\delta(0)\beta^3(0)}{4\beta^4(0)t^2 + (4\alpha(0)t + 1)^2}. \end{aligned} \quad (3.23)$$

In the special case $\mu(0) = \beta(0) = 1$, $\alpha(0) = \gamma(0) = \delta(0) = \varepsilon(0) = \kappa(0) = 0$ one gets the known transformation [54, 85, 82, 46, 50, 73]:

$$\psi(x, t) = \frac{1}{(4t^2 + 1)^{1/4}} \exp\left(i \frac{tx^2}{4t^2 + 1}\right) \chi\left(\frac{x}{\sqrt{4t^2 + 1}}, \frac{1}{2} \arctan 2t\right). \quad (3.24)$$

One can easily verify that transformations (3.16) and (3.24) are (local) inverses of each other.

Equations (3.2) and (3.17)–(3.23) provide a six parameter family of the “harmonic oscillator states” for the free particle (see also [46] and the references therein).

Transformation from the harmonic oscillator to the harmonic oscillator

In this section the case $a = b = c_0 = 1$, $c = d = f = g = 0$ is considered. The general solution of the corresponding Ermakov-type system is given by

$$\begin{aligned}
 \mu(t) &= \mu(0) \sqrt{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}, \\
 \alpha(t) &= \frac{\alpha(0) \cos 4t + \sin 4t (\beta^4(0) + 4\alpha^2(0) - 1) / 4}{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}, \\
 \beta(t) &= \frac{\beta(0)}{\sqrt{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}}, \\
 \gamma(t) &= \gamma(0) - \frac{1}{2} \arctan \frac{\beta^2(0) \sin 2t}{2\alpha(0) \sin 2t + \cos 2t}, \\
 \delta(t) &= \frac{\delta(0) (2\alpha(0) \sin 2t + \cos 2t) + \varepsilon(0) \beta^3(0) \sin 2t}{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}, \\
 \varepsilon(t) &= \frac{\varepsilon(0) (2\alpha(0) \sin 2t + \cos 2t) - \beta(0) \delta(0) \sin 2t}{\sqrt{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}}, \\
 \kappa(t) &= \kappa(0) + \sin^2 2t \frac{\varepsilon(0) \beta^2(0) (\alpha(0) \varepsilon(0) - \beta(0) \delta(0))}{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2} \\
 &\quad + \frac{1}{4} \sin 4t \frac{\varepsilon^2(0) \beta^2(0) - \delta^2(0)}{\beta^4(0) \sin^2 2t + (2\alpha(0) \sin 2t + \cos 2t)^2}.
 \end{aligned}$$

The Ansatz (2.3) together with these formulas explicitly determine the harmonic oscillator group introduced in Ref. [85]. The established connection with the corresponding Ermakov-type system offers an alternative to the traditional Lie algebra approach of the harmonic oscillator group [6, 14, 82, 85].

The use of the wave function (3.2) and our explicit solution (3.3)–(3.9) result in a six parameter family of the quantum oscillator state, which seems cannot be obtained by the standard separation of variables (the case $\beta(0) = 1$ and $\alpha(0) = \gamma(0) = \delta(0) = \varepsilon(0) = \kappa(0) = 0$ corresponds to the textbook oscillator solution). The corresponding quadratic dynamic invariant is found (in general) in Ref. [91].

3.5 Symmetry and Hidden Solutions

In section 3.2, the “dynamic harmonic oscillator states” (3.2)–(3.9) can be alternatively derived from the relation

$$E(t) \psi_n(x, t) = \left(n + \frac{1}{2}\right) \psi_n(x, t), \quad (3.25)$$

as they are eigenfunctions of the time-dependent quadratic invariant

$$\begin{aligned} E(t) &= \frac{1}{2} \left[\frac{(p - 2\alpha x - \delta)^2}{\beta^2} + (\beta x + \varepsilon)^2 \right] \\ &= \frac{1}{2} \left[\hat{a}(t) \hat{a}^\dagger(t) + \hat{a}^\dagger(t) \hat{a}(t) \right], \quad \frac{d}{dt} \langle E \rangle = 0. \end{aligned}$$

The required operator identity [32, 91] to find these dynamic harmonic states is given by

$$\frac{\partial E}{\partial t} + i^{-1} [E, H] = 0, \quad H = \frac{1}{2} (p^2 + x^2).$$

Here, the time-dependent annihilation $\hat{a}(t)$ and creation $\hat{a}^\dagger(t)$ operators are explicitly given by

$$\hat{a}(t) = \frac{1}{\sqrt{2}} \left(\beta x + \varepsilon + i \frac{p - 2\alpha x - \delta}{\beta} \right), \quad \hat{a}^\dagger(t) = \frac{1}{\sqrt{2}} \left(\beta x + \varepsilon - i \frac{p - 2\alpha x - \delta}{\beta} \right)$$

with $p = i^{-1} \partial / \partial x$ in terms of our solutions (3.4)–(3.9). These operators satisfy the canonical commutation relation,

$$\hat{a}(t) \hat{a}^\dagger(t) - \hat{a}^\dagger(t) \hat{a}(t) = 1,$$

and the oscillator-type spectrum (3.25) of the dynamic invariant E can be obtained in a standard way by using the Heisenberg–Weyl algebra of the raising and lowering operators (a “second quantization” [2, 71], the Fock states):

$$\hat{a}(t) \Psi_n(x, t) = \sqrt{n} \Psi_{n-1}(x, t), \quad \hat{a}^\dagger(t) \Psi_n(x, t) = \sqrt{n+1} \Psi_{n+1}(x, t). \quad (3.26)$$

(Important details on the Heisenberg representation of operators are given in Appendix C.) It can be noticed that

$$\psi_n(x, t) = e^{i(2n+1)\gamma(t)} \Psi_n(x, t)$$

is the relation to the wave functions (3.2) where

$$\varphi_n(t) = -(2n+1)\gamma(t)$$

is the nontrivial Lewis phase [71, 91].

This quadratic dynamic invariant and the corresponding creation and annihilation operators for the generalized harmonic oscillators have been introduced recently in Ref. [91] (see also [23, 32, 99] and the references therein for important special cases) and a generalization of the coherent states is discussed in Ref. [68].

3.6 The Momentum Representation

In continuous space, wavefunctions in momentum-space representation are derived by the inverse Fourier transform. By definition,

$$a_n(p, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ipx} \psi_n(x, t) dx, \quad (3.27)$$

Momentum representation is related to the position-space representation by a Fourier transform, where $x = i\hbar \frac{d}{dp}$, $p = -i\hbar \frac{d}{dx}$. Following, the corresponding wave functions in the momentum representation are derived by the Fourier transform of our solutions (3.2) and (3.3)–(3.9). For the wave functions in the momentum representation, the integral evaluation is similar to Ref. [66]. As a result, the functions $a_n(p, t)$ are of the same form as in (3.2)–(3.9), if $\psi_n \rightarrow a_n$ and $x \rightarrow p$, with the initial data

$$\begin{aligned} \alpha_1 &= -\frac{\alpha_0}{4\alpha_0^2 + \beta_0^2}, & \beta_1 &= \frac{\beta_0}{\sqrt{4\alpha_0^2 + \beta_0^2}}, \\ \gamma_1 &= \gamma_0 + \frac{1}{2} \operatorname{arccot} \frac{\beta_0^2}{2\alpha_0}, & \mu_1 &= \mu_0 \sqrt{4\alpha_0^2 + \beta_0^2}, \\ \delta_1 &= \frac{2\alpha_0\delta_0 + \beta_0^3\varepsilon_0}{4\alpha_0^2 + \beta_0^2}, & \varepsilon_1 &= \frac{2\alpha_0\varepsilon_0 - \beta_0\delta_0}{\sqrt{4\alpha_0^2 + \beta_0^2}}, \\ \kappa_1 &= \kappa_0 + \frac{\alpha_0(\beta_0^2\varepsilon_0^2 - \delta_0^2) + \beta_0^3\delta_0\varepsilon_0}{4\alpha_0^2 + \beta_0^2}. \end{aligned}$$

Again Mathematica was utilized with the calculations.

3.7 Conditions for Uncertainty Squeezed States

Mathematically the *Heisenberg uncertainty principle* says that every quantum state has the property that the root mean square (RMS) deviation of the position from its mean (the standard deviation of the x -distribution) $\sigma_x = \sqrt{\langle (x - \langle x \rangle)^2 \rangle} = \sqrt{(\Delta x)^2}$ times the RMS deviation of the momentum from its mean (the standard deviation of p): $\sigma_p = \sqrt{\langle (p - \langle p \rangle)^2 \rangle} = \sqrt{(\Delta p)^2}$ can never be smaller than a fixed fraction of Planck's constant (its minimum value) $\sigma_x \sigma_p \geq \hbar/2$. However, any state such that this principle is saturated (the product of the corresponding two operators takes on its minimum value) is called a *squeezed coherent state*, mathematically given by the quantity: $\Delta x \Delta p = \hbar/2$. Thus, to complement the Mathematica animations of our wavefunctions, we find the corresponding conditions that satisfy a squeezed coherent state. This mathematically provides conditions for localization of the particle.

