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Quantum first time-of-arrival operators

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Abstract

This paper undertakes the problem of constructing first time-of-arrival operators for arbitrary everywhere analytic potentials in the space of operators spanned by the Bender–Dunne basis (Bender and Dunne 1989 *Phys. Rev.* **D 40** 3504). The operators are conjugate with their respective system Hamiltonians and reduce to their corresponding classical time-of-arrival expressions for infinitesimal $\hbar$. The supraquantized time-of-arrival operators (Galapon 2004 *J. Math. Phys.* **45** 3180) and the confined time-of-arrival operators (Galapon *et al* 2004 *Phys. Rev. Lett.* **93** 180406, Galapon 2006 *J. Mod. Phys.* **A 21** 6351) are then shown to be two distinct representations of the time-of-arrival operators constructed in the Bender–Dunne space.

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

1. Introduction

The problem of calculating for the quantum time-of-arrival distribution of a quantum particle—known as the quantum time-of-arrival (QTOA) problem [1–3]—is one of the most studied aspects of the quantum time problem [4–13]. The QTOA problem is initially posed in the non-interacting case or for the quantum free particle. Kijowski is the first to give a solution within standard quantum mechanics (SQM) using an axiomatic approach [2]; his distribution is now known as the Kijowski distribution. Later attempts at addressing the free time-of-arrival problem in SQM have reproduced Kijowski's distribution [14–16]. Notably these attempts can be traced to a single formal operator—the free time-of-arrival operator, a quantized version of the classical free time-of-arrival observable. While there is a recognizable unity in the non-interacting case, there is a conspicuous variance in the interacting case. A variety of approaches in SQM have been introduced in the presence of an arbitrary interaction potential—approaches using Wigner's crossing states [17], current density [18, 19], operator normalization [20–22], complex potentials [23, 24] and Moller operators [25]. These solutions are non-time-operator based (except for the free case of Wigner's crossing states), that is, distributions are not computed from the spectral decomposition of a time-of-arrival operator, in sharp contrast to the free particle case.

The idea that the quantum time-of-arrival problem in the interacting case admits a solution in time-of-arrival operator form is not attractive and is laden with much skepticism [5, 25, 26]. It is for the following reason: the classical time of arrival in the interacting case is generally multiple and complex valued. Because there is no such thing as a multiple-valued operator and since quantum observables must have no complex spectra, it has been argued that no quantum time-of-arrival theory in the interacting case can be constructed via quantization of the classical expression [5, 25, 26]. It is believed that it is only for the free case that a time-of-arrival operator can be constructed because the classical expression is single and real valued in the entire phase space.

It is only recently that there is progress in the construction of time-of-arrival operators corresponding to the classical observable in the interacting case. In [27, 28] one of us, on addressing the circularity of quantization and the problem of obstruction to quantization [29–32], introduced the idea of supraquantization, the construction of quantum observables with classical counterparts without a direct quantization of the classical observable. There a quantum time-of-arrival operator, which we shall refer to as the supraquantized time-of-arrival (STOA) operator, has been constructed without quantization. This operator is conjugate with the system Hamiltonian in some generalized sense, and it derives the classical first time of arrival at a given arrival point. The STOA-operator for a given Hamiltonian is constructed in a rigged Hilbert space over the entire configuration space, that is, in coordinate representation in the entire real line. In this representation, the STOA-operator is in integral form. The expansion of the classical free time of arrival about the free time of arrival, which is a first time-of-arrival expression, is then recovered via Wigner transformation of the STOA-operator kernel followed by setting $\hbar^2 = 0$.

On another front, we have addressed the quantum first time-of-arrival problem for spatially confined particles leading to the concept of confined time-of-arrival (CTOA) operators, first for the non-interacting case [33, 34], and then for the interacting case [35]. The CTOA-operators are, for analytic potentials, compact and self-adjoint operators in the system Hilbert space. Their compactness implies that they possess a complete set of square integrable eigenfunctions with corresponding discrete spectra. It turns out that the proper interpretation of the eigenfunctions and eigenvalues of the CTOA-operators is tied with the internal unitary dynamics of the system. Numerical simulations show that the CTOA-eigenfunctions evolve according to Schrödinger equation such that the probability of locating the quantum particle in the neighborhood of the arrival point is maximum at their respective eigenvalues, justifying the identification of the CTOA-operators as first time-of-arrival operators. This dynamical behavior of the CTOA-operator eigenfunctions in relation to their respective eigenvalues is the first hint that time-of-arrival operators, despite the reservations of the majority, can have meaningful physical interpretation.

But these two works are actually preceded by a much earlier work of Bender and Dunne. In [36, 37], Bender and Dunne propose a technique for solving nonlinear Heisenberg equations of motion by deriving an operator $\hat{F}$ such that $\hat{F}$ and the system Hamiltonian $\hat{H}$ satisfy the canonical commutation relation $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$. Solving for $\hat{F}$ is equivalent to obtaining an implicit but exact solution to the equations of motion of the observables $\hat{p}$ and $\hat{q}$. In [37] they seek a particular solution $\hat{F}$ satisfying a certain condition; this solution they call the minimal solution. The fact that the time-of-arrival operator we seek is conjugate with the Hamiltonian in the sense of $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$ point to a relationship between Bender–Dunne's minimal solution and the operator we seek. This suspicion is motivated by Bender and Dunne's observation that their minimal solution for the harmonic oscillator is just the Weyl quantized form of the classical angle on the classical trajectory in phase space. But this angle, properly scaled, is just the negative of the classical time-of-arrival for the oscillator at the origin.

In this paper we undertake the problem of constructing representation-free first time-of-arrival operators for arbitrary analytic potentials, and consolidate the supraquantized local time-of-arrival and the confined time-of-arrival operators under a single framework built on the time-of-arrival operators constructed herein. The constructed operators have the properties of being conjugate with the system Hamiltonian and reducing to the classical time of arrival in the limit of infinitesimal $\hbar$, among other properties. The method is based on solving the operator equation $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$ for $\hat{T}$ given $\hat{H}$ in Liouville superoperator form $\hat{T} = \hat{\mathcal{L}}_{\hat{H}}^{-1}(\mathrm{i}\hbar\hat{I})$. Under certain conditions, the solution, which we refer to as the Liouville solution or Liouville time-of-arrival operator, is shown to exist for analytic potentials. The entire construction leans heavily on the properties of the Bender–Dunne basis set of operators [36, 37]. Our result unifies the supraquantized time-of-arrival operator and the confined time-of-arrival operators in the sense that these two operators are just different representations of the same operator $\hat{T}$. Our result is analogous to the theory of angular momentum in which there is just one underlying angular momentum algebra with distinct representations corresponding to distinct systems.

The rest of the paper is organized as follows. Section 2 reviews the concept of classical time of arrival and local time of arrival. Section 3 introduces the Bender–Dunne vector space of symmetrized products of momentum and position operators, and summarizes the algebra of the basis operators. Section 4 delineates the objectives of the paper. Section 5 discusses the quantization of the local time-of-arrival operator and highlights the problem of obstruction to quantization. Section 6 advances the method of inverse Liouville in superoperator form, and embodies the main results of the paper. Section 7 discusses the relationship between Bender–Dunne's minimal solution and our Liouville solution. Section 8 shows the relationship between the Liouville solution and the supraquantized local time of arrival. Section 9 shows how the Liouville solution can be extracted from the supraquantized local time-of-arrival operator. Section 10 discusses the relationship between the Liouville solutions and the confined time-of-arrival operators. Section 11 addresses the question of the physical content of the operators constructed. Section 12 provides the conclusion.

This paper is limited to the formal aspect of the construction of quantum first time-of-arrival operators. A separate paper is devoted on the problem of extracting time-of-arrival distributions from these constructed operators [40].

2. The classical time of arrival

Consider a particle with mass μ in one dimension whose Hamiltonian is $H(q, p)$. If at $t = 0$ the particle is at the point (q, p) in the phase space, the time $t = T_x$ at which the particle will arrive at the point $q(t = T_x) = x$ is given by

$$T_x(q, p) = -\mathrm{sgn}(p)\sqrt{\frac{\mu}{2}}\int_x^q \frac{\mathrm{d}q'}{\sqrt{H(q, p) - V(q')}}, \tag{1}$$

derived by inverting the equations of motion. For a given energy $H(q, p)$, the region in the phase space in which equation (1) is real valued is the classically accessible region to the particle for a given arrival point x. $T_x(q, p)$ can be multiple valued, indicating multiple arrivals at the given arrival point. An important property of $T_x(q, p)$ is its conjugacy with the Hamiltonian, $\{H(q, p), T_x(q, p)\} = 1$, where $\{,\}$ is the Poisson bracket.

Given the Hamiltonian $H = p^2/2\mu + V(q, p)$, consider all real-valued functions, $T(q, p)$, in the phase space that are conjugate to the Hamiltonian, i.e.,

$$\{H(q, p), T(q, p)\} = 1, \tag{2}$$

where the partials of $H(q, p)$ and $T(q, p)$ with respect to the canonical variables q and p exist. The time of arrival at some point in the configuration space is one such phase-space function. Out of all those $T(q, p)$'s, let us consider those that can be parameterized by x' and h, where x' is a point in the configuration axis and h is a fixed function of p alone. We denote these by $T_h^{x'}(q, p)$. The parameters x' and h are defined as follows. Let $K = p^2/2\mu$ be the kinetic energy, and $\mathcal{L}_K$ be the kinetic energy Liouville operator defined by $\mathcal{L}_K \cdot g = \{K, g\} = -\mu^{-1} p \partial_q g$. The pair of parameters x' and h fixes the inverse of $\mathcal{L}_K$, $\mathcal{L}_K^{-1}$, as follows:

$$\mathcal{L}_K^{-1} \cdot f(q, p) = -\frac{\mu}{p} \int_{x'}^{q} f(q', p)\, \mathrm{d}q' + h(p). \tag{3}$$

In other words, x' and h define the domain of $\mathcal{L}_K$ such that the inverse $\mathcal{L}_K^{-1}$ can be unambiguously defined.

Now given x' and h we construct $T_h^{x'}$ by the following prescription. With $\left\{H, T_h^{x'}\right\} = \mathcal{L}_H \cdot T_h^{x'}(q, p) = 1$, we express $T_h^{x'}$ in the form

$$T_h^{x'}(q, p) = \mathcal{L}_H^{-1} \cdot 1 = \frac{1}{\mathcal{L}_K + \mathcal{L}_V} \cdot 1, \tag{4}$$

where K and V are the kinetic and potential energy parts of the Hamiltonian, respectively. Geometric expansion of equation (4) yields

$$T_h^{x'}(q, p) = \mathcal{L}_K^{-1} \cdot 1 - \mathcal{L}_K^{-1} \cdot \mathcal{L}_V \cdot \mathcal{L}_K^{-1} \cdot 1 + \mathcal{L}_K^{-1} \cdot \mathcal{L}_V \cdot \mathcal{L}_K^{-1} \cdot \mathcal{L}_V \cdot \mathcal{L}_K^{-1} \cdot 1 + \cdots, \tag{5}$$

where $\mathcal{L}_K^{-1}$ is defined by equation (3). Assuming that there is a neighborhood in the phase space such that the right-hand side of (5) converges, equation (5) can be written in series form

$$T_h^{x'}(q, p) = \sum_{k=0}^{\infty} (-1)^k T_k(q, p, x'), \tag{6}$$

where the $T_k(q, p, x')$'s satisfy the recurrence relation

$$T_0(q, p, x') = \mathcal{L}_K^{-1} \cdot 1, \qquad T_k(q, p, x') = \mathcal{L}_K^{-1} \cdot \mathcal{L}_V \cdot T_{k-1}(q, p). \tag{7}$$

This system of recurrence relation is equivalent to the recurrence relation $\{K, T_k\} = \{V, T_{k-1}\}$, subject to the boundary condition $\{K, T_1\} = 1$.

Now let the system be autonomous so that the potential is only a function of q, $V(q, p) = V(q)$; moreover, let $h(p) = 0$ and $x' = x$. Then

$$T_0(q, p, x) = -\frac{\mu}{p}(q - x), \tag{8}$$

$$T_k(q, p, x) = -\frac{\mu}{p} \int_x^q \frac{\partial V}{\partial q'} \frac{\partial T_{k-1}}{\partial p}\, \mathrm{d}q'. \tag{9}$$

If $p \neq 0$ and $V(q)$ is continuous at q, then there exists a neighborhood of q determined by the neighborhood $|V(q) - V(q')| < K_\epsilon \leqslant \frac{p^2}{2\mu}$ such that for every x in this neighborhood, $T_{h=0}^x(q, p) \equiv t_x(q, p)$ converges absolutely and uniformly to the classical time of arrival $T_x(q, p)$. We referred to $t_x(q, p) = \sum_{k=0}^{\infty}(-1)^k T_k(q, p)$ as the local time of arrival (LTOA) at the arrival point x [27, 28]. The LTOA is a first time-of-arrival expression.

