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# Solutions for Time-Dependent Schrödinger Equations with Applications to Quantum Dots

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## 1. Introduction

In Ref.-(9), the authors study and solve the time-dependent Schrödinger equation

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

where

$$H = -a(t) \frac{\partial^2}{\partial x^2} + b(t) x^2 - i \left( c(t) x \frac{\partial}{\partial x} + d(t) \right) \quad (2)$$

and where  $a(t)$ ,  $b(t)$ ,  $c(t)$ , and  $d(t)$  are real-valued functions of time  $t$  only; see Refs.-(9), (10), (11), (29), (35), (39), (49), (50), and Ref.-(51) for a general approach and currently known explicit solutions. The solution (see Ref.-(9) for details) is given by

$$\psi(x, t) = \int_{-\infty}^{\infty} G(x, y, t) \psi_0(y) dy \quad (3)$$

where the Green's function, or particular solution is given by

$$G(x, y, t) = \frac{1}{\sqrt{2\pi i \mu(t)}} e^{i(\alpha(t)x^2 + \beta(t)xy + \gamma(t)y^2)}. \quad (4)$$

The time-dependent functions are found via a substitution method that reduces eqs.-(1)-(2) to a system of differential equations (see Ref. (9)):

$$\frac{d\alpha}{dt} + b(t) + 2c(t)\alpha + 4a(t)\alpha^2 = 0, \quad (5)$$

$$\frac{d\beta}{dt} + (c(t) + 4a(t)\alpha(t))\beta = 0, \quad (6)$$

$$\frac{d\gamma}{dt} + a(t)\beta^2(t) = 0, \quad (7)$$

where the first equation is the familiar Riccati nonlinear differential equation; see, for example, Refs.-(21), (45), (56). This system is explicitly integrable up to the function  $\mu(t)$  which satisfies the following so-called characteristic equation

$$\mu'' - \tau(t)\mu' + 4\sigma(t)\mu = 0 \quad (8)$$

with

$$\tau(t) = \frac{a'}{a} - 2c + 4d, \quad \sigma(t) = ab - cd + d^2 + \frac{d}{2} \left( \frac{a'}{a} - \frac{d'}{d} \right). \quad (9)$$

This equation must be solved subject to the initial data

$$\mu(0) = 0, \quad \mu'(0) = 2a(0) \neq 0 \quad (10)$$

in order to satisfy the initial condition for the corresponding Green's function. The time-dependent coefficients are given by the following equations:

$$\alpha(t) = \frac{1}{4a(t)} \frac{\mu'(t)}{\mu(t)} - \frac{d(t)}{2a(t)}, \quad (11)$$

$$\beta(t) = -\frac{1}{\mu(t)} \exp \left( -\int_0^t (c(\tau) - 2d(\tau)) d\tau \right), \quad (12)$$

$$\begin{aligned} \gamma(t) = & \frac{a(t)}{\mu(t)\mu'(t)} \exp \left( -2 \int_0^t (c(\tau) - 2d(\tau)) d\tau \right) + \frac{d(0)}{2a(0)} \\ & - 4 \int_0^t \frac{a(\tau)\sigma(\tau)}{(\mu'(\tau))^2} \left( \exp \left( -2 \int_0^\tau (c(\lambda) - 2d(\lambda)) d\lambda \right) \right) d\tau. \end{aligned} \quad (13)$$

Time dependence in the Hamiltonian has been studied in the context of various applications such as uniform magnetic fields Refs.-(9), (16), (28), (31), (32), (34), (36), time-periodic potentials and quantum dots Ref.-(8) (see also Ref.-(12) for a list of references and applications). Here, we present a general time-dependent Hamiltonian that has applications to the study of quantum devices such as quantum dots. Often described as artificial atoms, quantum dots are tools that allow the study of quantum behavior at the nanometer scale (see Ref.-(23)). This size is larger than the typical atomic scale that exhibits quantum behavior. Because of the larger size, the physics are closer to classical mechanics but still small enough to show quantum phenomena (see Ref.-(23)). Furthermore, their use extends into biological applications. In particular quantum dots are used as fluorescent probes in biological detection since these devices provide bright, stable, and sharp fluorescence (see Ref.-(6)).