First the expectation values of momentum and position are computed. Making use of (3.26), we derive the first and second moments of x and p . Consider working with $\hat{a}(t) \pm \hat{a}^\dagger(t)$. Notice first that the sum $\hat{a}(t) + \hat{a}^\dagger(t) = \sqrt{2}(\beta x + \varepsilon)$, such that $\hat{a}(t) + \hat{a}^\dagger(t)/\sqrt{2} = \beta x + \varepsilon$. Hence, an expression for x is the following:

$$x = \frac{\beta x + \varepsilon}{\sqrt{2}\beta} - \frac{\varepsilon}{\beta}. \quad (3.28)$$

Making use of wavefunctions (3.26) properties,

$$x\Psi_n = \frac{\hat{a}(t) + \hat{a}^\dagger(t)}{\sqrt{2}\beta}\Psi_n - \frac{\varepsilon}{\beta}\Psi_n.$$

Using the canonical commutation relations (3.26), the definition of expectation value and the inner and scalar product and ket properties it follows that

$$\begin{aligned} \langle x \rangle &= \langle \Psi_n | x \Psi_n \rangle = \langle \Psi_n | \frac{1}{\sqrt{2}\beta} (\hat{a}(t) + \hat{a}^\dagger(t)) \Psi_n - \frac{\varepsilon}{\beta} \Psi_n \rangle \\ &= \frac{1}{\sqrt{2}\beta} \langle \Psi_n | (\hat{a}(t) + \hat{a}^\dagger(t)) \Psi_n \rangle - \frac{\varepsilon}{\beta} \langle \Psi_n | \Psi_n \rangle \\ &= -\frac{\varepsilon}{\beta} \langle \Psi_n | \Psi_n \rangle. \end{aligned}$$

Since the Ψ_n form an orthonormal set, $\langle \Psi_n | \Psi_n \rangle = 1$ and thus the expectation value for x follows from (3.8) and (3.5).

Finding $\langle p \rangle$ tends to be a bit more tedious and requires the use of Mathematica for simplification. In this case, we consider the difference $\widehat{a}(t) - \widehat{a}^\dagger(t)$ and it gives

$$\frac{\widehat{a}(t) - \widehat{a}^\dagger(t)}{i\sqrt{2}} = \frac{p - 2\alpha x - \delta}{\beta};$$

which implies that

$$p = \frac{\widehat{a}(t) - \widehat{a}^\dagger(t)}{i\sqrt{2}} + \frac{2\alpha x}{\beta} + \frac{\delta}{\beta}.$$

Similar arguments as for finding $\langle x \rangle$ lead to the quantity

$$\langle p \rangle = \frac{2\alpha}{\beta} \langle x \rangle + \frac{\delta}{\beta}.$$

Therefore, the corresponding expectation values, following (3.26), are given by

$$\langle x \rangle = -\frac{1}{\beta_0} [(2\alpha_0 \varepsilon_0 - \beta_0 \delta_0) \sin t + \varepsilon_0 \cos t], \quad \frac{d}{dt} \langle x \rangle = \langle p \rangle, \quad (3.29)$$

$$\langle p \rangle = -\frac{1}{\beta_0} [(2\alpha_0 \varepsilon_0 - \beta_0 \delta_0) \cos t - \varepsilon_0 \sin t], \quad \frac{d}{dt} \langle p \rangle = -\langle x \rangle \quad (3.30)$$

with the initial data $\langle x \rangle|_{t=0} = -\varepsilon_0/\beta_0$ and $\langle p \rangle|_{t=0} = -(2\alpha_0 \varepsilon_0 - \beta_0 \delta_0)/\beta_0$. This provides a classical interpretation of our “hidden” parameters.

Moreover, the expectation values $\langle x \rangle$ and $\langle p \rangle$ satisfy the classical equation for harmonic motion, $y'' + y = 0$, with a total energy

$$\frac{1}{2} [\langle p \rangle^2 + \langle x \rangle^2] = \frac{(2\alpha_0 \varepsilon_0 - \beta_0 \delta_0)^2 + \varepsilon_0^2}{2\beta_0^2} = \frac{1}{2} [\langle p \rangle^2 + \langle x \rangle^2] \Big|_{t=0}.$$

Finally, we need to calculate standard deviations. Making use of the first moments (3.29)-(3.30), $\langle x^2 \rangle$ is calculated first as follows. Using equation (3.28),

$$\langle x^2 \rangle = \langle \Psi_n | x^2 \Psi_n \rangle = \langle \Psi_n | \frac{1}{2\beta^2} (\widehat{a}(t)^2 + \widehat{a}^\dagger(t)^2 + 2\widehat{a}(t)\widehat{a}^\dagger(t)) \Psi_n \rangle \quad (3.31)$$

$$- \frac{2\varepsilon}{\beta^2} \langle \Psi_n | \frac{\widehat{a}(t) + \widehat{a}^\dagger(t)}{\sqrt{2}} \rangle - \frac{\varepsilon^2}{\beta^2} \langle \Psi_n | \Psi_n \rangle; \quad (3.32)$$

as terms vanish,

$$\langle x^2 \rangle = \frac{1}{\beta^2} \langle \Psi_n | (\hat{a}(t)\hat{a}^\dagger(t) + \hat{a}^\dagger(t)\hat{a}(t)) \Psi_n \rangle - \frac{\varepsilon^2}{\beta^2} \langle \Psi_n | \Psi_n \rangle. \quad (3.33)$$

Yet $\hat{H}\Psi_n = E_n\Psi_n = (n + \frac{1}{2})\Psi_n$, and $\langle \Psi_n | \Psi_n \rangle = 1$,

$$\langle x^2 \rangle = \frac{1}{\beta^2} (n + \frac{1}{2}) - \frac{\varepsilon^2}{\beta^2}. \quad (3.34)$$

Now to find $\langle p^2 \rangle$ is a similar procedure and thus we arrive at the standard deviations:

$$\begin{aligned} \langle (\Delta p)^2 \rangle &= \langle p^2 \rangle - \langle p \rangle^2 \\ &= \left(n + \frac{1}{2} \right) \frac{1 + 4\alpha_0^2 + \beta_0^2 + (4\alpha_0^2 + \beta_0^2 - 1) \cos 2t - 4\alpha_0 \sin 2t}{2\beta_0^2}, \\ \langle (\Delta x)^2 \rangle &= \langle x^2 \rangle - \langle x \rangle^2 \\ &= \left(n + \frac{1}{2} \right) \frac{1 + 4\alpha_0^2 + \beta_0^2 - (4\alpha_0^2 + \beta_0^2 - 1) \cos 2t + 4\alpha_0 \sin 2t}{2\beta_0^2}. \end{aligned}$$

Their product is the general condition necessary to derive the saturated (or squeezed states), and it is

$$\langle (\Delta p)^2 \rangle \langle (\Delta x)^2 \rangle = \left(n + \frac{1}{2} \right)^2 \frac{1}{4\beta_0^4} \left[(1 + 4\alpha_0^2 + \beta_0^2)^2 - ((4\alpha_0^2 + \beta_0^2 - 1) \cos 2t - 4\alpha_0 \sin 2t)^2 \right].$$

In the case of the Schrödinger solution [93], when $\alpha_0 = \delta_0 = \varepsilon_0 = 0$ and $\beta_0 = 1$, we arrive at $\langle x \rangle = \langle p \rangle \equiv 0$ and

$$\langle (\Delta p)^2 \rangle = \langle (\Delta x)^2 \rangle = n + \frac{1}{2}$$

as presented in the textbooks [42, 45, 46, 65, 81]. The dependence on the quantum number n , which disappears from the Ehrenfest theorem [33, 52], is coming back at the level of the higher moments of the distribution.

3.8 Visualization of Solutions Using Mathematica

In this section, some numerical examples [76] are presented. The Mathematica algebra system has been used for the first time in this research, to elaborate on the “missing class” of solutions. Movie animations were developed for the space- and momentum-space wavefunctions. A few movie stills sequence of the dynamics are shown in Figures

(3.2)-(3.4). Each output in the source code is represented by a sequence of stills. Also, the Mathematica source code lines can be found in Appendix D. (complete lines with color are only available in the electronic version of the dissertation)

Examples: The following figures are numerical examples directly chosen from the Mathematica notebook. For all the states, the parameter values chosen are $\alpha_0 = \gamma_0 = \varepsilon_0 = 0$, $\beta_0 = 2/3$, and $\delta_0 = 3/2$. One will immediately recognize from these animations that the particle is the most localized at the turning points when its linear momentum is the least precisely determined, as required by the fundamental Heisenberg Uncertainty Principle [52] — The more precisely the position is determined, the less precisely the momentum is known in this instant, and vice versa (see also [17]). In its creator’s own words — “If the classical motion of the system is periodic, it may happen that the size of the wave packet at first undergoes only periodic changes” (see Ref. [52], p. 38).

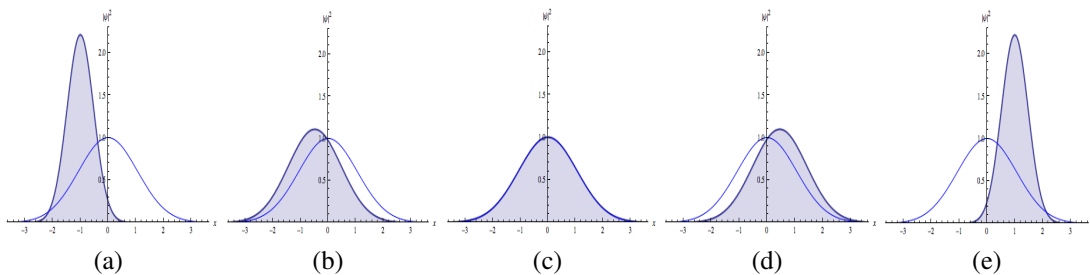


Figure 3.2: Figures (a)-(e) are a few *stills* taken from the mathematica movie animation [76]. Starting with (a) they denote the oscillating electron density (blue) of the ground “dynamic harmonic state” of the time-dependent Schrödinger equation (3.1). These space oscillations complement (with the help of Mathematica) the corresponding “static” textbook solution (clear)[93]. (The color version of this figure is available only in the electronic version of the dissertation, and the actual video animation is available on the dissertation author’s collaborator’s website: [http://hahn.la.asu.edu/~suslov/.](http://hahn.la.asu.edu/~suslov/))