Before we proceed let us reconsider the expression for the time of arrival for arbitrary arrival point x. Changing variables from (q, p) to $(\tilde{q} = q - x, \tilde{p} = p)$ in equation (1), we get

$$T(\tilde{q}, \tilde{p}) = -\mathrm{sgn}(\tilde{p})\sqrt{\frac{\mu}{2}}\int_0^{\tilde{q}} \frac{\mathrm{d}\tilde{q}'}{\sqrt{H(\tilde{q}+x, \tilde{p}) - V(\tilde{q}'+x)}}. \tag{10}$$

Comparing this expression with equation (1) we find that it is just the time of arrival at the origin for the potential $\tilde{V}(\tilde{q}) = V(\tilde{q}+x)$. Because of this it is sufficient for us to consider the time of arrival at the origin in the development to follow, for when the arrival point is different from the origin we only have to appropriately change variables.

The rest of the paper is devoted to constructing the quantum first time-of-arrival operator for a given arrival point. The geometric expansion behind equation (5) will serve as the fulcrum for the development to follow.

3. The Bender–Dunne space

In [36, 37] Bender and Dunne consider the problem of finding a certain operator $\hat{F}$ conjugate with the Hamiltonian in the sense of $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$. Their method hinges on the assumption of the existence of a complete set of basis operators, $\{\hat{T}_{m,n}\}$, for m, n integers, through which any operator can be expanded.

For $m, n \geqslant 0$ the operator $\hat{T}_{m,n}$ is defined as the Weyl-ordered product of the classical function $p^m q^n$,

$$\hat{T}_{m,n} = \frac{1}{2^n}\sum_{k=0}^{n} \frac{n!}{k!(n-k)!}\hat{q}^k \hat{p}^m \hat{q}^{n-k}. \tag{11}$$

Using the canonical commutation relation $[\hat{q}, \hat{p}] = \mathrm{i}\hbar\hat{I}$, this can be rewritten in the form

$$\hat{T}_{m,n} = \frac{1}{2^m}\sum_{k=0}^{m} \frac{m!}{k!(m-k)!}\hat{p}^k \hat{q}^n \hat{p}^{m-k}. \tag{12}$$

When $m < 0$ and $n \geqslant 0$, equation (11) defines $\hat{T}_{m,n}$; on the other hand, when $m \geqslant 0$ and $n < 0$, equation (12) defines $\hat{T}_{m,n}$. The definition of $\hat{T}_{m,n}$'s can be extended to cases when both m and n are negative by replacing the factorials with the gamma function,

$$\hat{T}_{m,n} = \frac{1}{2^n}\sum_{k=0}^{\infty} \frac{\Gamma(n+1)}{k!\Gamma(n-k+1)}\hat{q}^k \hat{p}^m \hat{q}^{n-k} = \frac{1}{2^m}\sum_{k=0}^{\infty} \frac{\Gamma(m+1)}{k!\Gamma(m-k+1)}\hat{p}^k \hat{q}^n \hat{p}^{m-k}. \tag{13}$$

These expressions reduce to equations (11) and (12) when m and n are both positive integers. $\hat{T}_{m,n}$'s satisfy the algebra

$$[\hat{T}_{m,n}, \hat{T}_{r,s}] = 2\sum_{j=0}^{\infty}\left(\frac{\mathrm{i}\hbar}{2}\right)^{2j+1}\sum_{l=0}^{2j+1} \frac{(-1)^l}{l!(2j+1-l)!}\frac{\Gamma(m+1)\Gamma(n+1)}{\Gamma(m-l+1)\Gamma(n+l-2j)} \times \frac{\Gamma(r+1)\Gamma(s+1)}{\Gamma(r+l-2j)\Gamma(s-l+1)}\hat{T}_{m+r-2j-1,n+s-2j-1}, \tag{14}$$

where we have inserted $\hbar$ in its appropriate place ($\hbar = 1$ in [36, 37]).

The assumption of completeness of $\hat{T}_{m,n}$'s, which requires introducing a suitable metric, can lead to technical issues that is well beyond the scope of this paper. So instead of assuming the completeness of $\hat{T}_{m,n}$'s, we introduce the infinite-dimensional complex linear space spanned by $\hat{T}_{m,n}$'s, which we refer to as the Bender–Dunne space $\mathcal{BD}$, and work exclusively in $\mathcal{BD}$. Then by definition $\hat{T}_{m,n}$'s already form a basis for the $\mathcal{BD}$-space. There will be a need for us to refer to the subspaces of $\mathcal{BD}$ corresponding to the four quadrants of the mn-lattice space, $D_{++} = (m > 0, n > 0)$, $D_{-+} = (m < 0, n > 0)$, $D_{--} = (m < 0, n < 0)$ and $D_{+-} = (m > 0, n < 0)$. The subspace D_{-+} will play a central role in the construction of time-of-arrival operators for analytic potentials.

4. The problem

Now we can state what we wish to accomplish in this paper: given a point x in the configuration space and given the system Hamiltonian $\hat{H}$ taken as an element of $\mathcal{BD}$, find the operator $\hat{T}$ in $\mathcal{BD}$ satisfying the following conditions: (1) $\hat{T}$ reduces to the local time-of-arrival expression, $t_x(q, p)$, in the limit of commuting $\hat{q}$ and $\hat{p}$ or as $\hbar \to 0$, (2) $\hat{T}$ is formally conjugate with the Hamiltonian $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$, (3) $\hat{T}$ is symmetric and (4) $\hat{T}$ satisfies the time-reversal symmetry $\Theta^{-1}\hat{T}\Theta = -\hat{T}$ where Θ is the time-reversal operator. The first condition follows from the requirement that the operator $\hat{T}$ must be identifiable as a quantum first time-of-arrival operator; the second from Heisenberg's equation of motion for a time-of-arrival operator; the third from the condition that quantum observables must have real expectation values; and the fourth from consistency with the identification of $\hat{T}$ as a time observable under time reversal.

In this paper we show that for everywhere analytic interaction potentials, that is potentials that can be expanded anywhere in the real line in Taylor series, in particular of the form $V = \sum_{k=0}^{\infty} v_k q^k$, the solution $\hat{T}$ exists. We will then study $\hat{T}$ in relation to Bender–Dunne's minimal solution, and to the supraquantized local time-of-arrival and the confined time-of-arrival operators. The last two lead us to consider the representation of $\hat{T}$ in the rigged Hilbert spaces $\Phi^{\times} \supset \mathcal{H} \supset \Phi$ and $\Phi_l^{\times} \supset \mathcal{H}_l \supset \Phi_l$, where Φ_l (Φ) is the fundamental space of infinitely differentiable complex-valued functions with compact supports in the interval $[-l, l]$ $((-\infty, \infty))$, $\mathcal{H}_l$ $(\mathcal{H})$ the associated Hilbert space of Φ_l (Φ) and $\Phi_l^{\times}$ $(\Phi^{\times})$ is the space of linear functionals of Φ_l (Φ). By representation of $\hat{T}$ in Φ_l (Φ) we mean taking the formal operator $\hat{T}$ as an operator in Φ_l (Φ). We will find that the Φ representation of $\hat{T}$ is generally an operator from Φ to $\Phi^{\times}$; while the Φ_l representation of $\hat{T}$ for continuous potentials is an operator from Φ_l to $\mathcal{H}_l$.

5. Quantized time-of-arrival operators

5.1. Weyl quantization of the local time of arrival

When the quantum version of a classical observable is sought, the first attempt at constructing the corresponding quantum observable is by quantization of the classical expression. So quantization of the classical time of arrival seems a reasonable approach at constructing quantum time-of-arrival operators. The objections discussed above on the quantization of the classical time of arrival can be addressed by quantizing not expression (1) but the local time of arrival as suggested in [35]. The LTOA is unambiguously a first time-of-arrival quantity, single and real-valued function of position and momentum. The only possible objection to quantizing the LTOA is that the LTOA is defined only in some small neighborhood of the arrival point, not in the entire phase space. Quantization presupposes the system Hilbert space is defined, say, in the entire configuration space. Our justification in quantizing the LTOA comes from the fact that the resulting operator can be given an unambiguous physical interpretation [40] (see section 11).

In general we propose to Weyl quantize a real-valued function $f(q,p)$ by expanding $f(q,p)$ in powers of $p^m q^n$ followed by the formal replacement

$$p^m q^n \xrightarrow{W} \hat{T}_{m,n}. \tag{15}$$

For potentials of the form $V(q) = \sum_{n=0}^{\infty} v_n q^n$ the local time of arrival at the origin is in expansion of $p^{-m}q^n$, with $m, n > 0$; this conclusion follows immediately from equations (8) and (9). For example, the potential $V(q) \propto \sin(kq)$ can lead to a term $p^{-m}\sin kq$, for some $m > 0$, in the local time of arrival. This term is Weyl quantized according to

$$p^{-m}\sin kq = \sum_{n=0}^{\infty} \frac{(-1)^n k^n}{(2n+1)!} p^{-m} q^n \xrightarrow{W} \sum_{n=0}^{\infty} \frac{(-1)^n k^n}{(2n+1)!} \hat{T}_{-m,n}.$$

It is clear that the quantized local time of arrivals for such potentials lie in the second quadrant, D_{-+}, of the mn-lattice space.

5.2. Examples

Let us consider deriving the local time of arrival at the origin for the potential $V = \beta q^n/n$ for some real constant β and some positive integer n. We will need this in the development to follow. Using equations (8) and (9) with $x = 0$, we arrive at the local time of arrival at the origin for the given potential

$$T(q,p) = -\sum_{k=0}^{\infty} (-1)^k \frac{\mu^{k+1}\beta^k 2^k \Gamma(k+1/2)\Gamma(1+1/n)}{n^k \Gamma(1+k+1/n)\sqrt{\pi}} \frac{q^{kn+1}}{p^{2k+1}}. \tag{16}$$

This series converges in some small neighborhood of the origin. The sum can be evaluated explicitly, but it is this series representation that we need.

Now we can perform the quantization of the local time of arrival via our formal replacement scheme. In particular, for the harmonic oscillator ($n = 2, \beta = \mu\omega^2$) and quartic oscillator ($n = 4$), we have their respective quantized local time-of-arrival operators

$$\hat{T}_{W,ho} = -\sum_{k=0}^{\infty} (-1)^k \frac{\mu^{2k+1}\omega^2 k}{(2k+1)} \hat{T}_{-2k-1,2k+1}, \tag{17}$$

$$\hat{T}_{W,qo} = -\frac{\Gamma(5/4)}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k}{2^k} \beta^k \mu^{k+1} \frac{\Gamma(k+1/2)}{\Gamma(k+5/4)} \hat{T}_{-2k-1,4k+1}. \tag{18}$$

We will be dealing with these two systems through out the paper.

By definition the quantized local time-of-arrival operators reduce to the classical expression in the limit of commuting momentum and position operators or as $\hbar \to 0$, and, by the symmetric nature of the basis operators, the quantized LTOA-operators are themselves symmetric; moreover, they have the correct time-reversal symmetry because they are odd in momentum operator. Then for the quantized LTO to satisfy all requirements, they must only now satisfy conjugacy with the Hamiltonian.

For the harmonic oscillator it is straightforward to show, using the commutators

$$[\hat{T}_{m,n}, \hat{q}^2] = -2\mathrm{i}m\hbar \hat{T}_{m-1,n+1} \tag{19}$$

$$[\hat{T}_{m,n}, \hat{p}^2] = 2\mathrm{i}n\hbar \hat{T}_{m+1,n-1}, \tag{20}$$

that $[\hat{H}_{ho}, \hat{T}_{W,ho}] = \mathrm{i}\hbar\hat{I}$. That is quantization of the local time of arrival for the harmonic oscillator gives an operator conjugate with the Hamiltonian.

On the other hand, for the quartic oscillator we can show, on using the commutator,

$$[\hat{T}_{m,n}, \hat{q}^4] = -4\mathrm{i}m\hbar\hat{T}_{m-1,n+3} + \mathrm{i}\hbar^3 m(m-1)(m-2)\hat{T}_{m-3,n+1} \tag{21}$$

that $\hat{H}_{qo}$ and $\hat{T}_{W,qo}$ have the commutator

$$[\hat{H}_{qo}, \hat{T}_{W,qo}] = \mathrm{i}\hbar\hat{I} - \mathrm{i}\hbar\cdot\hbar^2\sum_{k=0}^{\infty}\frac{\Gamma(5/4)}{\sqrt{\pi}}\frac{(-1)^k}{2^k}\beta^{k+1}\mu^{k+1}\frac{\Gamma(k+1/2)}{\Gamma(k+5/4)} \times (2k+1)(2k+2)(2k+3)\hat{T}_{-2k-4,4k+2}.$$

We find that the quantized local time of arrival of the quartic oscillator fails to be conjugate with the Hamiltonian. It is interesting though to find that $\hat{T}_{W,qo}$ is conjugate to the Hamiltonian for infinitesimal $\hbar$, that is $\hbar \neq 0$ but $\hbar^2 = 0$.