Using methods similar to the approach in Ref.-(12), we discuss the uniqueness of Schwartz solutions to the Schrödinger Equation of this quantum dot Hamiltonian. In Ref.-(12) the authors seek to find Quantum Integrals of motion of various time-dependent Hamiltonians. Specifically, the authors seek quantum integrals of motion for the time-dependent Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = H(t) \psi \quad (14)$$

with variable quadratic Hamiltonians of the form

$$H = a(t) p^2 + b(t) x^2 + d(t) (px + xp), \quad (15)$$

where  $p = -i\partial/\partial x$ ,  $\hbar = 1$  and  $a(t)$ ,  $b(t)$ ,  $d(t)$  are some real-valued functions of time only (see, for example, Refs.-(13), (30), (34), (36), (37), (57), (58) and references therein). A related energy operator  $E$  is defined in a traditional way as a quadratic in  $p$  and  $x$  operator that has constant expectation values (see Ref.-(16)):

$$\frac{d}{dt} \langle E \rangle = \frac{d}{dt} \int_{-\infty}^{\infty} \psi^* E \psi dx = 0. \quad (16)$$

Such quadratic invariants are not unique. In Ref.-(12), the simplest energy operators are constructed for several integrable models of the damped and modified quantum oscillators. Then an extension of the familiar Lewis–Riesenfeld quadratic invariant is given to the most general case of the variable non-self-adjoint quadratic Hamiltonian (see also Refs.-(30), (57), (58)). The authors use the Invariants to construct positive operators that help prove uniqueness of the corresponding Cauchy initial value problem (IVP) for the models as a small contribution to the area of evolution equations.

In the present paper, the author will follow a similar approach in first proving the uniqueness of the IVP for a reduced Hamiltonian (see eq.-(20)). Then the author will use a gauge transformation to extend the uniqueness to IVP of the Quantum Dot Hamiltonian, eq.-(17). Furthermore, the gauge transformation will also simplify the general solution previously obtained in Ref.-(9).

## 2. A quantum dot model

Essentially, a quantum dot is a small box with electrons. The box is coupled via tunnel barriers to a source and drain reservoir (see Refs.-(23), (17)) with which particles can be exchanged. When the size of this so-called box is comparable to the wavelength of the electrons that occupy it, the energy spectrum is discrete, resembling atoms. This is why quantum dots are artificial atoms in a sense. Vladimiro Mujica at Arizona State University has suggested that the following model is of use to Floquet Theory as well as the theory of Semiconductor quantum dots:

$$H = a(t) p^2 + b(t) x^2 - id(t). \quad (17)$$

This Hamiltonian is seen in photon-assisted tunneling in double-well structures and quantum dots (see Ref.-(8) and Refs.-(25), (26), (44), (19), (55)). In particular, the authors in Ref.-(8) consider a single-electron tunneling through double-well structures. The Schrödinger equation proposed by the authors has a Hamiltonian of the form of eq.-(17) where  $b(t) = 0$  and

$$d(t) = i(\nu + \zeta \cos \omega t).$$

Specifically, they use a single-electron Schrödinger equation with time-periodic potential with oscillating barriers. The potential with oscillating barriers is given by

$$V(x, t) = \begin{cases} 0 & \text{(emitter and collector)} \\ V_B + V_1 \cos \omega t & \text{(layers of barriers)} \\ V_W & \text{(layers of well)} \end{cases} \quad (18)$$

or with the oscillating wells it is given by

$$V(x, t) = \begin{cases} 0 & \text{(emitter and collector)} \\ V_B & \text{(layers of barriers)} \\ V_W + V_1 \cos \omega t & \text{(layers of well)} \end{cases} \quad (19)$$

where  $V_B$  and  $V_W$  are the height and depth of the static barrier and well respectively.  $V_1 \cos \omega t$  is the applied field with amplitude  $V_1$  and frequency  $\omega$ .