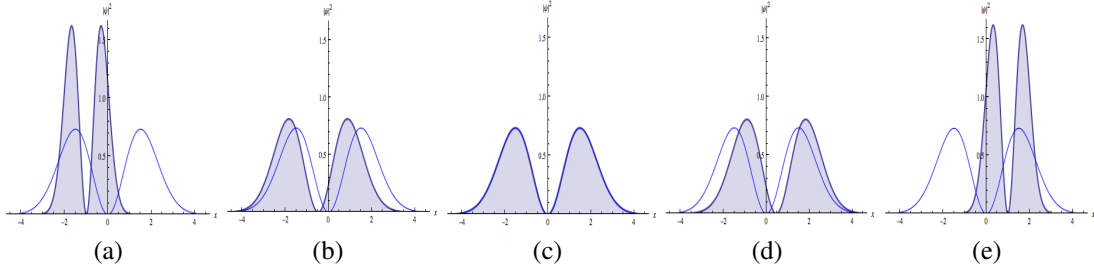


Figure 3.3: Figures (a)-(e) are a few *stills* taken from the mathematica movie animation [76]. Starting with (a) they denote the oscillating electron density (blue) of the first excited “dynamic harmonic state” of the time-dependent Schrödinger equation (3.1). These space oscillations complement (with the help of Mathematica) the corresponding “static” textbook solution (clear)[93]. (The color version of this figure is available only in the electronic version of the dissertation, and the actual video animation is available on the dissertation author’s collaborator’s website: <http://hahn.la.asu.edu/~suslov/>.)

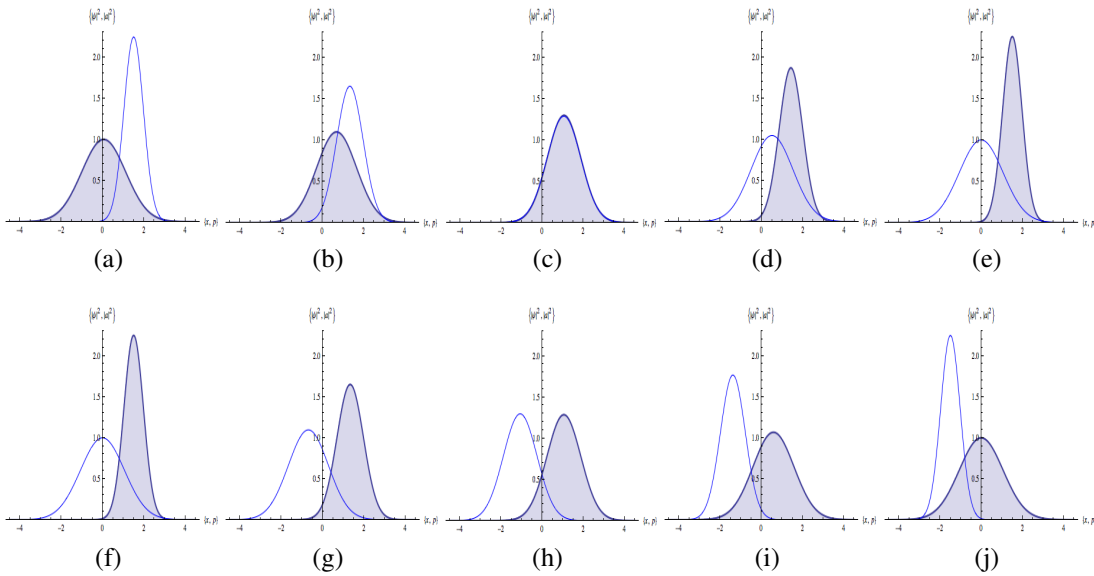


Figure 3.4: Figures (a)-(e) are a few *stills* taken from the mathematica movie animation [76]. Starting with (a) they denote simultaneous oscillations of electron density (blue) and probability distribution of momentum (clear) for the ground “dynamic harmonic state” of the time-dependent Schrödinger equation (3.1). These phase space oscillations complement (with the help of Mathematica) the corresponding “static” textbook solutions [45, 93]. (The color version of this figure is available only in the electronic version of the dissertation, and the actual video animation is available on the dissertation author’s collaborator’s website: <http://hahn.la.asu.edu/~suslov/>.)

Chapter 4

OVERVIEW AND DISCUSSION

4.1 Summary of the dissertation

Quantum systems with quadratic Hamiltonians (see, for example, [4, 12, 11, 23, 30, 32, 37, 41, 51, 77, 107, 109, 112] and the references therein) have attracted substantial attention over the years because of their great importance in many advanced quantum problems. Many examples of possible application of these systems are the coherent states and uncertainty relations, Berry's phase, quantization of mechanical systems and Hamiltonian cosmology. More applications include, but are not limited to charged particle traps and motion in uniform magnetic fields, molecular spectroscopy and polyatomic molecules in varying external fields, crystals through which an electron is passing and exciting the oscillator modes, and other mode interactions with external fields. Quadratic Hamiltonians have particular applications in quantum electrodynamics because the electromagnetic field can be represented as a set of forced harmonic oscillators [41].

Determined in **Chapter 2** of this dissertation is the explicit time evolution of the wave functions of generalized (driven) harmonic oscillators (3.2), known for their great importance in many advanced quantum problems (summarized in the above paragraph) [41], in terms of the solution to the Ermakov-type system (2.5)–(2.10) by means of a variant of the nonlinear superposition principle (2.42)–(2.48). An exact transformation of a linear second-order differential equation into the equation of motion of free particle was discussed by Arnold [8]. An extension of the later to the case of the time-dependent Schrödinger equation had been considered, for example, in Ref. [112] and recently it has been reproduced as the quantum Arnold transformation in [4] and [46] (see also [1, 18, 26, 44, 62, 82, 90] and [100] for similar transformations of nonlinear Schrödinger and other equations of mathematical physics). A relation of the quantum Arnold transformation is elaborated for the generalized (driven) harmonic oscillators

with a Riccati-type system when $c_0 = 0$ (transformation to the free particle) and an extension of this transformation (in terms of solutions of the corresponding Ermakov-type system) is considered to solve the case $c_0 = 1$ (transformation to the classical harmonic oscillator [112]). (In our approach, the standard solutions of equation (2.12) with $c_0 = 0$ should be found analytically or numerically for any given variable quadratic Hamiltonian.) Moreover, an relation of the transformation is discussed. It is also shown that the classical Arnold transformation turns out to be related to Ehrenfest's theorem of quantum mechanics – a theory which bridges classical and quantum mechanics via expectation values of operators.

Chapter 3 offers a new representation for the Schrödinger theoretical groups. Therein, a visualization of the Heisenberg Uncertainty Principle is clearly discussed and the use of *Mathematica* really helps with its dynamic visualisation. The maximal kinematical invariance group of the simple harmonic oscillator [85] provides the six-parameter family of solutions, namely (3.2) and (3.3)–(3.9), for an arbitrary choice of the initial data (of the corresponding Ermakov-type system [36, 66, 70, 75]). These “hidden parameters” usually disappear after evaluation of matrix elements and cannot be observed from the spectrum. Distinguishing between these “new dynamic” and the “standard static” harmonic oscillator states (and which of them is realized in a particular measurement) is thus a fundamental question and research problem.

Simultaneously, in **Chapter 3** it is demonstrated that the probability density $|\psi(x,t)|^2$ of the solution (3.2) is no longer a static result. Observed, are clear oscillations in time, something which somewhat contradicts the standard textbooks [42, 45, 65, 81, 93], – an elementary *Mathematica* simulation reveals such space oscillations for the simplest “dynamic oscillator states” [75, 76]. (The simple *Mathematica* source code is also included, although the full details and all notebooks of the symbolic computations are found at <http://hahn.la.asu.edu/~suslov/>.) The same is true for the probability distribution of the particle linear momentum due to the Heisenberg Un-

certainty Principle [52]. These effects, quite possibly, can be observed experimentally. One possibility might exist in Bose Einstein condensates, if the nonlinearity of the nonlinear Schrödinger equation (Gross–Pitaevskii equation) is turned off by the Feshbach resonance [20, 38, 59, 88, 97, 100]. An even more elementary example is an electron moving in a uniform magnetic field. If the magnetic field is slowly changed for example, from an initially occupied Landau level with the standard solution [65, 74], one may continuously follow the initial wave function evolution (with the quadratic invariant) until the magnetic field becomes a constant once again. This is called *parametric excitation* [21, 32, 67, 77]. The terminal state will end up with, in general, the initial conditions that are required for the “dynamic harmonic states” (3.2)–(3.9) and the probability density should oscillate on the corresponding Landau level just like the solution in this work predicts. However, how to perform experimental effects and observation are still unclear (but these “dynamic harmonic states” will have a nontrivial Berry’s phase [12, 11, 91, 101, 102]).

In this quest for physical relevance to this works, it is possible to consider possible applications in molecular spectroscopy, theory of crystals, quantum optics [46] and cavity quantum electrodynamics [31, 43, 110]. It is logical to believe that clearly nature has an inherent dynamic and unpredictable character [53], not static. Therefore, all of that puts into consideration all of the work in this dissertation to a much broader mathematical and physical context — This may help to better understand some intriguing features of quantum motion. Hence, the work in this dissertation shows that the separation of variables for the time-dependent Schrödinger equations may not always give us the “whole picture.”

4.2 Concluding Remarks

Overall, the research presented in this dissertation represents a continued study of the mathematical properties and physical applications of the time-dependent Schrödinger equation with quadratic Hamiltonians. In the quest for explicit solutions, the disserta-

tion took over and shed light to new results motivated by the works of other authors who started this quest for explicit integrability (see some of the references of this dissertation with authors: Ricardo Cordero-Soto, Erwin Suazo, and Sergei K. Suslov, for example). Physically, it is believed that the models constructed from the generalized harmonic oscillators may be used in quantum optics. But in general, endless possibilities for new research exists in the research of quantum oscillators or generalized quadratic Hamiltonians.