These two examples illustrate a general feature of the Weyl quantization of the local time of arrival. Later we will show in section 9.4 that only for linear systems, systems with linear (classical) equations of motion, that Weyl quantization of the local time-of-arrival preserves the classical algebra.

5.3. Obstruction to quantization

The above two examples illustrate the fact that quantization only preserves the classical algebra for a subset of classical observables. This is a consequence of the known obstruction to quantization in Euclidean space in which there exists no quantization that can consistently map Poisson brackets into commutators [29–32] for all observables. As a specific example in [29], in terms of Poisson brackets we have the equality $\frac{1}{3}\{q^3, p^3\} = \{q^2 p, qp^2\}$. Formally quantizing these canonical variables, we nevertheless obtain, $\frac{1}{3}[\hat{q}^3, \hat{p}^3] \neq \left[\frac{1}{2}(\hat{q}^2\hat{p} + \hat{p}\hat{q}^2), \frac{1}{2}(\hat{q}\hat{p}^2 + \hat{p}^2\hat{q})\right]$. Thus, the formal quantization $q \rightarrow \hat{q}$ and $p \rightarrow \hat{p}$ leads to an inconsistency. This is obviously a matter of general concern because the time evolution of classical and quantum observables are expressed in terms of Poisson and commutator relations respectively. Also, in the present context, a formal quantization $T \rightarrow \hat{T}$ may not necessarily lead to an observable that preserves the required algebra. So even if we assume that $\hat{T}$ is the observable corresponding to the classical expression $T(q, p)$, a direct approach via quantization is not sufficient. An alternative way is therefore needed.

6. The Liouville time-of-arrival operators

6.1. Quantum Liouville expansion

We now address the problem of constructing first time-of-arrival operators that satisfy all the requirements stated in section 4. We proceed in complete analogy to the classical case. Our problem is to find, for a given Hamiltonian $\hat{H}$ in $\mathcal{BD}$, the operator $\hat{T}$ in Bender–Dunne space $\mathcal{BD}$ that is formally conjugate with the Hamiltonian, $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$, and satisfying the other required properties discussed in section 4.

We likewise write the conjugacy relation $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$ in Liouville form $\mathcal{L}_{\hat{H}} \cdot \hat{T} = \mathrm{i}\hbar\hat{I}$, where $\mathcal{L}_{\hat{H}} = [\hat{H}, \cdot]$, as in the classical case. Assuming that we can define the inverse of $\mathcal{L}_{\hat{H}}$, then we have the solution $\hat{T} = \mathcal{L}_{\hat{H}}^{-1} \cdot (\mathrm{i}\hbar\hat{I})$. Breaking the Hamiltonian into its kinetic and potential energy parts enables us to express the inverse in geometric expansion in similar fashion to the classical expression. This leads to the formal solution

$$\hat{T} = \hat{\mathcal{L}}_{\hat{K}}^{-1}(\mathrm{i}\hbar I) - \hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}\hat{\mathcal{L}}_{\hat{K}}^{-1}(\mathrm{i}\hbar I) + \hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}\hat{\mathcal{L}}_{\hat{K}}^{-1}(\mathrm{i}\hbar I) - \cdots, \tag{22}$$

where $\mathcal{L}_{\hat{K}} = [\hat{K}, \cdot]$ and $\mathcal{L}_{\hat{V}} = [\hat{V}, \cdot]$. However, equation (22) is meaningful only if we can define the inverse $\mathcal{L}_{\hat{K}}^{-1}$ unambiguously. But since the kinetic energy operator commutes with any functional of the momentum operator, the null space of the superoperator $\mathcal{L}_{\hat{K}}$ is not empty. This makes the inverse of $\mathcal{L}_{\hat{K}}$ ill-defined.

However, by restricting the domain of $\mathcal{L}_{\hat{K}}$ to its kernel space, to operators of the form $\hat{B} = \sum_{n\neq 0,m} \beta_{m,n}\hat{T}_{m,n}$, its inverse can be defined. The fact that $T_{m,n}$'s form a basis for the operators in $\mathcal{BD}$ allows us to define the inverse of $\mathcal{L}_{\hat{K}}$ in terms of its action on the basis operators $\hat{T}_{m,n}$. From equation (20) we have

$$\mathcal{L}_{\hat{K}} \cdot \hat{T}_{m,n} = \frac{1}{2\mu}[\hat{p}^2, \hat{T}_{m,n}] = -\frac{\mathrm{i}\hbar}{\mu} n \hat{T}_{m+1,n-1}. \tag{23}$$

From this we can write the formal action of the inverse of the Liouville superoperator on the $\mathcal{BD}$ basis,

$$\mathcal{L}_{\hat{K}}^{-1} \cdot \hat{T}_{s,r} = \frac{\mathrm{i}\mu}{\hbar}\frac{\hat{T}_{s-1,r+1}}{(r+1)}. \tag{24}$$

It is immediate that the inverse is well defined if and only if $r \neq -1$, which is guaranteed if $\hat{\mathcal{L}}_K$ is restricted to its kernel space. Since $\mathcal{L}_{\hat{K}}$ is linear, $\hat{\mathcal{L}}_{\hat{K}}^{-1}$ must necessarily be linear; and by this linearity, its action on any given operator in $\mathcal{BD}$ is then defined in accordance with its action on the basis operators as given by equation (24). This allows us to assign a domain to $\hat{\mathcal{L}}_{\hat{K}}^{-1}$; and its domain consists of operators whose expansions are of the form $\hat{A} = \sum_{n\neq -1,m} \beta_{m,n}\hat{T}_{m,n}$.

The quantum Liouville expansion (22) can now be written as $\hat{T} = \sum_{k=0}^{\infty}(-1)^k\hat{T}_k$. The leading term in the expansion readily evaluates to $\hat{T}_0 = \mathcal{L}_{\hat{K}}^{-1}(\mathrm{i}\hbar\hat{T}_{0,0}) = -\mu\hat{T}_{-1,1}$, where we have used the equality $\hat{I} = \hat{T}_{0,0}$. The rest of $\hat{T}_k$'s are determined recursively through

$$\hat{T}_0 = -\mu\hat{T}_{-1,1}, \tag{25}$$

$$\hat{T}_k = \left(\mathcal{L}_{\hat{K}}^{-1}\mathcal{L}_{\hat{V}}\right)\cdot\hat{T}_{k-1}. \tag{26}$$

By repeated back substitution in equation (26), the Liouville expansion for the solution assumes the form

$$\hat{T} = -\mu\sum_{k=0}^{\infty}(-1)^k\left(\mathcal{L}_{\hat{K}}^{-1}\mathcal{L}_{\hat{V}}\right)^k\cdot\hat{T}_{-1,1}. \tag{27}$$

Comparing equations (25) and (8), we find that equation (25) is the quantization of equation (8) for arrival at the origin, $x = 0$; moreover, from the action of $\mathcal{L}_{\hat{K}}^{-1}$, we find that equation (26) reduces to the classical expression equation (9). Hence, equations (25)–(27) are the quantum versions of the classical expressions for arrival at the origin. These quantum expressions can be extended to arbitrary arrival point by a mere change of variable as pointed out earlier in section 2. Equation (27) is the central result of the paper.

We refer to the solution $\hat{T}$, whenever it exists, as the Liouville solution or Liouville time-of-arrival operator for the given interaction potential. Equation (27) implicitly assumes that the Liouville solution reduces to the free case in the limit of vanishingly small interaction potential. We will find later in section 7 that this rather innocent property of the Liouville solution determines whether a Liouville solution exists or not.

We point out that, while the classical expression for the local time of arrival has guided us in the construction of the Liouville solution, we have not performed a quantization of the local time of arrival to arrive at equation (27). We have actually proceeded in the spirit of supraquantization of a given classical observable [6]. In [6] we have suggested that to derive the operator corresponding to a classical observable, one does not quantize, instead, one imposes the required algebra or commutation relation and then solve the resulting operator equation under certain conditions that exactly determine the properties of the required solution. An important property that must be satisfied is that the classical expression must emerge from its corresponding quantum kind in the limit of vanishing $\hbar$. Our derivation of the Liouville solution in parallel to its classical counterpart is to ensure that this condition is satisfied.

6.2. Existence and non-existence of solution

Now the Liouville solution $\hat{T}$ exists if each $\hat{T}_k$ in the expansion belongs to the Bender–Dunne space. Let us see under what condition that the solution $\hat{T}$ exists. We denote the domain of $\hat{\mathcal{L}}_{\hat{K}}^{-1}$ by $D_{\hat{K}}$ and denote the subspace of this domain that is invariant under $\hat{\mathcal{L}}_{\hat{K}}^{-1}$ itself by $\tilde{D}_{\hat{K}}$. Not all of $D_{\hat{K}}$ belongs to $\tilde{D}_{\hat{K}}$; for example, the operator $\hat{T}_{m,-2}$, for any m, belongs to $D_{\hat{K}}$ but not to $\tilde{D}_{\hat{K}}$, because $\hat{\mathcal{L}}_{\hat{K}}^{-1}\cdot\hat{T}_{m,-2}\propto\hat{T}_{m-1,-1}$, which is no longer in $D_{\hat{K}}$. Now an element $\hat{A}$ of $D_{\hat{K}}$ belongs to $\tilde{D}_{\hat{K}}$ if and only if $\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\right)^n\cdot\hat{A}$ belongs to $D_{\hat{K}}$ for any positive integer n. Clearly elements of $\tilde{D}_{\hat{K}}$ are operators of the form $\hat{A}=\sum_{n\geqslant 0,m}a_{m,n}\hat{T}_{m,n}$ for some constants $a_{m,n}$. Now the leading term in the expansion for $\hat{T}$ is proportional to $\hat{T}_{-1,1}$; hence $\hat{T}_0$ belongs to the invariant subspace $\tilde{D}_{\hat{K}}$. The existence of each $\hat{T}_k$ in the expansion is then guaranteed by the condition that $\tilde{D}_{\hat{K}}$ is invariant under $\hat{\mathcal{L}}_{\hat{V}}$; that means no $\hat{A}$ in $\tilde{D}_{\hat{K}}$ such that $\hat{\mathcal{L}}_{\hat{V}}\cdot\hat{A}$ involves a term with $\hat{T}_{l,-j}$ for some $j>0$. Under this condition we are assured of the existence of the solution $\hat{T}$.

6.2.1. Example of potentials admitting solutions. So before we can proceed we must establish first that a wide class of potentials exists such that the above condition is satisfied. Let us consider the potential $\hat{V}\propto\hat{q}^s$ for some positive integer s. Then we have

$$\hat{\mathcal{L}}_{\hat{q}^s}\cdot\hat{T}_{m,n}=-\mathrm{i}\hbar\sum_{j=0}^{\lfloor\frac{s-1}{2}\rfloor}\frac{(-1)^j\hbar^{2j}}{4^j(2j+1)!}\frac{\Gamma(m+1)}{\Gamma(m-2j)}\frac{\Gamma(s+1)}{\Gamma(s-2j)}\hat{T}_{m-2j-1,n+s-2j-1}. \tag{28}$$

For $n\geqslant 0$ the least possible second index of the basis in the right-hand side is n; then it is not possible for $\hat{\mathcal{L}}_{\hat{q}^2}$ to map $\tilde{D}_{\hat{K}}$ outside itself. That means that $\tilde{D}_{\hat{K}}$ is invariant under $\hat{\mathcal{L}}_{\hat{q}^s}$. Then the solution $\hat{T}$ exists for potentials of the form $\hat{V}\propto\hat{q}^s$. Now because

$$\hat{\mathcal{L}}_{\hat{V}_1+\hat{V}_2}=\hat{\mathcal{L}}_{V_1}+\hat{\mathcal{L}}_{V_2},$$

we are assured that every polynomial potential admits a solution, and by extension, to everywhere analytic potentials.