### 2.1 Uniqueness

We wish to obtain uniqueness of solutions of eq.-(1) for eq.-(17) in Schwartz Space. We follow the approach of quantum integrals in Ref.-(12) to first prove the uniqueness of such solutions

for the following Hamiltonian:

$$H_0 = a(t) p^2 + b(t) x^2. \quad (20)$$

In particular, we will show that for eq.-(20),

$$\langle H_0 \rangle = 0 \text{ when } \psi(x, 0) = 0. \quad (21)$$

We first recall that

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) Q[\psi(x, t)] dx \quad (22)$$

Since, we have that  $\psi$  is in Schwartz space (see the Fourier Transform on  $\mathbb{R}$  in Ref.-(48)), it follows that

$$\langle H_0 \rangle = a(t) \langle p^2 \rangle + b(t) \langle x^2 \rangle < \infty. \quad (23)$$

as long as both functions  $a(t)$  and  $b(t)$  are bounded. Thus, to prove eq.-(21), we will show that

$$\langle p^2 \rangle = \langle x^2 \rangle = 0 \text{ when } \psi(x, 0) = 0. \quad (24)$$

Again, since  $\psi$  is in Schwartz space, we have that

$$\frac{d}{dt} \langle Q \rangle = \int_{-\infty}^{\infty} \frac{\partial}{\partial t} (\psi^*(x, t) Q[\psi(x, t)]) dx = \frac{1}{i} \langle QH - H^\dagger Q \rangle \quad (25)$$

for  $Q = p, x, px, xp, p^2$  and  $x^2$ .

Given eq.-(25) we have the following ODE system:

$$\begin{aligned} \frac{d}{dt} \langle p^2 \rangle &= -2b(t) \langle px + xp \rangle \\ \frac{d}{dt} \langle x^2 \rangle &= 2a(t) \langle px + xp \rangle \\ \frac{d}{dt} \langle px + xp \rangle &= 4a(t) \langle p^2 \rangle - 4b(t) \langle x^2 \rangle. \end{aligned} \quad (26)$$

If  $\psi(x, 0) = 0$ , then

$$\begin{aligned} \langle p^2 \rangle_0 &= 0 \\ \langle x^2 \rangle_0 &= 0 \\ \langle px + xp \rangle_0 &= 0. \end{aligned} \quad (27)$$

According to the general theory of homogeneous linear systems of ODE's, we have that

$$\begin{aligned} \langle p^2 \rangle &= 0 \\ \langle x^2 \rangle &= 0 \\ \langle px + xp \rangle &= 0. \end{aligned} \quad (28)$$

Thus, we have shown that eq.-(24) holds, thereby proving eq.-(21). We then use the following (see Ref.-(12)) lemma:

**Lemma 1.** Suppose that the expectation value

$$\langle H_0 \rangle = \langle \psi, H_0 \psi \rangle \geq 0 \quad (29)$$

for a positive quadratic operator

$$H_0 = f(t) (\alpha(t) p + \beta(t) x)^2 + g(t) x^2 \quad (f(t) \geq 0, g(t) > 0) \quad (30)$$

( $\alpha(t)$  and  $\beta(t)$  are real-valued functions) vanishes for all  $t \in [0, T)$  :

$$\langle H_0 \rangle = \langle H_0 \rangle(t) = \langle H_0 \rangle(0) = 0, \quad (31)$$

when  $\psi(x, 0) = 0$  almost everywhere. Then the corresponding Cauchy initial value problem

$$i \frac{\partial \psi}{\partial t} = H \psi, \quad \psi(x, 0) = \varphi(x) \quad (32)$$

may have only one solution in Schwartz space.

Since we have proven eq.-(21), we have that  $H_0$  satisfies this lemma, thus proving uniqueness of Schwartz solutions for eq.-(20). By using the gauge-transformation approach in Ref.-(11) we state the following lemma:

**Lemma 2.** Let  $\tilde{\psi}(x, t)$ , with  $\tilde{\psi}(x, 0)$  in Schwartz space, solve the following time-dependent Schrödinger equation:

$$i \frac{\partial \tilde{\psi}}{\partial t} = \tilde{H} \tilde{\psi}, \quad (33)$$

where

$$\tilde{H} = -a(t) \frac{\partial^2}{\partial x^2} + b(t) x^2 - ic(t) x \frac{\partial}{\partial x}. \quad (34)$$