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APPENDIX A

DERIVATION OF THE EMAKOV-TYPE SYSTEM

In this derivation, equations (2.17) and (2.26) will be used. Recall that the solution to the generalized Harmonic Oscillator system

$$-i\chi_\tau = -\chi_\xi \xi + c_0 \xi^2 \chi$$

for the case $c_0 = 1$ is given by the exact oscillator wavefunctions (2.17),

$$\psi_n(x, t) = \frac{e^{i(\alpha x^2 + \delta x + \kappa) + 2i(n + \frac{1}{2})\gamma}}{\sqrt{2^n n! \mu(t) \sqrt{\pi}}} H_n(\beta x + \varepsilon) e^{-\frac{1}{2}(\beta x + \varepsilon)^2}. \quad (\text{A.1})$$

The Green's function (free particle propagator) adopted from [21] is given by

$$G(x, y, t) = \frac{1}{\sqrt{2\pi\mu_0}} e^{i(\alpha_0 x^2 + \beta_0 xy + \gamma_0 y^2 + \delta_0 x + \varepsilon_0 y + \kappa_0)},$$

where the time dependent coefficients are the Riccati-type solution functions. Using arbitrary initial data $\psi(y, 0) = \varphi(y)$ it follows that the fundamental solution to the Schrödinger equation is given in generalized form by the Superposition principle (2.17):

$$\psi_n(x, t) = \int_{-\infty}^{\infty} G(x, y, t) \psi_n(y, 0) dy. \quad (\text{A.2})$$

In the resulting equation (A.2), the integral right hand side is evaluated as a *Gaussian Hermite Integral Transform*; it is known already in literature to have an analytically explicit solution on the complex plane and it is expressed as follows

$$\int_{-\infty}^{\infty} e^{\lambda^2(x-y)^2} H_n(ay) dy = \sqrt{\frac{\pi}{\lambda^2}} \left(\frac{\lambda^2 - a^2}{\lambda^2} \right)^{n/2} \times H_n \left(ax \sqrt{\frac{\lambda^2}{\lambda^2 - a^2}} \right).$$

We want to find all the possible solutions by the Superposition principle over the real space $-\infty < x < \infty$. Using the Green's function integral and exact wavefunctions (A.1) we construct a similar Gaussian Hermite-type integral transform

$$\int_{-\infty}^{\infty} e^{Z - \lambda^2(X-Y)^2} H_n(aY) = \frac{\sqrt{\pi}}{\lambda^{n+1}} (\lambda^2 - a^2)^{n/2} H_n \left(\frac{a\lambda X}{\sqrt{\lambda^2 - a^2}} \right), \quad a > 0, a \in \mathbb{R},$$

where again H_n represent the orthogonal Hermite polynomials of degree (or quantum number) $n = 0, 1, 2, 3, \dots$. The following computations demonstrate how the expressions for the time dependent functions $\alpha(t)$, $\beta(t)$, $\gamma(t)$, $\delta(t)$, $\varepsilon(t)$ and $\kappa(t)$ are computed.

To initialize, let us compute the integrand $G(x, y, t) \psi_n(x, 0)$. At some initial time $t_0 = 0$, the states ψ_n are given by

$$\psi_n(x, 0) = \frac{e^{i(\alpha(0)x^2 + \delta(0)x + \kappa(0)) + 2i(n + \frac{1}{2})\gamma(0)}}{\sqrt{2^n n! \mu(0)} \sqrt{\pi}} H_n(\beta(0)x + \varepsilon(0)) e^{-\frac{1}{2}(\beta(0)x + \varepsilon(0))^2}.$$

Substituting this initial data into the right hand side of equation (A.2) shows that

$$\begin{aligned} \psi_n(x, t) &= \frac{1}{\sqrt{2i\pi\mu_0 2^n n! \mu(0)} \sqrt{\pi}} \int_{-\infty}^{\infty} e^{i(\alpha_0 x^2 + \delta_0 x + \kappa_0)} \\ &\times e^{i(\beta_0 x y + \gamma_0 y^2 + \varepsilon_0 y) + i(\alpha(0)y^2 + \delta(0)y + \kappa(0) + 2(n + \frac{1}{2})\gamma(0))} \\ &\times e^{-\frac{1}{2}(\beta(0)y + \varepsilon(0))^2} H_n(\beta(0)y + \varepsilon(0)) dy. \end{aligned}$$

Extracting terms dependent on x (they are treated as constants in the integral), constant and time-dependent terms leaves us with the following relation

$$\begin{aligned} \psi_n(x, t) &= \frac{e^{i(\alpha_0 x^2 + \delta_0 x + \kappa_0 + \kappa(0) + 2(n + \frac{1}{2})\gamma(0))}}{\sqrt{2i\pi\mu_0 2^n n! \mu(0)} \sqrt{\pi}} \int_{-\infty}^{\infty} e^{i(\beta_0 x y + \gamma_0 y^2 + \varepsilon_0 y + \alpha(0)y^2 + \delta(0)y)} \\ &\times e^{-\frac{1}{2}(\beta(0)y + \varepsilon(0))^2} H_n(\beta(0)y + \varepsilon(0)), \end{aligned} \quad (\text{A.3})$$

which is equivalent to the expansion

$$\begin{aligned} \psi_n(x, t) &= \int_{-\infty}^{\infty} e^{Z - \lambda^2(X - Y)^2} H_n(aY) dY = e^Z \int_{-\infty}^{\infty} e^{-\lambda^2(X - Y)^2} H_n(aY) dY \\ &= \frac{e^{i(\alpha_0 x^2 + \delta_0 x + \kappa_0 + \kappa(0) + 2(n + \frac{1}{2})\gamma(0))}}{\sqrt{2i\pi\mu_0 2^n n! \mu(0)} \sqrt{\pi}} e^Z \frac{\sqrt{\pi}}{\lambda^{n+1}} (\lambda^2 + a^2)^{n/2} H_n\left(\frac{a\lambda X}{\sqrt{\lambda^2 - a^2}}\right) dy. \end{aligned}$$

Yet the right hand side

$$\frac{e^{i(\alpha_0 x^2 + \delta_0 x + \kappa_0 + \kappa(0) + 2(n + \frac{1}{2})\gamma(0))}}{\sqrt{2\mu_0 2^n n! \mu(0)} \sqrt{\pi}} \times \frac{e^Z}{\sqrt{i\lambda^{n+1}}} (\lambda^2 + a^2)^{n/2} H_n\left(\frac{a\lambda X}{\sqrt{\lambda^2 - a^2}}\right)$$

can be computed by matching terms with

$$\frac{e^{i(\alpha x^2 + \delta x \kappa + 2(n + \frac{1}{2})\gamma)}}{\sqrt{2^n n! \mu} \sqrt{\pi}} e^{-\frac{1}{2}(\beta x + \varepsilon)^2} H_n(\beta x + \varepsilon)$$

whenever

$$\lambda^2 = \frac{1}{2}\beta^2(0) - i(\gamma_0 + \alpha(0)) \quad (\text{A.4})$$

$$X = i \frac{\beta_0 x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\gamma_0 + \alpha(0))}{2\lambda^2} \quad (\text{A.5})$$

$$Z = \lambda^2 X^2 + \frac{\varepsilon^2(0)}{\beta^2(0)}(\gamma_0 + \alpha(0)) - i \frac{\varepsilon(0)}{\beta(0)}(\beta_0 x + \varepsilon_0 + \delta(0)). \quad (\text{A.6})$$

Derivation of equations (A.4)-(A.6)

Notice that the Hermite polynomial expression $H_n(\beta(0)y + \varepsilon(0)) = H_n\left(\beta(0)\left(y + \frac{\varepsilon(0)}{\beta(0)}\right)\right)$, and one can compute a , and Y such that $aY = \beta(0)\left(y + \frac{\varepsilon(0)}{\beta(0)}\right)$. Thus one can see that $y = Y - \frac{\varepsilon(0)}{\beta(0)}$, and $a = \beta(0) \neq 0$. Introducing these relations into the expression $i(\beta_0xy + \varepsilon_0y + \alpha(0)y^2 + \gamma_0y^2 + \delta(0)y) - \frac{1}{2}(\beta(0)y + \varepsilon(0))^2$ which comes from the exponential constant terms of the wavefunctions (A.3), allows us to obtain another quadratic relation in Y , that is

$$\begin{aligned} \left(i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)\right)Y^2 + i\left(\beta_0x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\gamma_0 + \alpha(0))\right)Y \\ - i\frac{\varepsilon(0)}{\beta(0)}(\beta_0x + \varepsilon_0 + \delta(0)) + \frac{\varepsilon^2(0)}{\beta^2(0)}(\gamma_0 + \alpha(0)) \end{aligned} \quad (\text{A.7})$$

that is equivalent to the exponential expression $Z - \lambda^2(X - Y)^2 = Z - \lambda^2(Y - X)^2$ for some elementary functions X , λ and Z obtained explicitly by completion of the square in the integral. We proceed by rewriting equation (A.7) as

$$\begin{aligned} Y^2 + i\left(\frac{\beta_0x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\gamma_0 + \alpha(0))}{i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)}\right)Y - \frac{i\frac{\varepsilon(0)}{\beta(0)}(\beta_0x + \varepsilon_0 + \delta(0))}{i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)} \\ - \frac{i\frac{\varepsilon^2(0)}{\beta^2(0)}(\gamma_0 + \alpha(0))}{i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)}. \end{aligned}$$