6.2.2. Example of potentials not admitting solutions. But not all potentials assure that $\hat{\mathcal{L}}_{\hat{V}}$ leaves the domain $\tilde{D}_{\hat{K}}$ invariant, and that may lead to non-existent $\hat{T}$. Consider the potential $\hat{V}\propto\hat{q}^{-1}$. Then we have [37]

$$\hat{\mathcal{L}}_{\hat{q}^{-1}}\cdot\hat{T}_{m,n}=-\mathrm{i}\hbar\sum_{j=0}^{\infty}(-1)^j\frac{\hbar^{2j}}{4^j}\frac{\Gamma(m+1)}{\Gamma(m-2j)}\hat{T}_{m-2j-1,n-2j-2}.$$

For $n=1$ the $j=0$ term is proportional to $\hat{T}_{m-1,-1}$; then this is outside the domain of $\hat{\mathcal{L}}_{\hat{K}}^{-1}$. Then $\tilde{D}_{\hat{K}}$ is not invariant under $\hat{\mathcal{L}}_{\hat{V}}$. Because of this the time-of-arrival operator for this potential does not exist. This follows because $\hat{T}_1\propto\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}\cdot\hat{T}_{-1,1}$ will be undefined. In fact it can be shown that the potentials $\hat{q}^{-s}$, for every positive integer s, do not preserve $\tilde{D}_{\hat{K}}$, and the corresponding Liouville solution does not exist. Later in section 7 we will address the question whether this is a failure of the method or not. (It is not clear if non-invariance of $\tilde{D}_{\hat{K}}$

under $\hat{\mathcal{L}}_{\hat{V}}$ strongly implies the non-existence of the Louiville solution. We leave that problem open.)

6.3. The structure of Liouville solutions for analytic potentials

According to our discussion above, we are assured that the Liouville solution exists for analytic potentials of the form $\hat{V} = \sum_{s=0}^{\infty} v_s \hat{q}^s$. Let us see the general structure of the solution for these potentials. It is sufficient to consider a particular power $s > 0$ in the expansion for the potential. For $k, \ell \geqslant 0$, we have from equations (24) and (28),

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{q}^s}\right)\cdot\hat{T}_{-k,\ell} = -\mu\sum_{j=0}^{\left\lfloor\frac{s-1}{2}\right\rfloor}\frac{(-1)^j\hbar^{2j}}{4^j(2j+1)!}\frac{(k+2j)!}{(k-1)!}\frac{\Gamma(s+1)}{\Gamma(s-2j)}\frac{\hat{T}_{-k-2j-2,\ell+s-2j}}{(\ell+s-2j)}. \tag{29}$$

It is clear from this expression that the Liouville solution will be expanded in the basis $\hat{T}_{-r,s}$ for $r, s > 0$, because the terms in the expansion for $\hat{T}$ are all generated from $\hat{T}_{-1,1}$ via equations (25) and (26); that is, the solution will lie in the second quadrant, D_{-+}, of the mn-lattice space. Moreover, since $m = -1$ in the leading term $\hat{T}_{-1,1}$, all basis elements $\hat{T}_{-r,s}$'s involved in the expansion for $\hat{T}$ will be odd in $r > 0$. This implies the time-reversal symmetry $\Theta^{-1}\hat{T}\Theta = -\hat{T}$ because $\Theta^{-1}\hat{p}\Theta = -\hat{p}$ and $\Theta^{-1}\hat{q}\Theta = \hat{q}$.

By construction the Liouville solution is conjugate with the Hamiltonian, and is symmetric by virtue of the symmetric nature of the basis operators, and is time-reversal antisymmetric. It only remains to show that $\hat{T}$ reduces to the classical time-of-arrival expression in the limit of commuting $\hat{q}$ and $\hat{p}$. The following examples will demonstrate that this is the case. But we have to wait until section 9 to prove that indeed $\hat{T}$ reduces to the classical expression for everywhere analytic potentials.

6.4. Examples

6.4.1. Harmonic oscillator. We now derive the time-of-arrival operator, $\hat{T}_{ho}$, for the harmonic oscillator using our inverse Liouville approach. Given the harmonic oscillator potential $\hat{V}_{ho} = (1/2)\mu\omega^2 q^2$, we apply $\hat{\mathcal{L}}_{\hat{V}_{ho}}$ on the basis elements of $\tilde{D}_{\hat{K}}$, in particular $\hat{T}_{-m,n}$'s with $m, n > 0$, using equation (23), then followed by $\hat{\mathcal{L}}_{\hat{K}}^{-1}$ using equation (24), to arrive at

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{ho}}\right)\cdot\hat{T}_{-m,n} = \mu^2\omega^2\frac{m}{(n+2)}\hat{T}_{-m-2,n+2}. \tag{30}$$

Equation (30) allows us to find $\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{ho}}\right)^k\cdot\hat{T}_{-m,n}$ recursively for any $k > 1$. It yields

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{ho}}\right)^k\cdot\hat{T}_{-m,n} = (\mu\omega)^{2k}\frac{m(m+2)\cdots(m+2k-2)}{(n+2)(n+4)\cdots(n+2k)}\hat{T}_{-m-2k,n+2k} \tag{31}$$

for a given integer $k \geqslant 0$. This can be proven by induction.

For the specific case of $m = n = 1$ for the construction of $\hat{T}_k$ (see equation (25)), we obtain the Liouville time-of-arrival operator for the harmonic oscillator

$$\begin{aligned}\hat{T}_{ho} &= -\mu\sum_{k=0}^{\infty}(-1)^k\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{ho}}\right)^k\cdot\hat{T}_{-1,1}\\ &= -\sum_{k=0}^{\infty}(-1)^k\frac{\mu^{2k+1}\omega^{2k}}{2k+1}\hat{T}_{-2k-1,2k+1}.\end{aligned} \tag{32}$$

This recovers our previous result (17) applying Weyl quantization on the local time of arrival at the origin. As what we have said earlier, this operator is confirmed to be conjugate with the Hamiltonian. Moreover, $\hat{T}_{ho}$ reduces to the classical local time of arrival in the classical limit.

6.4.2. Quartic oscillator. Following similar steps, we derive an explicit expression for the quantum time-of-arrival operator $\hat{T}_{qo}$ for the quartic oscillator. Given the potential $\hat{V}_{qo} = (1/4)\beta\hat{q}^4$, we obtain

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)\cdot\hat{T}_{-m,n} = 4\beta\mu\frac{m}{(n+4)}\hat{T}_{-m-2,n+4} - \beta\mu\hbar^2\frac{m(m+1)(m+2)}{(n+2)}\hat{T}_{-m-4,n+2} \tag{33}$$

for $m > 0$ and $n > 0$, where we have used the commutation relation (21) to arrive at this expression. Repeated application of equation (33) for the specific case of $m, n = 1$, we obtain

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^k\cdot\hat{T}_{-1,1} = (\beta\mu)^k\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\hat{T}_{-2k-2j-1,4k-2j+1} \tag{34}$$

for $k \geqslant 0$, for some constants $c_{k,j}$'s to be determined.

We now prove by induction that equation (34) holds for all $k \geqslant 0$ and in the process determine the recurrence relation that determines the unknown coefficients $c_{k,j}$. With $c_{0,0} = 1$, equation (34) holds for $k = 0$. Now let us assume that equation (34) holds for some $k > 0$. Then

$$\begin{aligned}\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^{k+1}\cdot\hat{T}_{-1,1} &= \left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)\cdot\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^k\cdot\hat{T}_{-1,1}\\ &= (\beta\mu)^k\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)\cdot\hat{T}_{-2k-2j-1,4k-2j+1},\end{aligned} \tag{35}$$

where we have used equation (34) and the linearity of $\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}$. Using equation (33) we have

$$\begin{aligned}\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)\cdot\hat{T}_{-2k-2j-1,4k-2j+1} &= (\beta\mu)\frac{(2k+2j+1)}{(4k-2j+5)}\hat{T}_{-2k-2j-3,4k-2j+5}\\ &\quad-(\beta\mu)\frac{(2k+2j+1)(2k+2j+2)(2k+2j+3)}{4(4k-2j+3)}\hbar^2\hat{T}_{-2k-2j-5,4k-2j+3}.\end{aligned}$$

Substituting this back into equation (35), we have

$$\begin{aligned}\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^{k+1}\cdot\hat{T}_{-1,1} &= (\beta\mu)^{k+1}\sum_{j=0}^{k}(-1)^k\hbar^{2j}c_{k,j}\frac{(2k+2j+1)}{(4k-2j+5)}\hat{T}_{-2k-2j-3,4k-2j+5}\\ &\quad+(\beta\mu)^{k+1}\sum_{j=0}^{k}(-1)^{k+1}\hbar^{2j+2}c_{k,j}\frac{(2k+2j+1)(2k+2j+2)(2k+2j+3)}{4(4k-2j+3)}\\ &\quad\times\hat{T}_{-2k-2j-5,4k+3-2j}.\end{aligned}$$

We now wish to combine the two summations into one summation. This is achieved by shifting index in the second term from $j \rightarrow (j-1)$, which gives

$$\begin{aligned}\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^{k+1}\cdot\hat{T}_{-1,1} &= (\beta\mu)^{k+1}\sum_{j=0}^{k}(-1)^k\hbar^{2j}c_{k,j}\frac{(2k+2j+1)}{(4k-2j+5)}\hat{T}_{-2k-2j-3,4k-2j+5}\\ &\quad+(\beta\mu)^{k+1}\sum_{j=1}^{k+1}(-1)^{k+1}\hbar^{2j}c_{k,j-1}\frac{(2k+2j-1)(2k+2j)(2k+2j+1)}{4(4k-2j+5)}\\ &\quad\times\hat{T}_{-2k-2j-3,4k-2j+5}.\end{aligned}$$

Since $c_{k,j} = 0$ for $j > k$ we can extend the upper limit of the first summation to $(k+1)$; also since $c_{k,j} = 0$ for $j < 0$ we can extend the lower limit of the second summation to $j = 0$.

This allows us to combine the two summations into the single summation

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^{k+1}\cdot\hat{T}_{-1,1} = (\beta\mu)^{k+1}\sum_{j=0}^{k+1}(-1)^j\hbar^{2j}\left[\frac{(2k+2j+1)}{(4k-2j+5)}c_{k,j} + \frac{(2k+2j-1)(2k+2j)(2k+2j+1)}{4(4k-2j+5)}c_{k,j-1}\right]\hat{T}_{-2k-2j-3,4k-2j+5}. \quad (36)$$

Comparing equations (34) and (36), we find that the form of equation (36) follows from equation (34) by changing power from $k \to (k+1)$.

This means that equation (34) holds for any k since k is arbitrary. This in turn yields the recurrence relation satisfied by the coefficients $c_{k,j}$'s. Shifting power from $k \to (k+1)$ in equation (34) and requiring equality of the resulting expression with equation (36) yield the recurrence relation

$$c_{k+1,j} = \frac{(2k+2j+1)}{(4k-2j+5)}c_{k,j} + \frac{(2k+2j-1)(2k+2j)(2k+2j+1)}{4(4k-2j+5)}c_{k,j-1}. \quad (37)$$

An equivalent expression, which is more convenient to solve, can be obtained by shifting index from k to $k-1$,

$$c_{k,j} = \frac{(2k+2j-1)}{(4k-2j+1)}c_{k-1,j} + \frac{(2k+2j-3)(2k+2j-2)(2k+2j-1)}{4(4k-2j+1)}c_{k-1,j-1}. \quad (38)$$

This relation, together with the boundary condition $c_{0,0} = 1$, determine uniquely the coefficients $c_{k,j}$.

The above recurrence relation can be solved by back substitution. That is, by assuming that $c_{k,j}$ is known we can solve for $c_{k+1,j}$. The first few coefficients are given by

$$\begin{aligned}
c_{k,0} &= \frac{\sqrt{2\pi}\,\Gamma(k+1/2)}{4\Gamma(3/4)2^k\Gamma(k+5/4)}\\
c_{k,1} &= \frac{\sqrt{2\pi}\,\Gamma(k+5/2)}{6\Gamma(3/4)2^k\Gamma(k+1/4)} - \frac{\Gamma(3/4)\Gamma(k+5/2)}{2\sqrt{\pi}2^k(2k+3)\Gamma(k+3/4)}\\
c_{k,2} &= \frac{\sqrt{2\pi}\,(8k^3+30k^2+34k-33)\Gamma(k+5/2)}{144\Gamma(3/4)2^k\Gamma(k+1/4)} - \frac{\Gamma(3/4)(2k+11)\Gamma(k+5/2)}{12\times 2^k\sqrt{\pi}\,\Gamma(k-1/4)}\\
c_{k,3} &= \frac{\sqrt{2\pi}\,(8k^4+58k^3+163k^2+143k-705)\Gamma(k+7/2)\Gamma(k+3/4)}{162\Gamma(3/4)2^k(4k-1)\Gamma(k-3/4)\Gamma(k-1/4)}\\
&\quad - \frac{\Gamma(3/4)(4k^3+45k^2+149k-235)\Gamma(k+7/2)\Gamma(k+1/4)}{18\sqrt{\pi}2^k(4k-1)\Gamma(k-3/4)\Gamma(k-1/4)}.
\end{aligned} \quad (39)$$

In principle the recurrence relation can be solved for the rest of the coefficients for a given j.