Then

$$\psi(x, t) = \tilde{\psi}(x, t) \exp \left( - \int_0^t d(s) ds \right) \quad (35)$$

solves eqs.-(1)-(2) for

$$\psi(x, 0) = \tilde{\psi}(x, 0). \quad (36)$$

**Proof.** Let  $\psi(x, t) = \tilde{\psi}(x, t) \exp \left( - \int_0^t d(s) ds \right)$  and assume  $\tilde{\psi}(x, t)$  solves (33)-(34), where  $\tilde{\psi}(x, 0)$  is in Schwartz space. We differentiate  $\psi(x, t)$  with respect to time:

$$i \frac{\partial \psi}{\partial t} = i \frac{\partial \tilde{\psi}}{\partial t} \exp \left( - \int_0^t d(s) ds \right) - id(t) \tilde{\psi}(x, t) \exp \left( - \int_0^t d(s) ds \right). \quad (37)$$

For  $H$  given by (2) and  $\tilde{H}$  given by (34), we have

$$H = \tilde{H} - id(t), \quad (38)$$

and

$$i \frac{\partial \psi}{\partial t} = \tilde{H} [\tilde{\psi}] \exp \left( - \int_0^t d(s) ds \right) - id(t) \psi. \quad (39)$$

Since

$$\tilde{H} [\tilde{\psi}] \exp \left( - \int_0^t d(s) ds \right) = \tilde{H} \left[ \tilde{\psi} \exp \left( - \int_0^t d(s) ds \right) \right] = \tilde{H} [\psi], \quad (40)$$

we have that

$$i \frac{\partial \psi}{\partial t} = \tilde{H}[\psi] - id(t) \psi = H\psi. \quad (41)$$

■

By the method of Ref.-(9) for  $d = 0$  we can find  $\tilde{\psi}(x, t)$ : We simply generate the Green's function for  $\tilde{\psi}(x, t)$  by substituting  $d = 0$  in eq.-(2). This leads us to a simpler form of the solution previously obtained in Ref.-(9) for eqs.-(1)-(2). Namely,

$$\psi(x, t) = \exp\left(-\int_0^t d(s) ds\right) \int_{-\infty}^{\infty} G(x, y, t) \psi_0(y) dy \quad (42)$$

where

$$G(x, y, t) = \frac{1}{\sqrt{2\pi i \mu(t)}} e^{i(\alpha(t)x^2 + \beta(t)xy + \gamma(t)y^2)} \quad (43)$$

with

$$\alpha(t) = \frac{1}{4a(t)} \frac{\mu'(t)}{\mu(t)}, \quad (44)$$

$$\beta(t) = -\frac{1}{\mu(t)} \exp\left(-\int_0^t c(\tau) d\tau\right), \quad (45)$$

$$\gamma(t) = \frac{a(t)}{\mu(t) \mu'(t)} \exp\left(-2 \int_0^t c(\tau) d\tau\right) - 4 \int_0^t \frac{a(\tau) \tilde{\sigma}(\tau)}{(\mu'(\tau))^2} \left( \exp\left(-2 \int_0^\tau c(\lambda) d\lambda\right) \right) d\tau.$$

and  $\mu(t)$  is the solution of a *reduced characteristic equation* given by

$$\mu'' - \tilde{\tau}(t) \mu' + 4\tilde{\sigma}(t) \mu = 0, \quad (46)$$

where

$$\tilde{\tau}(t) = \frac{a'}{a} - 2c, \quad (47)$$

$$\tilde{\sigma}(t) = ab \quad (48)$$

and initial conditions are given by eq.-(10).

The Schwartz requirement on the initial condition is necessary to show that eq.-(3) is in fact the solution of eqs.-(1)-(2) since we can justify the interchanging of the time-derivative and integral operators. In particular, we note that

$$\left| \frac{\partial}{\partial t} G(x, y, t) \psi_0(y) \right| = \left| \frac{\partial}{\partial t} \left[ A(t) e^{i(\alpha(t)x^2 + \beta(t)xy + \gamma(t)y^2)} \psi_0(y) \right] \right|. \quad (49)$$

Here,

$$A(t) = \frac{1}{\sqrt{2\pi i \mu(t)}}. \quad (50)$$

Thus, eq.-(49) reduces to

$$\left| \left( \frac{\partial A}{\partial t} + Ai \frac{\partial S}{\partial t} \right) \psi_0(y) \right|, \quad (51)$$

where

$$S(x, y, t) = \alpha(t)x^2 + \beta(t)xy + \gamma(t)y^2. \quad (52)$$

Since  $\psi_0(y)$  is in Schwartz space, eq.-(51) is also in Schwartz space. It follows that the time-derivative operator can be exchanged with the integral (see Ref.-(1)).