By completing the square then,

$$\begin{aligned} Z - \lambda^2(Y - X)^2 &= \left(i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)\right) \\ &\times \left(Y + \frac{i\beta_0x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\gamma_0 + \alpha(0))}{i(\gamma_0 + \alpha(0)) - \frac{1}{2}\beta^2(0)}\right)^2 \\ &+ i\frac{\beta_0x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\gamma_0 + \alpha(0))}{4i(\gamma_0 + \alpha(0)) - 2\beta^2(0)} - i\frac{\varepsilon(0)}{\beta(0)}(\beta_0x + \varepsilon_0 + \delta(0)) \\ &+ \frac{\varepsilon^2(0)}{\beta^2(0)}(\gamma_0 + \alpha(0)). \end{aligned}$$

Thus,

$$\begin{aligned}\lambda^2 &= \frac{1}{2}\beta^2(0) - i(\gamma_0 + \alpha(0)), \\ X &= i \frac{\beta_0 x + \varepsilon_0 + \delta(0) - 2 \frac{\varepsilon(0)}{\beta(0)} (\gamma_0 + \alpha(0))}{2\lambda^2}, \\ Z &= \lambda^2 X^2 + \frac{\varepsilon^2(0)}{\beta^2(0)} (\gamma_0 + \alpha(0)) - i \frac{\varepsilon(0)}{\beta(0)} (\beta_0 x + \varepsilon_0 + \delta(0)).\end{aligned}$$

Derivation of solutions μ , $\beta(t)$, $\gamma(t)$ and $\varepsilon(t)$

Because the solution to the Schrödinger equation is complex valued, it is necessary to define a positive complex number as $\zeta = \frac{1}{2}\beta^2(0) + i(\gamma_0 + \alpha(0))$, where $\frac{1}{2}\beta^2(0) \in \mathbb{R}$, and $\frac{1}{2}\beta^2(0) \geq 0$. One can represent ζ in Polar form $\zeta = |\zeta| (\cos \varphi + i \sin \varphi)$, however, the Euler form $\zeta = |\zeta| e^{i\varphi + 2\pi ik}$ where $k \in \mathbb{W}$, is preferred, where $|\zeta| = \zeta^* \zeta$ is the complex modulus (a positive quantity), and φ is the usual Argument (the phase angle) of ζ . This suggests that $|\zeta| = \frac{1}{4}\beta^4(0) + (\gamma_0 + \alpha(0))^2$, so in complex Euler form we define $\zeta = \lambda^2 = |\zeta| e^{i\varphi + 2\pi ik}$. Consequently, using the ground value $k = 0$, we obtain

$$\lambda^2 = \frac{1}{2}\beta^2(0) - i(\alpha(0) + \gamma_0).$$

One can observe due to the positiveness of ζ , the useful relationship

$$\varphi = \arctan \left(2 \cdot \frac{\alpha(0) - \gamma_0}{\beta^2(0)} \right).$$

With the elementary definition $\perp_x + \varphi + (\frac{\pi}{2} - \varphi) = 180^\circ$, one can deduce the most useful relation to our calculations:

$$\varphi - \frac{\pi}{2} = -\arctan \left(\frac{1}{2} \cdot \frac{\beta^2(0)}{\gamma_0 + \alpha(0)} \right).$$

Hence using all these defined quantities, trigonometric identities, and by choosing the negative branch $-\sqrt{\lambda^2 - a^2}$ in the integral solution, one obtains a simplified expression for the constant terms in the Hermite integral transform as

$$\frac{1}{\lambda^{n+1}} (\lambda^2 - a^2)^{n/2} = \frac{1}{|\zeta|^{1/2}} e^{i(\varphi - \frac{\pi}{2}) \cdot (n + \frac{1}{2})}.$$

Therefore, from this we are able to derive the Ermakov-type system solution to the differential equation for $\frac{d\gamma}{dt}$:

$$\gamma(t) = \gamma(0) - \frac{\pi}{4} + \frac{1}{2} \arctan \left(2 \cdot \frac{\alpha(0) + \gamma_0}{\beta^2(0)} \right).$$

With the already defined expressions for X , λ^2 and Z (found by substituting y into the integrand and completing the square in the exponential terms), one can find the time dependent function coefficients $\beta(t)$ and $\varepsilon(t)$ by matching argument terms in the Hermite polynomial from both sides of the integral relations. We have defined a complex number $\lambda^2 = \frac{1}{2}\beta^2(0) - i(\alpha(0) + \gamma_0) = \zeta^*$ as the complex conjugate of ζ . By definition, an improper complex number in the fractional form $\frac{a+ib}{a-ib} = \frac{z}{z^*}$ can be reduced to the proper complex form $c + id$ if the algebraic operation $c + id = \frac{z}{z^*} \cdot \frac{z}{z}$ is performed. These operations yield that $c + id = \frac{a^2-b^2}{a^2+b^2} + i \frac{2ab}{a^2+b^2}$ where $a, b \in \mathbb{R}$ and $|z|^2 = z^*z = a^2 + b^2$. Keeping these elementary rules on hand, one can express Z as a proper complex number, and this results in the quantity

$$Z = - \frac{\left(\frac{1}{2}\beta^2(0) + i(\alpha(0) + \gamma_0)\right) \left(\beta_0 x + \varepsilon_0 + \delta(0) - 2 \frac{\varepsilon(0)}{\beta(0)} (\alpha(0) + \gamma_0)\right)^2}{4(\alpha(0) + \gamma_0)^2 + \beta^4(0)}.$$

Thus, the Hermite polynomial argument,

$$\frac{a\lambda X}{\sqrt{\lambda^2 - a^2}} = - \frac{\beta(0) \beta_0 x + \varepsilon_0 + \delta(0) - 2 \frac{\varepsilon(0)}{\beta(0)} (\alpha(0) + \gamma_0)}{2 \sqrt{\frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2}},$$

where

$$|z| = \frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2,$$

implies that

$$\beta(t) = - \frac{\beta(0)\beta_0}{2\sqrt{\frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2}},$$

and

$$\varepsilon(t) = - \frac{\beta(0)(\delta(0) + \varepsilon_0)}{\sqrt{\frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2}} + \frac{\varepsilon(0)(\alpha(0) + \gamma_0)}{\sqrt{\frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2}}.$$

These calculations culminate the search for $\beta(t)$ and $\varepsilon(t)$.

Finally, from the relationship

$$\begin{aligned} & \frac{e^{-\frac{1}{2}(\beta x + \varepsilon)^2}}{\sqrt{2^n n! \mu(t) \sqrt{\pi}}} e^{i(\alpha x^2 + \delta x + \kappa + 2(n + \frac{1}{2})\gamma)} H_n(\beta x + \varepsilon) \\ &= \frac{e^{i(\alpha_0 x^2 + \delta_0 x + \kappa_0 + \kappa(0) + 2(n + \frac{1}{2})\gamma(0))}}{\sqrt{2\mu_0 2^n n! \mu(0)}} \frac{1}{|z|^{1/2}} e^{i(\varphi - \frac{\pi}{2})(n + \frac{1}{2})} \\ & \times H_n \left(-\frac{\beta(0) \left(\beta_0 x + \varepsilon_0 + \delta(0) - 2\frac{\varepsilon(0)}{\beta(0)}(\alpha(0) + \gamma_0) \right)}{2\sqrt{\frac{1}{4}\beta^4(0) + (\alpha(0) + \gamma_0)^2}} \right) \end{aligned}$$

we notice that

$$\frac{1}{\sqrt{2\mu_0 2^n n! \mu(0)}} = \frac{|z|^{1/2}}{\sqrt{2^n n! \mu \sqrt{\pi}}}$$

hold in equality if

$$\mu(t) = 2\mu(0)\mu_0 \left(\frac{\beta^4(0)}{4} + (\alpha(0) + \gamma_0)^2 \right).$$

This concludes the search for the solution $\mu(t)$. The use of Mathematica is used to verify that these calculations are correct, and the remaining calculations are tedious and left to the interested reader. The mathematica notebooks for the symbolic derivations are also found in <http://hahn.la.asu.edu/~suslov/>.

APPENDIX B

DERIVATIONS FROM EHRENFEST'S THEOREM

B.1 Review of the Theory

Ehrenfest's theorems shows that the motion of a wave packet agrees with the motion of a particle in classical mechanics if the *position* and *momentum* vectors of the wave packet are taken to denote the weighted average or expectation values of these quantities. It can be shown that the time rate of change of the expectation value of the position coordinate x corresponds to the velocity of the particle [29]. Dynamical variables are real quantities that are measurable and so they are represented by Hermitian operators which yield real eigenvalues. Since the wave function yields only the probability distribution, one can obtain only a probability distribution for the dynamical variable. Ehrenfest theorems deal with expectation values, and the formal definition follows.

Definition *Given a quantum mechanical Hermitian operator A (a random dynamical variable), its mean or expectation value is defined by*

$$\langle A \rangle = \int \psi^* A \psi d\mathbf{r} \quad (\text{B.1})$$

if ψ is normalized ($\int \psi^*(\mathbf{r},t)\psi(\mathbf{r},t) d\mathbf{r} = 1$). Otherwise,

$$\langle A \rangle = \frac{\int \psi^* A \psi d\mathbf{r}}{\int \psi^*(\mathbf{r},t)\psi(\mathbf{r},t) d\mathbf{r}}. \quad (\text{B.2})$$

The reduction of quantum mechanical dynamics to the classical trajectories is known as the Ehrenfest's theorems. It only holds for expectation values (averages of the measurements) and not the eigenvalues themselves. Mathematically, they relate the time derivative of an expectation value for a quantum mechanical operator to the commutator of that operator with the Hamiltonian of the system by the equation

$$\frac{d}{dt}\langle A \rangle = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i\hbar}\langle AH - H^\dagger A \rangle,$$

where A is some quantum mechanical operator, and $\langle A \rangle$ is its expectation value. The symbol \dagger represents the Hermiticity of the Hamiltonian.