Assuming that we have solved for the coefficients, the time-of-arrival operator for the quartic oscillator now assumes the form

$$\begin{aligned}
\hat{T}_{qo} &= -\mu\sum_{k=0}^{\infty}(-1)^k\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}_{qo}}\right)^k\cdot\hat{T}_{-1,1}\\
&= -\sum_{k=0}^{\infty}(-1)^k\beta^k\mu^{k+1}\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\hat{T}_{-2k-2j-1,4k-2j+1}.
\end{aligned} \quad (40)$$

This time our solution and the quantized local time of arrival do not coincide, in contrast to that of the harmonic oscillator. We can see the relationship between the two by rearranging equation (40) so that it is instead summed for a given j. This leads us to

$$\begin{aligned}\hat{T}_{qo} &= -\sum_{r=0}^{\infty}\hbar^{2r}\sum_{s=0}^{\infty}(-1)^s\beta^{r+s}\mu^{r+2+1}c_{s+r,r}\hat{T}_{-2s-1,4s+1}\\ &= -\sum_{s=0}^{\infty}(-1)^s\beta^s\mu^{k+1}c_{s,0}\hat{T}_{-2k-1,4k+1} - \hbar^2\sum_{s=0}^{\infty}(-1)^s\beta^{s+2}\mu^{s+3}c_{s+1,1}\hat{T}_{-2s-5,4k+3}\\ &\qquad -\hbar^4\sum_{s=0}^{\infty}(-1)^s\beta^{s+3}\mu^{s+4}c_{s+2,2}\hat{T}_{-2s-9,4k+5} - \cdots. \end{aligned} \tag{41}$$

Note that the leading term is independent of $\hbar$ and the succeeding terms are in increasing order of $\hbar^2$. Given $c_{k,0}$, equation (39), the leading term is explicitly given by

$$\hat{T}_{qo,\hbar^{0.2}} = -\frac{\Gamma(5/4)}{\sqrt{\pi}}\sum_{k=0}^{\infty}\frac{(-1)^k}{2^k}\beta^k\mu^{k+1}\frac{\Gamma(k+1/2)}{\Gamma(k+5/4)}\hat{T}_{-2k-1,4k+1}, \tag{42}$$

where we have used the identity $\Gamma(3/4) = \pi\sqrt{2}/4\Gamma(5/4)$. Comparing this with the Weyl-quantized local time of arrival for the quartic oscillator, $\hat{T}_{0,qo}$, we find that they are the same. That is the leading term of $\hat{T}_{qo}$ is just the failed solution. The separation of the operator $\hat{T}_{qo}$ in this manner shows clearly that correction terms of order $\hbar^2$ and above are required if the complementary relation with the Hamiltonian $\hat{H}_{qo}$ is to hold. Clearly $\hat{T}_{qo}$ reduces to the classical local time of arrival in the classical limit.

Earlier we have shown that the quantized local time of arrival for the quartic oscillator fails to be conjugate with the Hamiltonian. This time it can be shown that $\hat{T}_{qo}$ is conjugate with the Hamiltonian.

7. The Liouville solution and the Bender–Dunne minimal solution

7.1. The Bender–Dunne minimal solution

In [37] Bender and Dunne propose a technique for solving nonlinear Heisenberg equations of motion by deriving an operator function $\hat{F}$ such that $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$. This general procedure consists of employing the operator basis elements $\hat{T}_{m,n}$ so that we obtain an operator expansion

$$\hat{F} = \sum_{m,n}\alpha_{m,n}\hat{T}_{m,n}, \tag{43}$$

where $\alpha_{m,n}$'s are real constants determined by the Hamiltonian. However, a solution $\hat{F}$ that satisfies the commutator relation $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$ is not necessarily unique, i.e. if $\hat{F}_1$ commutes with $\hat{H}$ then so does $\hat{F}_2 = \hat{F}_1 + \phi(\hat{H})$ where ϕ is some function of the Hamiltonian operator. The non-uniqueness of $\hat{F}$ allows one to choose the simplest particular solution satisfying the recursion relation generated from the expansion coefficients $\alpha_{m,n}$. Bender and Dunne call this the 'minimal solution'.

In subsequent examples, we will show the relationship between our Liouville solution $\hat{T}$ and the Bender–Dunne minimal solution.

7.2. Examples

7.2.1. Harmonic oscillator. Assuming an expansion of the form given by equation (43) and imposing the requirement $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$ give us the partial difference equation satisfied by the coefficients

$$(n+1)\alpha_{m-1,n+1} - \mu^2\omega^2(m+1)\alpha_{m+1,n-1} = \mu\delta_{m,0}\delta_{n,0}. \tag{44}$$

Following [37] the minimal solution is the solution that has the 'least' number of coefficients. We quote Bender and Dunne: 'The simplest solution to (44) consists of taking as many $\alpha_{m,n}$'s as possible to vanish . . .. We construct what we call the *minimal solution* by starting with the partial difference equation (44) with $m = n = 0$, in which the inhomogeneous term is present, and deduce the smallest set of $\alpha_{m,n}$'s which are non-vanishing as a consequence of this partial difference equation. All other $\alpha_{m,n}$'s are set to zero'.

Hence setting $m = n = 0$ in the recurrence relation gives the constraint relation $\alpha_{-1,1} - \mu^2\omega^2\alpha_{1,-1} = \mu$. There are three possible cases: $(\alpha_{-1,1} \neq 0, \alpha_{1,-1} = 0)$, $(\alpha_{-1,1} = 0, \alpha_{1,-1} \neq 0)$ and $(\alpha_{-1,1} \neq 0, \alpha_{1,-1} \neq 0)$. The first gives us a solution lying in D_{-+}, the second in D_{+-}, the third connecting D_{-+} and D_{+-}. The third case obviously cannot give a minimal solution because there is one 'more' non-vanishing coefficient. It is useful at this point to introduce the concept of free solutions to the canonical relation $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$. We define a free solution to be a solution of $[\hat{F}, \hat{H}] = \mathrm{i}\hbar\hat{I}$ generated from the constraint relation without involving a free coefficient. Thus, by definition, the third case $(\alpha_{-1,1} \neq 0, \alpha_{1,-1} \neq 0)$ does not generate a free solution because the corresponding solution will involve a free coefficient, either $\alpha_{-1,1}$ or $\alpha_{1,-1}$. On the other hand, the first two cases generate two free solutions.

The two free solutions corresponding to $(\alpha_{-1,1} \neq 0, \alpha_{1,-1} = 0)$ and $(\alpha_{-1,1} = 0, \alpha_{1,-1} \neq 0)$ are respectively given by

$$\hat{F}_{ho,1} = \sum_{k=0}^{\infty}(-1)^k \frac{\mu^{2k+1}\omega^{2k}}{2k+1}\hat{T}_{-2k-1,2k+1} \tag{45}$$

$$\hat{F}_{ho,2} = \sum_{k=0}^{\infty}(-1)^k \frac{\mu^{-2k-1}\omega^{-2k-2}}{2k+1}\hat{T}_{2k+1,-2k-1}. \tag{46}$$

These two solutions have the same density of coefficients in the entire mn-lattice space, and they represent solutions that give the minimum number of non-vanishing coefficients. By Bender–Dunne's definition of minimal solution, both qualify as minimal solutions in the entire $\mathcal{BD}$-space. Bender and Dunne, however, limited their solutions in D_{-+}, leading only to the solution $\hat{F}_{ho,1}$.

By inspection it is immediate that the Liouville solution and Bender–Dunne's minimal solution in D_{-+} are just the negatives of each other. And this implies that, at least for the harmonic oscillator, the Liouville solution is the minimal operator conjugate with the Hamiltonian that reduces to the classical expression in the limit of commuting $\hat{q}$ and $\hat{p}$.

7.2.2. Constant force potential. Now let us consider the potential $\hat{V} = \lambda\hat{q}$. Again assuming a solution in series of the basis $\hat{T}_{m,n}$, we arrive at the recurrence relation $\alpha_{m-1,n+1} + \mu\lambda\alpha_{m+1,n} = \mu\delta_{m,0}\delta_{n,0}$. For $m = n = 0$ this reduces to the constraint relation $\alpha_{-1,1} + \mu\lambda\alpha_{1,0} = \mu$. Again this gives us two free solutions corresponding to $(\alpha_{-1,1} \neq 0, \alpha_{1,0} = 0)$ and $(\alpha_{-1,1} = 0, \alpha_{1,0} \neq 0)$. They yield the two solutions

$$\hat{F}_{cf,1} = \sum_{k=0}^{\infty}(-1)^k\mu^{k+1}\lambda^k \frac{2^k\Gamma(k+1/2)}{\Gamma(1/2)\Gamma(k+2)}\hat{T}_{-2k-1,k+1}, \tag{47}$$

$$\hat{F}_{cf,2} = \frac{1}{\lambda}\hat{T}_{1,0}, \tag{48}$$

the second of which is obviously, by definition, the minimal solution. The minimal solution in the entire Bender–Dunne space does not lie in D_{-+}, but in the boundary of D_{++} and D_{+-}.

But, following Bender and Dunne, if we restrict solving the commutation relation in D_{-+} we arrive at $\hat{F}_{cf,1}$ as the minimal solution. And for this case the Liouville solution and the minimal solution in D_{-+} are negatives of each other again.

7.3. *The Liouville, minimal and free solutions*

The free solutions give us the set of parameter-free solutions to $[\hat{F}, \hat{H}] = i\hbar\hat{I}$ in the entire Bender–Dunne space $\mathcal{BD}$. We have seen in the above two examples that if the Liouville solution exists, then it is a free solution. Moreover, as long as we restrict our solution to the subspace D_{-+} of $\mathcal{BD}$, Bender–Dunne's minimal solution may coincide up to a sign with our Liouville solution, at least for the given examples, including the quartic oscillator (considered in [36, 37]) which we have not given any detail. If we inspect the above examples closer, we find that the crucial condition that makes the Liouville solution and Bender–Dunne's minimal solution coincide (up to a sign) is that they both satisfy the initial condition

$$\alpha_{-1,1} = \mu. \tag{49}$$

The above two minimal solutions, $\hat{F}_{h0,2}$ and $\hat{F}_{cf,2}$, do not satisfy equation (49) and we find that they differ from the Liouville solutions. However, note that when we impose equation (49) on the Bender–Dunne equation for the linear potential, we arrive at the Liouville solution (47). This suggests that we may be able determine the Liouville solution by solving the Bender–Dunne equation under the initial condition given by equation (49).

However, the examples above do not constitute a proof that the Liouville solution and the Bender–Dunne minimal solution agree (up to a sign). It is not clear at the moment if the minimal solution is unique in the D_{-+} quadrant; at least it is for the examples considered here. The situation is not as straightforward for nonlinear systems, because of the many possible solutions that satisfy equation (49). If it turns out that the minimal solution is unique in D_{-+} and that the minimal solution coincide with the Liouville solution, then the Liouville solution is already the minimal solution that satisfies all the required conditions of a quantum first time-of-arrival operator in D_{-+}. In other words, there is no simpler solution than the Liouville solution satisfying all our stated required properties in D_{-+}. (Simpler in the sense of $\hat{F}_{cf,2}$ is a simpler solution to $[\hat{F}, \hat{H}] = i\hbar\hat{I}$ than $\hat{F}_{cf,1}$ in the entire $\mathcal{BD}$.)

But then this leads us to the question of the uniqueness of the solution to the problem as stated in section 4. If $\hat{T}$ is the Liouville solution for a given Hamiltonian $\hat{H}$, then the operator $\hat{T}' = \hat{T} + f[\hat{H}]$, where f is a function that maps $\hat{H}$ into an element of $\mathcal{BD}$, is conjugate with the Hamiltonian and is another solution to the problem by an appropriate choice of the function f; that is f is chosen such that $\hat{T}'$ is symmetric and carries the correct time-reversal symmetry and $\hat{T}'$ reduces to the classical local time of arrival. Then should we accept $\hat{T}'$ as a solution to the problem? If we require that the solution must be the minimal solution in D_{-+} and if the minimal solution is unique in D_{-+} and coincides with the Liouville solution (up to a sign), then we are left with the Liouville solution as the only solution. But that, of course, leads to the question of why the minimal solution and not some other solution. We leave this important problem open in the mean time.

7.3.1. The non-existence of Liouville solution. Earlier we have argued that there cannot be a Liouville solution to the potential $V = \lambda q^{-1}$ because the domain of $\hat{\mathcal{L}}_{\hat{K}}^{-1}$ is not invariant under $\mathcal{L}_{\hat{V}}$. The non-existence of Liouville solution may be construed as a failure of the method. Whether it is a failure of the method or not can be decided upon by inspecting the free solutions. If the free solution contains a solution with the required properties of the Liouville solution, then it is the method's failure to yield this solution. That required property is equation (49) itself.