We state the following extension Corollary:

**Corollary 3.** *Let  $\tilde{\psi}(x, t)$ , with  $\tilde{\psi}(x, 0)$  uniquely solve eqs.-(33)-(34). Then eq.-(35) uniquely solves eqs.-(1)-(2) for eq.-(36).*

This extends the uniqueness of Schwartz Space solutions to eq.-(1) for eq.-(17).

### 3. Invariants

In Ref.-(12), the authors seek the quantum integrals of motion or dynamical invariants for different time-dependent Hamiltonians. We recall a familiar definition (see, for example, Refs.-(16), (38)). We say that a quadratic operator

$$E = A(t) p^2 + B(t) x^2 + C(t) (px + xp) \quad (53)$$

is a quadratic dynamical invariant of eq.-(2) if

$$\frac{d\langle E \rangle}{dt} = 0 \quad (54)$$

for eq.-(2). We recall from Ref.-(11) that the expectation value of an operator  $A$  in quantum mechanics is given by the formula

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) E(t) \psi(x, t) dx, \quad (55)$$

where the wave function satisfies the time-dependent Schrödinger equation

$$i \frac{\partial \psi}{\partial t} = H\psi. \quad (56)$$

The time derivative of this expectation value can be written as

$$i \frac{d}{dt} \langle E \rangle = i \left\langle \frac{\partial E}{\partial t} \right\rangle + \langle EH - H^\dagger E \rangle, \quad (57)$$

where  $H^\dagger$  is the Hermitian adjoint of the Hamiltonian operator  $H$ . Our formula is a simple extension of the well-known expression Refs.-(28), (40), (47) to the case of a nonself-adjoint Hamiltonian.

Lemma 1 provides us with a Corollary regarding the relationship between invariants of gauge-related Hamiltonians.

**Corollary 4.** *Let  $\tilde{E}$  be a dynamical invariant of eq.-(34). If  $d(t)$  is a real-valued function, then*

$$E = \tilde{E} \exp \left( \int_0^t 2d(s) ds \right) \quad (58)$$

*is an invariant of eq.-(2). If  $d(t) = i\tilde{d}(t)$  where  $\tilde{d}(t)$  is a real-valued function, then  $\tilde{E}$  is an invariant of eq.-(2).*

**Conclusion 5.** *While Schrödinger equations have been widely used in quantum mechanics and other related fields such as quantum electrodynamics, Schrödinger equations with time-dependent*



*Hamiltonians continue to have applications in a wide area of related fields. It is thus appropriate to consider IVPs that have potential applications to devices such as Quantum Dots. It is thus important to understand the physics of these devices as we realize their great potential in the usage of imaging and other biological applications. Furthermore, quantum dots give us a glimpse of phenomena that unifies classical mechanics with quantum mechanics and thus deserve study in order to further the theoretical understandings of the laws that govern the universe.*

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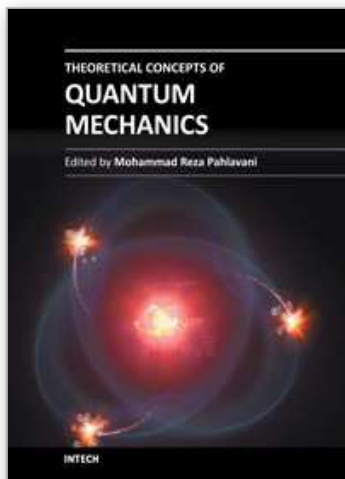
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## **Theoretical Concepts of Quantum Mechanics**

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Quantum theory as a scientific revolution profoundly influenced human thought about the universe and governed forces of nature. Perhaps the historical development of quantum mechanics mimics the history of human scientific struggles from their beginning. This book, which brought together an international community of invited authors, represents a rich account of foundation, scientific history of quantum mechanics, relativistic quantum mechanics and field theory, and different methods to solve the Schrodinger equation. We wish for this collected volume to become an important reference for students and researchers.

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