In classical mechanics we know that $(\text{mass}) \times (\text{velocity}) = (\text{momentum})$, which translates to the quantum result

$$m \frac{d}{dt} \langle x \rangle = \int_{\mathbb{R}} \psi^* p \psi dx = \langle p \rangle \quad (\text{B.3})$$

whenever ψ satisfies the Schrödinger equation. Equation (B.3) reads that $(\text{mass}) \times (\text{average of velocity}) = (\text{average of momentum})$ in quantum mechanics. Inversely one might understand that this result justifies the definition of the momentum in quantum mechanics, (that is $p = -i\hbar \frac{\partial}{\partial x}$). Observe that the second differentiation with respect to t of the equation for average momentum, gives the second Ehrenfest's theorem

$$m \frac{d^2}{dt^2} \langle x \rangle = \int_{\mathbb{R}} \psi^* \left(-\frac{dV}{dx} \right) \psi dx = \langle F \rangle. \quad (\text{B.4})$$

Equation (B.4) confirms the wave packet description of the particle for which the rate of change of momentum corresponds to the negative gradient of the potential, which is equal to the impressed force acting on the particle. Therefore, the wave packet description reproduces Newton's second law of motion in the form of averages. This is just the same form as that of Newtonian equation of motion $m\ddot{x} = F$. In this sense, we can say that quantum mechanics involves the classical mechanics. Hence, Equations (B.4) and (B.3) are known as Ehrenfest theorem, which give a correspondence between the wave packet formalism and the classical dynamics describing particle motion. The averages of the measurements are equivalent to the physical quantities describing the motion of a real particle.

B.2 Classical Parametric Oscillator Derivation via Ehrenfest's Theorems

Here we propose a new transformation to derive Ehrenfest's Theorems—a bridge from quantum to classical mechanics—for the time-dependent Schrödinger equation with a quadratic Hamiltonian. Consider the following assumption or claim.

Claim: *Using a change of variables from Lemma 2.2.1, the transformation of expec-*

tation values

$$\bar{\xi} = \beta(t)\bar{x} + \varepsilon(t), \quad \bar{\xi} = \langle \xi \rangle = \int_{\mathbb{R}} |\chi|^2 d\xi,$$

reduces the parametric classical equation of motion (Ehrenfest's Theorems)

$$\frac{d^2\bar{x}}{dt^2} - \frac{a'}{a} \frac{d\bar{x}}{dt} + \left(4ab - c^2 + c \frac{a'}{a} - c'\right) \bar{x} = 2af - g' + g \frac{a'}{a} - cg$$

into

$$\frac{d^2\bar{\xi}}{d\tau^2} + 4c_0\bar{\xi} = 0, \quad c_0 \in \{0, 1\}$$

which is another version of the free particle and harmonic oscillator map.

The free particle case is solved in terms of solutions of a Riccati-type system ($c_0 = 0$) and if $c_0 = 1$, the linear harmonic oscillator is solved via the solutions to an Ermakov-type system. Recall, the master evolution equation is given by

$$i \frac{\partial}{\partial t} \psi = -a(t) \frac{\partial^2 \psi}{\partial x^2} + bx^2 \psi - c(t)x \frac{\partial \psi}{\partial x} - id(t)\psi - f(t)x\psi + ig(t) \frac{\partial \psi}{\partial x}.$$

In the derivation of Ehrenfest's theorems, we need to use the following commutation relations from the Schrödinger Lie Algebra sets [4] (with $\hbar = 1$):

$$\begin{aligned} [x, p] &= i, & [x, p^2] &= 2ip, & [x^2, p] &= 2ix, \\ [x^2, p^2] &= 2i(px + xp), & [px + xp, p^2] &= 4ip^2, & [x^2, px + xp] &= 4ix^2 \end{aligned}$$

along with the Hermitian transpose definitions for two operators (or matrices), \widehat{X} , \widehat{P} , $(\widehat{X}\widehat{P})^\dagger = \widehat{P}^\dagger\widehat{X}^\dagger$, and $(\widehat{X}^\dagger)^\dagger = \widehat{X}$, $\widehat{X}^\dagger = \widehat{X}$, etc. Introducing some randomly selected quantum mechanical position and momentum operators, with $\hbar = 1$, we calculate that

$$\frac{d}{dt} \langle x \rangle = \left\langle \frac{\partial x}{\partial t} \right\rangle + \frac{1}{i} \langle xH - H^\dagger x \rangle,$$

and

$$\frac{d}{dt} \langle p \rangle = \left\langle \frac{\partial p}{\partial t} \right\rangle + \frac{1}{i} \langle pH - H^\dagger p \rangle.$$

Taking the Hermitian transpose of the Hamiltonian only transforms the quantities $(px)^\dagger \rightarrow xp$, and $(xp)^\dagger \rightarrow px$. The remaining terms in the master equation remain invariant. Notice in addition that $\langle \partial_t x \rangle$, $\langle \partial_t p \rangle$ vanish. Now using the lie algebra commutation relations yields the following

$$xH - H^\dagger x = a[x, p^2] + d[x^2, p] + f[x, p] = 2iap + 2idx + if.$$

Because *bras* and *kets* are linear functionals, and since the expectation value of a linear combination of two random operators is the linear combination of two random operators, the expectation value of the previous equation is

$$\frac{d}{dt}\langle x \rangle = \frac{1}{i}\langle xH - H^\dagger x \rangle = 2a\langle p \rangle + 2d\langle x \rangle + f\langle 1 \rangle.$$

In a similar fashion we calculate that

$$\frac{d}{dt}\langle p \rangle = \frac{1}{i}\langle pH - H^\dagger p \rangle = -2b\langle x \rangle - 2c\langle p \rangle - g\langle 1 \rangle.$$

In short,

$$\frac{d}{dt}\langle x \rangle = 2a\langle p \rangle + 2d\langle x \rangle + f\langle 1 \rangle, \quad \frac{d}{dt}\langle p \rangle = -2b\langle x \rangle - 2c\langle p \rangle - g\langle 1 \rangle.$$

Since $\langle 1 \rangle$ is the unit operator, we also calculate its instantaneous rate of change, which is the simple expression

$$\frac{d}{dt}\langle 1 \rangle = (d - c)\langle 1 \rangle. \tag{B.5}$$

At this point we introduce the relations

$$\bar{x} = \frac{\langle x \rangle}{\langle 1 \rangle}, \quad \text{and} \quad \bar{p} = \frac{\langle p \rangle}{\langle 1 \rangle}. \tag{B.6}$$

Differentiating equations (B.6), and using (B.5) brings us to the following set of equations:

$$\frac{1}{\langle 1 \rangle} \frac{d}{dt}\langle x \rangle = \frac{d}{dt}\bar{x} + (d - c)\bar{x} \tag{B.7}$$

$$\frac{1}{\langle 1 \rangle} \frac{d}{dt}\langle p \rangle = \frac{d}{dt}\bar{p} + (d - c)\bar{p}. \tag{B.8}$$

From (B.7-B.8), utilizing the relations (B.5) we derive *symmetry relations* for the time derivatives of \bar{x} and \bar{p} , and as a result,

$$\frac{d}{dt}\bar{x} = 2a\bar{p} + (c+d)\bar{x} + f \quad (\text{B.9})$$

$$\frac{d}{dt}\bar{p} = -2b\bar{x} - (c+d)\bar{p} + g. \quad (\text{B.10})$$

Here these represent the average rates of change of change in \bar{x} , \bar{p} . We proceed to derive Newton's second law of motion for the generalized (driven) harmonic oscillators.

Taking an extra derivative of the equations (B.9-B.10) gives us

$$\frac{d^2\bar{x}}{dt^2} = 2a'\bar{p} + 2a\frac{d\bar{p}}{dt} + (c' + d')\bar{x} + (c+d)\frac{d\bar{x}}{dt} + f'. \quad (\text{B.11})$$

Equation (B.9) can be expressed as

$$\bar{p} = \frac{\frac{d\bar{x}}{dt} - (c+d)\bar{x} - f}{2a}, \quad (\text{B.12})$$

so combining (B.12) along with (B.10) we get the parametric, classical equation of motion of \bar{x} . It is given by

$$\begin{aligned} \frac{d^2\bar{x}}{dt^2} - \frac{a'}{a} + \frac{d\bar{x}}{dt} + \left(4ab + \left(\frac{a'}{a} - c - d\right)(c+d) - c' - d'\right)\bar{x} \\ = f' - \left(\frac{a'}{a} - c - d\right)f - 2ag. \end{aligned} \quad (\text{B.13})$$

Following similar steps to find the equation of motion (B.13), we derive Ehrenfest's evolution equation of momentum \bar{p} :

$$\begin{aligned} \frac{d^2\bar{p}}{dt^2} - \frac{b'}{b} + \frac{d\bar{p}}{dt} + \left(4ab + \left(\frac{b'}{b} + c + d\right)(c+d) + c' + d'\right)\bar{p} \\ = -g' + \left(\frac{b'}{b} + c + d\right)g - 2bf. \end{aligned}$$

In both relations, the time dependent coefficients a, b, c, d, f, g satisfy the Riccati-type system.