Again assuming a solution expanded in terms of $\hat{T}_{m,n}$'s, the coefficients satisfy the recurrence relation

$$\frac{1}{\mu}(n+1)\alpha_{m-1,n+1} + \lambda \sum_{j=0}^{\infty} \left(-\frac{\hbar^2}{4}\right)^j \frac{\Gamma(m+2j+2)}{\Gamma(m+1)} \alpha_{m+2j+1,n+2j+2} = \delta_{m,0}\delta_{n,0}, \tag{50}$$

where we have arrived at this by imposing conjugacy with the Hamiltonian again. Observe that for $m = -2$ and $n = -1$ equation (50) reduces to $\alpha_{-1,1} = 0$. The vanishing of $\alpha_{-1,1}$ implies that, whenever a solution to equation (50) exists, the solution for the free particle cannot be recovered continuously from $\hat{F}$ in the limit as $\lambda \to 0$. This is so because the free solution is $\hat{F}' = \mu \hat{T}_{-1,1}$. The singularity of the problem that makes our Liouville solution non-existent is reflected in this vanishing of the coefficient $\alpha_{-1,1}$. The free solution space does not then accommodate a solution satisfying (49). The noted earlier non-existence of solution is then not a failure of the method but a reflection of the fact that indeed no such solution exists in the Bender–Dunne space.

To show that the free solution space is not empty, it is sufficient to give one solution. A solution lying in D_{++} and D_{+-} is given by

$$\hat{F} = \sum_{J=0}^{\infty} \sum_{k=0}^{\infty} \frac{(-1)^{k+J}}{\mu^{k+J} \lambda^{k+J+1}} \beta_{J,k} \left(\frac{\hbar^2}{4}\right)^J \hat{T}_{2k+1,k+2-J},$$

where the coefficients $\beta_{J,k}$ are determined recursively through

$$\beta_{J,k} = \frac{(k+1-J)}{(2k+1)} \beta_{J,k-1} + \sum_{j=1}^{J} \frac{\Gamma(2k+2j+2)}{(2k+1)\Gamma(2k+1)} \beta_{J-j,k+j}$$

with $\beta_{J,k} = 0$ for either $J < 0$ or $k < 0$ and $\beta_{0,0} = 1$. The first few coefficients can be solved

$$\beta_{0,k} = \frac{(k+1)!}{(2k+1)!!}, \qquad \beta_{1,k} = \frac{\Gamma(1/2)\Gamma(2k+4)(3k+4)}{12 \cdot 2^k \Gamma(k+3/2)}.$$

Observe that $\hat{F}$ is in powers of λ^{-1}, which implies that $\hat{F}$ has no meaningful limit as $\lambda \to 0$.

8. The Liouville solution in Φ-representation and the supraquantized local time of arrival

8.1. Supraquantization of the LTOA

In [27] we addressed the circularity of quantization and the problem of obstruction to quantization by proposing the method of supraquantization in which the quantum observable corresponding to a given classical observable is derived not by quantization of the classical observable but by starting from first principles and the axioms of quantum mechanics. There in the classical observable takes the role of a boundary condition as $\hbar$ approaches zero or becomes infinitesimal. The major first principle that is taken is the algebra satisfied by the observable.

There the problem of constructing a quantum time-of-arrival operator conjugate with the system Hamiltonian that derives the classical time of arrival is addressed. This appears similar to the problem being addressed by the paper at hand. However, the difference is that in [27] the problem is directly treated in coordinate representation, in particular, in the rigged Hilbert space $\Phi^{\times} \supset \mathcal{H} \supset \Phi$. There an operator $\hat{\mathcal{T}} : \Phi \mapsto \Phi^{\times}$ is sought with the property of being conjugate with the system Hamiltonian in the generalized sense,

$$\langle\phi|[\hat{H}^{\times}, \hat{\mathcal{T}}]|\varphi\rangle = \mathrm{i}\hbar\langle\phi|\varphi\rangle, \tag{51}$$

where $\phi(q)$ and $\varphi(q)$'s are elements of Φ, and $\hat{H}^{\times}$ is the rigged Hilbert space extension of the Hamiltonian $\hat{H}$ in $\Phi^{\times}$. The operator $\hat{\mathcal{T}}$ is found by appealing to a transfer principle applied to a class of observables, such as to time-of-arrival operators. The principle can be stated as: each element of a class of observables shares a common set of properties with the rest of its class such that when a particular property is identified for a specific element of the class that property can be transferred to the rest of the class without discrimination.

The problem is solved by determining the free particle time-of-arrival operator, and, from this particular result, the rest of the time-of-arrival operators are found by an appropriate use of the transfer principle. It is then determined in [27] that the sought operator $\hat{\mathcal{T}}$ for a given interaction potential $V(q)$ and for arrival at the origin takes the integral operator form

$$(\hat{\mathcal{T}}\varphi)(q) = \int_{-\infty}^{\infty} \langle q|\mathcal{T}|q'\rangle\varphi(q')\,\mathrm{d}q', \tag{52}$$

where the kernel is given by

$$\langle q|\hat{\mathcal{T}}|q'\rangle = \frac{\mu}{\mathrm{i}\hbar}T(q, q')\,\mathrm{sgn}(q - q') \tag{53}$$

and $T(q, q')$, which we refer to as the kernel factor, depends on the Hamiltonian, and is required to be real valued, symmetric and analytic. The kernel factor is the solution to the second-order partial differential equation

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 T(q, q')}{\partial q^2} + \frac{\hbar^2}{2\mu}\frac{\partial^2 T(q, q')}{\partial q'^2} + (V(q) - V(q'))T(q, q') = 0 \tag{54}$$

subject to the boundary conditions

$$T(q, q') = \frac{q}{2}, \qquad T(q, -q) = 0, \tag{55}$$

assuming that the solution exists; we refer to equation (54) as the time kernel equation (TKE). For arrival points other than at the origin, say at x, the operator is found by changing variables in the above equations from $q \to (q + x)$; this is in effect changing the potential from $V(q)$ to $V(q + x)$ and then taking the origin as the arrival point.

The local time of arrival at the origin is then recovered from the time-of-arrival operator $\hat{\mathcal{T}}$ by Wigner transforming the kernel

$$\mathcal{T}_{\hbar}(q, p) = \int_{-\infty}^{\infty} \left\langle q + \frac{v}{2}\right| \mathcal{T} \left|q - \frac{v}{2}\right\rangle \exp\left(-\mathrm{i}\frac{vp}{\hbar}\right)\,\mathrm{d}v. \tag{56}$$

For linear systems, we have $\mathcal{T}_{\hbar}(q, p) = t_0(q, p)$; for nonlinear systems, $\mathcal{T}_{\hbar}(q, p) = t_0(q, p) + \mathcal{O}(\hbar^2)$. That is the local time of arrival derives from the operator $\mathcal{T}$ for infinitesimal $\hbar$, i.e. $\hbar \neq 0$ but $\hbar^2 = 0$.

In this section, we establish the relationship between the Liouville solution and the supraquantized local time of arrival. We show, in particular, that the Φ-representation of the Liouville solution gives the operator $\hat{\mathcal{T}}$. We will do this by showing that the kernels of the operator $\hat{T}$ is just the kernel $\langle q|\hat{\mathcal{T}}|q'\rangle$. Later we will determine the relationship between quantized local time of arrival and $\hat{\mathcal{T}}$.

8.2. The existence and uniqueness of solution for continuous potentials

To establish the existence and uniqueness of solution to the time kernel equation, we transform equation (54) in canonical form by performing a change in variable from (q, q') to $(u = q + q', v = q - q')$. The differential equation (54) and its accompanying boundary conditions (55) assume the canonical form

$$-2\frac{\hbar^2}{\mu}\frac{\partial^2 T}{\partial u \partial v} + \left(V\left(\frac{u+v}{2}\right) - V\left(\frac{u-v}{2}\right)\right) T(u, v) = 0, \tag{57}$$

$$T(u, 0) = \frac{u}{4}, \qquad T(0, v) = 0. \tag{58}$$

Equation (57) is an everywhere hyperbolic differential equation belonging to a known type [38]. Since equation (57) is linear and the potential is continuous, reference [38] assures us that there exists exactly one solution to equation (57) subject to the boundary condition (58) in the square $0 \leqslant u, v \leqslant h$ for arbitrary positive number h. Moreover, the solution is both continuous in u and v. The solution in the rest of the uv-plane is found by extension of $T(u, v)$.

8.3. Liouville solutions in Φ-representation

We now consider the Φ-representation of the Liouville solutions; that is the projection of $\hat{T}$ in Φ as the operator $\hat{T} : \Phi \mapsto \Phi^{\times}$. In this representation the Liouville solution $\hat{T}$ assumes the integral operator

$$(\hat{T}\varphi)(q) = \int_{-\infty}^{\infty} \langle q|\hat{T}|q'\rangle \varphi(q')\, \mathrm{d}q'.$$

If there is a relationship between the Liouville solution and the STOA-operator, this relationship should manifest in the kernels of the two operators. Our goal now is to find the explicit form of the kernel $\langle q|\hat{T}|q'\rangle$ and compare it to the kernel $\langle q|\hat{\mathcal{T}}|q'\rangle$.

If we restrict the interaction potential $\hat{V}$ to those such that $\hat{\mathcal{L}}_{\hat{V}}$ leaves $\tilde{D}_{\hat{K}}$ invariant, then we know that the Liouville solution will only involve sums of the basis vectors $\hat{T}_{-m,n}$ for positive m and n's. Then we are led to find the coordinate representation of the basis vectors $\hat{T}_{-m,n}$. The kernel is

$$\begin{aligned}
\langle q|\hat{T}_{-m,n}|q'\rangle &= \frac{1}{2^n}\sum_{k=0}^{n}\frac{n!}{k!(n-k)!} q^k q'^{n-k}\langle q|\hat{p}^{-m}|q'\rangle \\
&= \frac{(q+q')^n}{2^n}\langle q|\hat{p}^{-m}|q'\rangle \\
&= \frac{(q+q')^n}{2^n}\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\frac{1}{p^m}\,\mathrm{e}^{\mathrm{i}(q-q')p/\hbar} \\
&= \mathrm{i}(-1)^{\frac{1}{2}(m-1)}\frac{(q+q')^n(q-q')^{m-1}}{2^{n+1}\hbar^m(m-1)!}\,\mathrm{sgn}(q-q'),
\end{aligned} \tag{59}$$

where the second line follows from the generalized eigenvalue relation $\hat{q}|q\rangle = q|q\rangle$ and from the binomial theorem; the last line follows with the identification of p^{-m} as a distribution in Φ [39]. Factoring out common factors in the kernel, the kernel of $\hat{T}$ in coordinate representation must take the form

$$\langle q|\hat{T}|q'\rangle = \frac{\mu}{\mathrm{i}\hbar} W(q, q')\,\mathrm{sgn}(q - q') \tag{60}$$

for some function $W(q, q')$ determined by the potential; we will refer to $W(q, q')$ as the Liouville kernel factor. Comparing equation (60) with equation (53), we find an obvious functional similarity between the two kernels. The operator $\hat{T}$ is the Φ-representation of $\hat{T}$ if $W(q,q')$ solves the time kernel equation and satisfies the boundary conditions. We now illustrate that this is the case for the harmonic and quartic oscillators.

8.3.1. Kernel of the harmonic oscillator. Given the explicit form of the Liouville solution, the kernel is given by

$$\begin{aligned}\langle q|\hat{T}_{ho}|q'\rangle &= -\sum_{k=0}^{\infty}(-1)^k\frac{\mu^{2k+1}\omega^{2k}}{2k+1}\langle q|\hat{T}_{-2k-1,2k+1}|q'\rangle\\ &= \frac{\mu}{\mathrm{i}\hbar}\sum_{k=0}^{\infty}\frac{1}{4}\left(\frac{\mu\omega}{2\hbar}\right)^{2k}\frac{(q+q')^{2k+1}(q-q')^{2k}}{(2k+1)!}\operatorname{sgn}(q-q')\\ &= \frac{1}{\mathrm{i}2\omega}\frac{\sinh\left(\frac{\mu\omega}{2\hbar}(q^2-q'^2)\right)}{(q-q')}\operatorname{sgn}(q-q'),\end{aligned}$$

where it is understood that the value along the diagonal in the second line is obtained via the limit $q'\to q$. Comparing this with equation (60), we find that the Liouville kernel factor $W(q,q')$ is

$$W_{ho}(q,q') = \frac{\hbar}{2\mu\omega}\frac{\sinh\left(\frac{\mu\omega}{2\hbar}(q^2-q'^2)\right)}{(q-q')}. \tag{61}$$

Direct substitution of equation (61) back into the time kernel equation (54) shows that it is a solution; moreover, it satisfies the boundary conditions. Since the solution is unique, equation (61) is the sought solution for the harmonic oscillator.