Direct substitution approach for the free particle

The free particle equation $i\chi_\tau = \chi_\xi\xi$, for $c_0 = 0$ obtained by transformation, is considered. The expectation value of the new variable $\bar{\xi} = \langle \xi \rangle$ according to our previous lemma 2.2.1, should be defined as

$$\bar{\xi} = \langle \beta(t)x + \varepsilon(t) \rangle.$$

The original time t is now treated as a constant in this new transformation and this means $\frac{\partial^2 \bar{\xi}}{\partial \tau^2} = 0$. The definition of an expectation value for the new change of variables $\xi = \beta(t)x + \varepsilon(t)$ and $\tau = \gamma(t)$ is given by

$$\langle \xi \rangle = \int_{\mathbb{R}} |\chi|^2 \xi d\xi, \quad (\text{B.14})$$

where $\chi = \sqrt{\mu}\psi e^{-iS}$. Thus equation (B.14) becomes

$$\langle \xi \rangle = \int_{\mathbb{R}} \mu |\psi|^2 (\beta x + \varepsilon) \beta dx = \mu \beta (\beta \langle x \rangle + \varepsilon \langle 1 \rangle).$$

However, more generally if we compute

$$\frac{\langle \xi \rangle}{\langle 1 \rangle} = \frac{\mu \beta}{\langle 1 \rangle^{-1}} \left(\beta \frac{\langle x \rangle}{\langle 1 \rangle} + \varepsilon \right),$$

the resulting relation is

$$\begin{aligned} \bar{\xi} &= \beta \mu \langle 1 \rangle (\beta \bar{x} + \varepsilon) \\ &= \beta(0) \mu(0) \lambda \langle 1 \rangle (\beta \bar{x} + \varepsilon) \\ &= \beta(0) \mu(0) \langle 1 \rangle_0 (\beta \bar{x} + \varepsilon). \end{aligned}$$

Choosing $\beta(0)\mu(0)\langle 1 \rangle_0 = 1$, we demonstrate a more direct, alternate derivation of Ehrenfest's Theorems. For computational purposes in this derivation, we choose to rename $\bar{x} \rightarrow x$ and $\bar{\xi} \rightarrow \xi$. By directly substituting Riccati-type system equations we derive first the free-particle expectation relation. Since

$$\frac{d\xi}{dt} = \frac{d\xi}{d\tau} \frac{d\tau}{dt}, \quad \frac{d\tau}{dt} = \gamma' = -a\beta^2, \quad (\text{B.15})$$

the left hand side of (B.15) implies

$$\frac{d}{dt}(\beta x + \varepsilon) = \beta' x + \beta \frac{dx}{dt} + \varepsilon';$$

Equation (B.15) also gives us

$$-a\beta \frac{d\xi}{d\tau} = -(c + 4a\alpha)x + \frac{dx}{dt} + g - 2a\delta. \quad (\text{B.16})$$

A second differentiation of (B.15) and using the definition of the case $c_0 = 0$ yields

$$\frac{d}{dt}(-a\beta) \frac{d\xi}{d\tau} + (-a\beta) \frac{d^2\xi}{d\tau^2} \frac{d\tau}{dt} = -(c + 4a\alpha) \frac{dx}{dt} + \frac{d^2x}{dt^2} + (g - 2a\delta)'. \quad (\text{B.17})$$

Using a mathematical trick, we reduce equation (B.19) into

$$-\frac{(a\beta)'}{a\beta} \left(a\beta \frac{d\xi}{d\tau} \right) = \frac{dx^2}{dt^2} - (c + 4a\alpha) \frac{dx}{dt} - (c' + 4a'\alpha + 4a\alpha')x + g' - 2a'\delta - 2a\delta'.$$

Now we invoke equations α' , β' and α' in the Riccati-type system to eliminate the derivatives as follows.

$$\begin{aligned} & \left(\frac{a'}{a} - c - 4a\alpha \right) \frac{dx}{dt} + \left(\frac{a'}{a} - c - 4a\alpha \right) (-(c + 4a\alpha)x + g - 2a\delta) \\ & = \frac{d^2x}{dt^2} - (c + 4a\alpha) \frac{dx}{dt} - (c' + 4a'\alpha + 4a\alpha')x \\ & \quad + g' - 2a'\delta + 2a(c + 4a\alpha)\delta - 2af - 4ag\alpha, \\ & -\frac{d^2x}{dt^2} + \frac{a'}{a} \frac{dx}{dt} - \frac{a'}{a} (c + 4a\alpha)x + \frac{a'}{a} g + (c + 4a\alpha)^2 x - (c + 4a\alpha)(g - 2a\delta) \\ & = -x(c' + 4a'\alpha + 4a(-b - 2c\alpha - 4a\alpha^2)) \\ & \quad + g' + 2ac\delta + \delta a^2 \alpha \delta - 2af - 4ag\alpha. \end{aligned}$$

After cancellations, and grouping terms in order, we derive again the parametric classical equation of motion,

$$\frac{d^2\bar{x}}{dt^2} - \frac{a'}{a} \frac{d\bar{x}}{dt} + \left(\frac{a'}{a} c - c^2 - c' + 4ab \right) \bar{x} = 2af - g' + \frac{a'}{a} g - cg, \quad (\text{B.18})$$

where $\frac{d^2\bar{\xi}}{d\tau^2} = 0$. Finally, we will link the classical equation of motion to Lemma 2.2.1 of the classical equation of the Simple Harmonic Oscillator using the Ermakov-type equations (the case $c_0 = 0$).

Direct substitution approach for the harmonic oscillator

In this section we use the Ermakov-type system to derive a relation that maps the free particle to Harmonic Oscillator, and vice versa. That is, we transform the classical equation of motion given by

$$\frac{d^2\bar{x}}{dt^2} - \frac{a'}{a} \frac{d\bar{x}}{dt} + \left(\frac{a'}{a}c - c^2 - c' + 4ab \right) \bar{x} = 2af - g' + \frac{a'}{a}g - cg,$$

into the following classical equation for harmonic or free particle motion

$$\frac{d^2\bar{\xi}}{d\tau^2} + 4c_0\bar{\xi} = 0, \quad c_0 = \{0, 1\}.$$

Proof We substitute the Ermakov-type equations

$$\begin{aligned} \delta' &= f + 2g\alpha + 2c_0a\beta^3\varepsilon - (c + 4a\alpha)\delta, \\ \alpha' + b + 2c\alpha + 4a\alpha^2 &= c_0a\beta^4, \end{aligned}$$

into

$$\frac{d}{dt}(-a\beta) \frac{d\xi}{d\tau} + (-a\beta) \frac{d^2\xi}{d\tau^2} \frac{d\tau}{dt} = -(c + 4a\alpha) \frac{dx}{dt} + \frac{d^2x}{dt^2} + (g - 2a\delta)'. \quad (\text{B.19})$$

Computing derivatives and manipulating algebraically gives

$$\begin{aligned} a^2\beta^3 \frac{d^2\xi}{d\tau^2} &= \frac{d^2}{dt^2} - (c + 4a\alpha) \frac{dx}{dt} - g' - 2a'\delta - 2a\delta' - (c' + (4a\alpha)')x \\ &\quad - \left(-a\beta \frac{d\xi}{d\tau} \right) \left(\frac{a'}{a} + \frac{\beta'}{\beta} \right), \end{aligned}$$

$$\begin{aligned} a^2\beta^3 \frac{d^2\xi}{d\tau^2} &= \frac{d^2x}{dt^2} - \frac{a'}{a} \frac{dx}{dt} + \left(\frac{a'}{a}c + 4a'\alpha - (c + 4a\alpha)^2 - c' - (4a\alpha)' \right) x \\ &\quad - \frac{a'}{a}g + (c + 4a\alpha)g - 2a\delta(c + 4a\alpha) - g' - 2a\delta', \end{aligned}$$

$$\begin{aligned} a^2\beta^3 \frac{d^2\xi}{d\tau^2} &= \frac{d^2x}{dt^2} - \frac{a'}{a} \frac{dx}{dt} + \left(44ab - \frac{a'}{a}c - c' - c^2 \right) x \\ &\quad - 4c_0a^2\beta^4x - 4a^2c_0\beta^3\varepsilon - \frac{a'}{a}g + cg - g' - 2af \end{aligned}$$

This finally reduces to our goal

$$\frac{d^2\xi}{d\tau^2} + 4c_0\xi = 0, \quad c_0 = \{0, 1\} \quad \square$$

An example: the united model

We have derived parametric classical equations of motion for the position and momentum operators. An example can be derived using the Hamiltonian in the article [23], Ann Phys. p. 1888. The non-self adjoint Hamiltonian (where λ and μ are constant),

$$H = \frac{\omega_0}{2} \left(e^{-2\lambda t} p^2 + e^{2\lambda t} x^2 \right) - \mu x p, \quad (\text{B.20})$$

coincides with the original Caldirola-Kanai model when $\mu = 0$ and the Hamiltonian is self-adjoint. Another special case $\lambda = 0$ corresponds to the quantum damped oscillator discussed in [22] as an example of a simple quantum system with the non-self-adjoint Hamiltonian. (This is an alternative way to introduce dissipation of energy to the quantum harmonic oscillator.) Combining both cases we refer to (B.20) as the united Hamiltonian. The variable coefficients are

$$a = \frac{\omega_0}{2} e^{-2\lambda t}, \quad b = \frac{\omega_0}{2} e^{2\lambda t}, \quad c = 0$$

$$d = -\mu, \quad f = g = 0.$$

We derive Ehrenfest's theorem for the united model by computing the coefficient of \bar{x}' and \bar{x} . Given the values above, calculating these coefficients give us

$$\frac{d'}{a} = -2\lambda$$

$$4ab + \left(\frac{d'}{a} - c - d \right) (c + d) - c' - d' = \omega_0^2 - \mu(\mu - 2\lambda)$$

which will give us Ehrenfest theorem for the united model:

$$\bar{x}'' + 2\lambda \bar{x}' + (\omega_0^2 + \mu(2\lambda - \mu)) \bar{x} = 0.$$