8.3.2. Kernel of the quartic oscillator. Similarly given the explicit form of the Liouville solution for the quartic oscillator, the kernel is given by

$$\begin{aligned}\langle q|\hat{T}_{qo}|q'\rangle &= -\sum_{k=0}^{\infty}(-1)^k\beta^k\mu^{k+1}\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\langle q|\hat{T}_{-2k-2j-1,4k-2j+1}|q'\rangle\\ &= \frac{\mu}{\mathrm{i}\hbar}\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k\sum_{j=0}^{k}c_{k,j}\frac{4^j(q+q')^{4k-2j+1}(q-q')^{2k+2j}}{(2k+2j)!}\operatorname{sgn}(q-q')\end{aligned}$$

From this kernel we extract the Liouville kernel factor

$$W_{qo}(q,q') = \frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k\sum_{j=0}^{k}\frac{c_{k,j}4^j}{(2k+2j)!}(q+q')^{4k-2j+1}(q-q')^{2k+2j}. \tag{62}$$

Note that this satisfies the boundary conditions. It remains to show that it is a solution to the time kernel equation.

To show that indeed it is a solution to the time kernel equation, we work in the uv-plane. Under this coordinates the Liouville kernel factor assumes the form

$$W_{qo}(u,v) = \frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k\sum_{j=0}^{k}\frac{4^jc_{k,j}}{(2k+2j)!}u^{4k-2j+1}v^{2k+2j}. \tag{63}$$

We then use the time kernel equation in canonical form. To that end we need

$$A(u,v)\equiv\left[V\left(\frac{u+v}{2}\right)-V\left(\frac{u-v}{2}\right)\right]=\frac{\beta}{8}(u^3v+uv^3), \tag{64}$$

where we have used the potential $V(q) = \beta q^4/4$ to arrive at this expression. Substituting equations (63) and (64) back into equation (57) and performing some straightforward simplifications, we arrive at

$$-\frac{2\hbar^2}{\mu}\frac{\partial^2 W_{qo}}{\partial u \partial v} + \frac{\beta}{8}(u^3 v + u v^3) W_{qo}(u, v) = \frac{1}{2}\frac{\hbar^2}{\mu}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^{k+1}$$

$$\times \sum_{j=0}^{k+1}\frac{4^j}{(2k+2j+1)!}[-(4k-2j+5)c_{k+1,j} + (2k+2j+1)c_{k,j}$$

$$+4^{-1}(2k+2j-1)(2k+2j)(2k+2j+1)c_{k,j-1}]u^{4k-2j+4}v^{2k+2j+1}. \tag{65}$$

But the quantity in brackets vanishes for all k and j by virtue of the recurrence relation (37) satisfied by the coefficients $c_{k,j}$. Hence equation (65) vanishes identically; that is, $W_{qo}(u, v)$ is a solution to the time kernel equation for the quartic oscillator.

8.4. The equality of $\langle q|\hat{T}|q'\rangle$ and $\langle q|\hat{\mathcal{T}}|q'\rangle$ in Φ

We now show the equality of $\langle q|\hat{T}|q'\rangle$ and $\langle q|\hat{\mathcal{T}}|q'\rangle$ for everywhere analytic potentials of the form $V(q) = \sum_{k=1}^{\infty} v_n q^n$. Under this potential we know that the Liouville solution $\hat{\mathcal{T}}$ exists, and that it is expanded in terms of $\hat{T}_{-m,n}$'s for $m, n > 0$. From the action of $\hat{\mathcal{L}}_{\hat{V}}$ on $\hat{T}_{-m,n}$'s, it is not difficult to see that the Liouville kernel factor has the leading terms

$$W(u, v) = \frac{u}{4} + \text{increasing positive powers of } u \text{ and } v^2 \ldots,$$

where the leading term follows directly from $\hat{T}_0 = -\mu\hat{T}_{-1,1}$. That $W(u, v)$ is in powers of v^2 follows from the time-reversal symmetry property of $\hat{\mathcal{T}}$, that is, every basis vector $\hat{T}_{-m,n}$ involved in the expansion for $\hat{\mathcal{T}}$ is odd in m; since m is odd, then from equation (59), $W(u, v)$ must be even in v. Immediately we find that $W(u, v)$ satisfies the boundary conditions $W(u, 0) = (1/4)u$ and $W(0, v) = 0$. These are just the boundary conditions imposed upon the solutions of the time kernel equation. The harmonic and quartic oscillators above demonstrate this behavior of $W(u, v)$. It then remains to show that $W(u, v)$ solves the time kernel equation; for if it does, it follows from the uniqueness of the solution of the TKE for continuous potentials that $W(u, v)$ is the sought solution for the time kernel equation, or $W(u, v) = T(u, v)$.

If there is any chance that $W(q, q')$ solves the time kernel equation for arbitrary potential, the commutation relation $[\hat{H}, \hat{\mathcal{T}}] = \mathrm{i}\hbar\hat{I}$ must carry over in Φ. That means for all ϕ and φ in Φ we must have

$$\langle\varphi|[\hat{H}, \hat{\mathcal{T}}]|\phi\rangle = \mathrm{i}\hbar\langle\varphi|\phi\rangle. \tag{66}$$

This holds if and only if the algebra of the basis operators $\hat{T}_{m,n}$ carry over in Φ. Since $\hat{\mathcal{T}}$ is expanded in terms of $\hat{T}_{-m,n}$'s for $m, n > 0$ and the Hamiltonian is in the form

$$\hat{H} = \frac{1}{2\mu}\hat{p}^2 + \sum_{s=0}^{\infty} v_s \hat{q}^s$$

it is sufficient to show that $\hat{T}_{-m,n}$'s satisfy the correct commutation relation for $[\hat{p}^2, \hat{T}_{-m,n}]$ and $[\hat{q}^s, \hat{T}_{-m,n}]$ for every positive integer s.

Now the operator basis $\hat{T}_{-m,n}$ is the integral operator $(\hat{T}_{-m,n}\varphi)(q) = \int_{-\infty}^{\infty}\langle q|\hat{T}_{-m,n}|q'\rangle\varphi(q')\,\mathrm{d}q'$ in Φ into $\Phi^{\times}$, whose kernel is given by equation (59). First let us compute the commutator $[\hat{p}^2, \hat{T}_{-m,n}]\Phi$. Now

$$(\hat{p}^2\hat{T}_{-m,n}\varphi)(q) = -\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}q^2}\int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{2^{n+1}\hbar^m(m-1)!}(q+q')^n(q-q')^{m-1}\,\mathrm{sgn}(q-q')\varphi(q')\,\mathrm{d}q'$$
$$= -\hbar^2\int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{2^{n+1}\hbar^m(m-1)!}[n(n-1)(q+q')^{n-2}(q-q')^{m-1}$$
$$+2n(m-1)(q+q')^{n-1}(q-q')^{m-2}$$
$$+(m-1)(m-2)(q+q')^n(q-q')^{m-3}]\,\mathrm{sgn}(q-q')\varphi(q')\,\mathrm{d}q'$$
$$-\frac{3}{2}\mathrm{i}\hbar nq^{n-1}\varphi(q)\delta_{m,1}+q^n\varphi(q)\delta_{m,2}-\mathrm{i}\hbar q^n\varphi'(q)\delta_{m,1}. \tag{67}$$

Also by performing two successive integration by parts, we have

$$(\hat{T}_{-m,n}\hat{p}^2\varphi)(q) = \int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{2^{n+1}\hbar^m(m-1)!}(q+q')^n(q-q')^{m-1}\,\mathrm{sgn}(q-q')(-\hbar^2)\varphi''(q')\,\mathrm{d}q'$$
$$= -\hbar^2\int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{2^{n+1}\hbar^m(m-1)!}[n(n-1)(q+q')^{n-2}(q-q')^{m-1}$$
$$-2n(m-1)(q+q')^{n-1}(q-q')^{m-2}$$
$$+(m-1)(m-2)(q+q')^n(q-q')^{m-3}]\,\mathrm{sgn}(q-q')\varphi(q')\,\mathrm{d}q'$$
$$+\frac{1}{2}\mathrm{i}\hbar nq^{n-1}\varphi(q)\delta_{m,1}+q^n\varphi(q)\delta_{m,2}-\mathrm{i}\hbar q^n\varphi'(q)\delta_{m,1}, \tag{68}$$

where we have dropped surface terms because $\varphi(q)$ and its derivatives have compact supports. Subtracting equation (68) from equation (67) yields the commutator

$$([\hat{p}^2, \hat{T}_{-m,n}]\varphi)(q) = \mathrm{i}\hbar 2n\int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}((m-1)-1)}}{2^{(n-1)+1}\hbar^{(m-1)}((m-1)-1)!}$$
$$\times(q+q')^{(n-1)}(q-q')^{(m-1)-1}\,\mathrm{sgn}(q-q')\varphi(q')\,\mathrm{d}q'+\mathrm{i}\hbar 2q^{n-1}\varphi(q)\delta_{m,1}$$
$$= (\mathrm{i}\hbar 2n\hat{T}_{-m+1,n-1}\varphi)(q),$$

which is just the correct commutation relation (20).

Now let us compute for the commutator $[\hat{q}^s, \hat{T}_{-m,n}]$ for arbitrary positive integer s. We will need the identity

$$(q^s - q'^s) = 2\sum_{j=0}^{\lfloor\frac{s-1}{2}\rfloor}\frac{s!}{2^s(s-2j-1)!(2j+1)!}(q+q')^{s-2j-1}(q-q')^{2j+1}. \tag{69}$$

This identity can be established by changing variables in the left-hand side of equation (69), in particular, $q = (1/2)(u+v)$ and $q' = (1/2)(u-v)$, followed by expanding the resulting binomial series, and then going back to the original variables. The commutator can now be computed,

$$([\hat{q}^s, \hat{T}_{-m,n}]\varphi)(q) = \int_{-\infty}^{\infty}\frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{2^{n+1}\hbar^m(m-1)!}(q+q')^n(q-q')^{m-1}\,\mathrm{sgn}(q-q')$$
$$\times(q^s-q'^s)\varphi(q')\,\mathrm{d}q'$$
$$= \frac{\hbar}{-\mathrm{i}}\sum_{j=0}^{\lfloor\frac{s-1}{2}\rfloor}\frac{s!(2j+m)!}{(s-2j-1)!(2j+1)!(m-1)!}(\hat{T}_{-m-2j-1,n+s-2j-1}\varphi)(q), \tag{70}$$

where we have arrive at the second line by substituting equation (69) for $(q^s - q'^s)$ in the first line, and then performing some simplifications. This is exactly what equation (14) will yield.

We are then assured that the canonical commutation relation $[\hat{H}, \hat{T}] = \mathrm{i}\hbar\hat{I}$ is carried over in Φ; that is, equation (66) holds in the entire Φ. Then we can proceed in showing that $W(q, q')$ is a solution to the time kernel equation. Substituting equation (60) back into the left-hand side of equation (66) and performing two successive integration by parts, we arrive at

$$\langle\varphi|[\hat{H}, \hat{T}]|\phi\rangle = \mathrm{i}\hbar\int_\Sigma \phi^*(q)\left(\frac{\mathrm{d}W(q,q)}{\mathrm{d}q} + \frac{\partial W(q',q')}{\partial q} + \frac{\partial W(q,q)}{\partial q'}\right)\varphi(q)\,\mathrm{d}q$$
$$-\mathrm{i}\frac{\mu}{\hbar}\int_\Sigma \phi^*(q)\left[\left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q^2} + V(q)\right)W(q,q')\right.$$
$$\left. - \left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial q'^2} + V(q')\right)W(q,q')\right]\operatorname{sgn}(q-q')\varphi(q')\,\mathrm{d}q'\,\mathrm{d}q, \tag{71}$$

where Σ is the common support of $\varphi(q)$ and $\phi(q)$. But equation (71) must be equal to the right-hand side of equation (66). Already we have from the boundary condition satisfied by $W(q, q')$ that

$$\frac{\mathrm{d}W(q,q)}{\mathrm{d}q} + \frac{\partial W(q',q')}{\partial q} + \frac{\partial W(q,q)}{\partial q'} = 1. \tag{72}$$

This is true because the first term of equation (72) evaluates to $1/2$ and the last two terms evaluate each to $1/4$; we owe the value $1/4$ from the even powerness of $W(u, v)$ in v. Then the second term must necessarily vanish. But $\phi(q)$ and $\varphi(q)$ are arbitrary; hence, the second term vanishes if and only if the bracketed quantity in the second line identically vanishes

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2 W(q,q')}{\partial q^2} + \frac{\hbar^2}{2\mu}\frac{\partial^2 W(q,q')}{\partial q'^2} + (V(q) - V(q'))W(q,q') = 0. \tag{73}$$

This implies that $W(q, q')$ solves the time kernel equation and it is the required solution because it satisfies the required boundary conditions. Therefore $W(q, q') = T(q, q')$. Or $\langle q|\hat{T}|q'\rangle$ and $\langle q|\hat{\mathcal{T}}|q'\rangle$ are equal for analytic potentials.