The characteristic equation is

$$\Gamma^2 + 2\lambda \Gamma + (\omega_0^2 + \mu(2\lambda - \mu)) = 0,$$

where the roots are the following complex quantities,

$$\Gamma_{1,2} = -\lambda \pm \sqrt{-\omega_0^2 + (\mu - \lambda)^2}$$

$$= -\lambda \pm i\sqrt{\omega_0^2 + (\lambda - \mu)^2}.$$

Therefore, we find an explicit general solution

$$\bar{x} = e^{-\lambda t} (c_1 \cos \omega t + c_2 \sin \omega t), \quad \omega = \sqrt{\omega_0^2 + (\lambda - \mu)^2},$$

best represented by

$$\bar{x} = A e^{-\lambda t} \sin(\omega t + \delta), \quad \omega = \sqrt{\omega_0^2 + (\lambda - \mu)^2}.$$

APPENDIX C

HEISENBERG REPRESENTATION

C.1 Time Dependence of Creation and Annihilation Operators

Until now, the time dependence of an evolving quantum system (with $\hbar = 1$) like

$$H\psi(t) = i\frac{\partial}{\partial t}\psi(t) \quad (\text{C.1})$$

has been placed within the wavefunction while the operators have remained constant—this is the Schrödinger picture or representation. However, it is sometimes useful to transfer the time-dependence to the operators. This alternative approach in which operators take on time-dependence and wavefunctions become time-independent is called the *Heisenberg Representation*. Note, meanwhile, that equation (C.1) can be also represented as

$$\psi(t) = e^{-iHt}\psi(0). \quad (\text{C.2})$$

This result (C.2) suggests a new viewpoint. Because in quantum mechanics we want to predict outcome of experiments, we will be interested in calculating expectation values or mean value of the measurement of a time-dependent operator. To see how to transfer time dependence, consider the expectation value of some operator A , defined as

$$\langle A \rangle = \langle \psi | A | \psi \rangle = \int \psi^* A \psi dt. \quad (\text{C.3})$$

According to rules of associativity, we can multiply operators together before using them. Thus, the definition (C.3) is equivalent to

$$\begin{aligned} \langle A \rangle &= \int e^{iHt}\psi(0)Ae^{-iHt}\psi(0) dt \\ &= \int \psi(0)e^{iHt}Ae^{-iHt}\psi(0) dt \\ &= \int \psi(0)\hat{A}\psi(0) dt. \end{aligned}$$

If the relation (C.2) is defined by the operator

$$\hat{A}(t) = e^{iHt}Ae^{-iHt}, \quad (\text{C.4})$$

the time-dependence of the expectation values has been transferred from the wave function. In this Heisenberg picture or representation, the operators evolve with time while

the wave functions remain constant. Furthermore, the time derivative of the operator itself is given by

$$\begin{aligned}
\frac{\partial}{\partial t}\hat{A}(t) &= iHe^{iHt}\hat{A}e^{-iHt} + e^{iHt}\hat{A}(-iH)e^{-iHt} \\
&= ie^{iHt}(H\hat{A} - \hat{A}H)e^{-iHt} \\
&= ie^{iHt}[H, \hat{A}]e^{-iHt} \\
&= i[H, \hat{A}(t)].
\end{aligned}$$

Sometimes it is useful to know the time dependence of commutation relations \hat{a} , \hat{a}^\dagger for the Harmonic oscillator. In the Heisenberg representation the time development is given by equation (C.4), where \hat{A} is an operator such as \hat{a} or \hat{a}^\dagger . Time dependence for any operator \hat{a} becomes

$$\frac{d}{dt}\hat{a}(t) = i[H, \hat{a}(t)]. \tag{C.5}$$

In summary, the canonical equation for time dependence of an operator, like creation and annihilation, is given by

$$\frac{\partial}{\partial t}\hat{A}(t) - \frac{i}{\hbar}[H(t), \hat{A}(t)] = 0.$$

This relation is also the formal definition of an *invariant*, with $H(t)$ the Hamiltonian of the system. (These time dependence of operators has the most importance in the area of quantum field theory.)

APPENDIX D

MATHEMATICA SOURCE CODE

The following animation lines are for the ground state $n = 0$:

```

output = Animate [ Plot [ {  $\frac{9\sqrt{2} e^{-\frac{72(x-\sin[\frac{1}{500}\pi(-1+T)])^2}}{97+65\cos[\frac{1}{250}\pi(-1+T)]}}{\sqrt{97+65\cos[\frac{1}{250}\pi(-1+T)]}}$ ,  $e^{-\frac{4x^2}{9}}$  },
    { x, -3.5, 3.5 }, AxesLabel -> { x, (Abs[ψ])^2 },
    PlotRange -> {0, 2.3}, Filling -> {1 -> Bottom},
    PlotStyle -> {Blue, Red} ], {T, 1001}, AnimationRate -> 100 ];

```

(* These will output a .avi and .mov file. However, they will contain the frame controls from Animate. You can control the AnimationRate by adjusting the parameter. *)

```
Export["groundstate_s.mov", output];
```

groundstate_s.mov

```

output2 = Table [ Plot [ {  $\frac{9\sqrt{2} e^{-\frac{72(x-\sin[\frac{1}{500}\pi(-1+T)])^2}}{97+65\cos[\frac{1}{250}\pi(-1+T)]}}{\sqrt{97+65\cos[\frac{1}{250}\pi(-1+T)]}}$ ,  $e^{-\frac{4x^2}{9}}$  }, { x, -3.5, 3.5 },
    AxesLabel -> { x, (Abs[ψ])^2 }, PlotRange -> {0, 2.3}, Filling -> {1 -> Bottom},
    PlotStyle -> {Blue, Red} ], {T, 0, 1001, 10} ];

```

(* These are a frameless version. You can control the smoothness of the animation by adjusting the step size in the T loop *)

```
Export["groundstate_f.mov", output2];
```

The second animation lines correspond to the first excited state $n = 1$:

`output =`

```

Animate [Plot [ {  $\frac{1296 \sqrt{2} e^{-\frac{72 \left( x - \sin \left[ \frac{1}{500} \pi (-1+T) \right] \right)^2}}{97+65 \cos \left[ \frac{1}{250} \pi (-1+T) \right]} \left( x - \sin \left[ \frac{1}{500} \pi (-1+T) \right] \right)^2}{\left( 97 + 65 \cos \left[ \frac{1}{250} \pi (-1+T) \right] \right)^{3/2}}$ ,
 $\frac{8}{9} e^{-\frac{4x^2}{9}} x^2$  }, {x, -4.5, 4.5}, AxesLabel -> {x, (Abs[ψ])^2},
PlotRange -> {0, 1.67}, Filling -> {1 -> Bottom}, PlotStyle -> {Blue, Red}],
{T, 1001}, AnimationRate -> 100 ];

```

```
Export["firstexcitedstate_s.mov", output];
```

`output2 =`

```

Table [Plot [ {  $\frac{1296 \sqrt{2} e^{-\frac{72 \left( x - \sin \left[ \frac{1}{500} \pi (-1+T) \right] \right)^2}}{97+65 \cos \left[ \frac{1}{250} \pi (-1+T) \right]} \left( x - \sin \left[ \frac{1}{500} \pi (-1+T) \right] \right)^2}{\left( 97 + 65 \cos \left[ \frac{1}{250} \pi (-1+T) \right] \right)^{3/2}}$ ,
 $\frac{8}{9} e^{-\frac{4x^2}{9}} x^2$  }, {x, -4.5, 4.5}, AxesLabel -> {x, (Abs[ψ])^2},
PlotRange -> {0, 1.67}, Filling -> {1 -> Bottom}, PlotStyle -> {Blue, Red}],
{T, 0, 1001, 10} ];

```

```
Export["firstexcitedstate_f.mov", output2];
```

The Heisenberg Uncertainty Principle - The more precisely the position is determined, the less precisely the momentum is known at an instant, and vice versa.

The following animation shows (simultaneous) phase space oscillations of the electron density (blue) and the probability distribution of momentum (red), according to the Heisenberg Uncertainty Principle, for the dynamic ground state $n = 0$ of the harmonic oscillator with parameters $\alpha_0 = \gamma_0 = \varepsilon_0 = \hbar_0 = 0$, $\beta_0 = 2/3$ and $\delta_0 = 3/2$:

output =

$$\text{Animate} \left[\text{Plot} \left[\left\{ \frac{9 \sqrt{2} e^{-\left(\frac{6 \sqrt{2} x}{\sqrt{97+65 \cos\left[\frac{1}{250} \pi (-1+T)\right]} - \frac{9 \sqrt{2} \sin\left[\frac{1}{500} \pi (-1+T)\right]} \right)^2}}{\sqrt{97+65 \cos\left[\frac{1}{250} \pi (-1+T)\right]}}, \right. \right. \\ \left. \left. \frac{18 e^{-\frac{18 \left(-2x+3 \cos\left[\frac{1}{500} \pi (-1+T)\right]\right)^2}}{-97+65 \cos\left[\frac{1}{250} \pi (-1+T)\right]}}{\sqrt{97+65 \cos\left[\frac{1}{250} \pi (-1+T)\right]}}, \right. \right. \\ \left. \left. \frac{18 e^{-\frac{18 \left(-2x+3 \cos\left[\frac{1}{500} \pi (-1+T)\right]\right)^2}}{-97+65 \cos\left[\frac{1}{250} \pi (-1+T)\right]}}{\sqrt{14593-4225 \cos\left[\frac{1}{125} \pi (-1+T)\right]}} \right\}, \right. \\ \left. \{x, -4.5, 4.5\}, \text{AxesLabel} \rightarrow \{\{x, p\}, \{(Abs[\psi])^2, (Abs[a])^2\}\}, \right. \\ \left. \text{PlotRange} \rightarrow \{0, 2.3\}, \text{Filling} \rightarrow \{1 \rightarrow \text{Bottom}\}, \right. \\ \left. \text{PlotStyle} \rightarrow \{\text{Blue}, \text{Red}\}\right], \{T, 1001\}, \text{AnimationRate} \rightarrow 100];$$

Export["heisenberg_s.mov", output];