9. From Φ-representation to Liouville solution

9.1. Weyl quantization of $\mathcal{T}_\hbar(q, p)$

The previous section has established that one can solve the time kernel equation by solving for the Liouville solution and then extracting the corresponding kernel factor by writing the Liouville solution in coordinate representation. The process is completely reversible. That is starting from the time kernel equation we can construct the Liouville solution.

It is a two step process. First, we take the Wigner transform of the kernel $\langle q|\hat{T}|q'\rangle$ to yield

$$\mathcal{T}_\hbar(q,p) = \int_{-\infty}^{\infty}\left\langle q + \frac{v}{2}\right|\mathcal{T}\left|q - \frac{v}{2}\right\rangle \exp\left(-\mathrm{i}\frac{vp}{\hbar}\right)\mathrm{d}v. \tag{74}$$

And then Weyl quantize $\mathcal{T}_\hbar(q, p)$ using our earlier prescription $p^m q^n \mapsto \hat{T}_{m,n}$. It is not immediately obvious why this prescription should work, but a careful analysis of the above equivalence of $\langle q|\hat{T}|q'\rangle$ and $\langle q|\hat{\mathcal{T}}|q'\rangle$ suggests this prescription. This in turn indicates a way of writing formally the Liouville solution in terms of the supraquantized local time-of-arrival operator

$$\hat{\mathcal{T}} = \int_{-\infty}^{\infty}\mathrm{d}q\int_{-\infty}^{\infty}\mathrm{d}p\,\mathcal{T}_\hbar(q,p)\exp\left[\frac{\mathrm{i}}{\hbar}(q\hat{p} + p\hat{q})\right].$$

This expression should be interpreted more of a symbolic representation of the above prescription of deriving $\hat{T}$ from the time kernel equation or of the relationship between the Liouville solution and the supraquantized local time of arrival.

In this section we demonstrate how the prescription can be implemented, and use the scheme in elaborating the relationship between the Weyl-quantized local time of arrival and the Liouville solution.

9.2. Iterative solution to the time kernel equation

To accomplish our purpose, we need to solve the time kernel equation in a form that is amenable to comparison with the results of the Liouville method. In [27] we solved the time kernel equation by means of the Frobenius method in two dimensions; but this method is not helpful in our goal. We instead solve the time kernel equation in integral form, in particular, in uv-coordinates.

The partial differential equation (57) and the associated boundary conditions (58) are equivalent to the integral equation

$$T(u, v) = \frac{1}{4}u + \left(\frac{\mu}{2\hbar^2}\right)\int_0^u \int_0^v A(x, y)T(x, y)\,\mathrm{d}x\,\mathrm{d}y, \tag{75}$$

obtained by integrating equation (57) twice and then imposing the boundary conditions [41, 42]. Then we attempt at solving this iteratively, that is, by successive approximation of the true solution. With $u/4$ as the leading approximation, we get the following sequence of approximations,

$$\begin{aligned} T_0(u, v) &= \frac{1}{4}u \\ T_n(u, v) &= \frac{1}{4}u + \left(\frac{\mu}{2\hbar^2}\right)\int_0^u \int_0^v A(x, y)T_{n-1}(x, y)\,\mathrm{d}x\,\mathrm{d}y. \end{aligned} \tag{76}$$

The solution is found in the limit as $n \to \infty$ and is given by

$$T(u, v) = \frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\mu}{2\hbar^2}\right)^k R_k(u, v), \tag{77}$$

where $R_k(u, v)$ is solved recursively through

$$R_0(u, v) = u \tag{78}$$

$$R_{k+1}(u, v) = \int_0^u \int_0^v \mathrm{d}x\,\mathrm{d}y\,A(x, y)R_k(x, y). \tag{79}$$

This recursion relation follows from the observation that the last term in the $(n + 1)$st iterate is completely determined by the last term nth iterate. For continuous potentials this iterative solution is known to exist and is unique [38, 41].

9.3. Example

9.3.1. The potential $V(q) = \lambda q^3$. We now demonstrate how we can arrive at the Liouville solution using the time kernel equation for the potential $V(q) = \lambda q^3$. For this potential, we have

$$A(u, v) = \frac{\lambda}{4}(3u^2 v + v^3).$$

Using equations (78) and (79), we can work out the first few $R_k(u, v)$'s and from them infer that

$$R_k(u, v) = \left(\frac{\lambda}{4}\right)^k \sum_{j=0}^{k} \sigma_{k,j} u^{3k-2j+1} v^{2k+2j}, \tag{80}$$

for arbitrary k, where $\sigma_{k,j}$'s are constants. By induction these constants can be shown to satisfy the recurrence relation

$$\sigma_{0,0} = 1, \qquad \sigma_{k+1,j} = \frac{3\sigma_{k,j} + \sigma_{k,j-1}}{(3k - 2j + 4)(2k + 2k + 2)}, \tag{81}$$

which we do not need to solve explicitly. Assuming that we have already solved for the coefficients, we can now write the kernel factor

$$T(u, v) = \frac{1}{4} \sum_{k=0}^{\infty} \frac{1}{2^{2k}} \left(\frac{\mu\lambda}{2\hbar^2}\right)^k \sum_{j=0}^{k} \sigma_{k,j} u^{3k-2j+4} v^{2k+2j}.$$

From this we obtain the kernel of our operator $\hat{\mathcal{T}}$,

$$\langle q|\hat{\mathcal{T}}|q'\rangle = \frac{\mu}{4i\hbar} \left[\sum_{k=0}^{\infty} \frac{1}{2^{2k}} \left(\frac{\mu\lambda}{2\hbar^2}\right)^k \sum_{j=0}^{k} \sigma_{k,j} (q + q')^{3k-2j+4} (q - q')^{2k+2j}\right] \operatorname{sgn}(q - q'), \tag{82}$$

where we have reverted back from uv to qq' coordinates.

9.3.2. The Liouville solution. We now show how the Liouville solution follows from the kernel (82). The Wigner transform of the kernel is given by

$$\begin{aligned} \mathcal{T}_\hbar(q, p) &= \int_{-\infty}^{\infty} \left\langle q + \frac{v}{2} \right| \mathcal{T} \left| q - \frac{v}{2} \right\rangle \exp\left(-i\frac{vp}{\hbar}\right) \mathrm{d}v \\ &= -\mu \sum_{k=0}^{\infty} (-1)^k (\mu\lambda)^k \sum_{j=0}^{k} (-1)^j \sigma_{k,j} \left(\frac{\hbar}{2}\right)^{2j} (2k + 2j)! \frac{q^{3k-2j+1}}{p^{2k+2j+1}}, \end{aligned} \tag{83}$$

where we have used the identity [39]

$$\int_{-\infty}^{\infty} \sigma^{m-1} \operatorname{sgn}(v) \exp(ix\sigma)\, \mathrm{d}\sigma = \frac{2(m-1)!}{i^m} \frac{1}{x^m}$$

to arrive at the second line. Weyl-quantizing equation (83) using the replacement scheme $p^m q^n \to \hat{T}_{m,n}$ yields the operator

$$\hat{\mathcal{T}} = -\mu \sum_{k=0}^{\infty} (-1)^k \hat{S}_k, \tag{84}$$

where

$$\hat{S}_k = (\mu\lambda)^k \sum_{j=0}^{k} (-1)^j \sigma_{k,j} \left(\frac{\hbar}{2}\right)^{2j} (2k + 2j)! \hat{T}_{-2k-2j-1,3k-2j+1}.$$

Comparing the explicit form of the Liouville solution given by equation (27) and equation (84), we find that equation (84) is the Liouville solution if and only if $\hat{S}_k$'s satisfy the recurrence relation

$$\hat{S}_{k+1} = \left(\hat{\mathcal{L}}_{\hat{K}}^{-1} \hat{\mathcal{L}}_{\hat{V}}\right) \cdot \hat{S}_k. \tag{85}$$

and satisfy the boundary condition $\hat{S}_0 = \hat{T}_{-1,1}$. With $c_{0,0} = 1$ the boundary condition is satisfied. To show that recurrence relation (85) holds for $k > 0$ we apply similar method that we have used in the earlier sections. With the commutation relation

$$[\hat{T}_{m,n}, \hat{q}^3] = -\mathrm{i}\hbar 3m\hat{T}_{m-1,n+2} + \tfrac{1}{4}\,\mathrm{i}\hbar^3 m(m-1)(m-2)\hat{T}_{m-3,n},$$

we get after a straightforward calculation

$$\left(\hat{\mathcal{L}}_{\hat{K}}^{-1}\hat{\mathcal{L}}_{\hat{V}}\right)\cdot\hat{S}_k = (\mu\lambda)^{k+1}\sum_{j=0}^{k+1}(-1)^j\left(\frac{\hbar}{2}\right)^{2j}(2k+2j+1)!\left[\frac{3\sigma_{k,j}+\sigma_{k,j-1}}{(3k-2j+4)}\right] \times \hat{T}_{-2k-2j-3,3k-2j+4}. \tag{86}$$

Shifting index in equation (85) from k to $k+1$, we have

$$\hat{S}_{k+1} = (\mu\lambda)^{k+1}\sum_{j=0}^{k+1}(-1)^j\left(\frac{\hbar}{2}\right)^{2j}\sigma_{k+1,j}(2k+2j+2)!\hat{T}_{-2k-2j-3,3k-2j+4}. \tag{87}$$

Subtracting equation (87) from equation (86) gives zero, by virtue of the recurrence relation (81) satisfied by $\sigma_{k,j}$'s; $\hat{S}_k$'s then satisfy the recurrence relation (85). That means the operator, given by equation (84), is the Liouville solution and is arrive at by Weyl-quantizing $\mathcal{T}_\hbar(q,p)$.

9.4. The Weyl-quantized local time of arrival and the Liouville solution

Earlier we have solved for the Liouville time-of-arrival operator for the quartic oscillator and found that the leading term in the solution is the quantized local time of arrival. That result is not peculiar to the quartic oscillator but a general result for nonlinear systems. In [27] we have established the result

$$\mathcal{T}_\hbar(q,p) = t_0(q,p) \qquad \text{for linear systems}$$

$$\mathcal{T}_\hbar(q,p) = t_0(q,p) + \mathcal{O}(\hbar^2) \qquad \text{for nonlinear systems,}$$

where $t_0(q,p)$ is the local time of arrival at the origin. Then by appealing to our result that $\hat{T}$ is the Weyl quantization of $\mathcal{T}_\hbar(q,p)$, we have the general result

$$\hat{T} = \hat{T}_W \qquad \text{for linear systems}$$

$$\hat{T} = \hat{T}_W + \hat{\mathcal{O}}(\hbar^2) \qquad \text{for nonlinear systems,}$$

where $\hat{T}_W$ is the Weyl-quantized local time of arrival. Immediately the Liouville solution reduces to the quantized local time of arrival for infinitesimal $\hbar$, $\hbar^2 = 0$, or the leading term of the Liouville solution is the quantized local time of arrival. This completes our proof that the Liouville solution satisfies all the stated condition for a time-of-arrival operator. Moreover, this constitutes proof of our earlier claim that Weyl quantization of the local time of arrival for linear systems preserves the classical algebra.

The corrections appearing in the Liouville solutions for nonlinear systems maybe interpreted as contributions coming from the Weyl-quantized quantum corrections to the classical equations of motion.

10. The Liouville solution in Φ_l-representation and the confined time-of-arrival operators

10.1. The confined time-of-arrival operators

In [35] one of us developed the theory of confined time-of-arrival operators in one dimension, the quantum arrival theory for spatially confined quantum particles in the interval $[-l, l]$, with the arrival point serving as the origin of the interval. Two classes of confined time-of-arrival operators have been introduced there: the quantized confined time-of-arrival (QCTOA) operators and the algebra preserving confined time-of-arrival (APCTOA) operators. In the language of the current paper, the QCTOA-operators are the Φ_l-representations of the Weyl-quantized local time of arrival in the rigged Hilbert space $\Phi_l^\times \supset \mathcal{H}_l \supset \Phi_l$. The APCTOA-operators are then obtained by appropriately generalizing the functional forms of the QCTOA-operators using the idea of supraquantization. While the QCTOA-operators admits the interpretation as Φ_l-representations of the quantized local time of arrival, the APCTOA-operators do not have similar interpretation there. However, our current results now allow us to give similar interpretation to the APCTOA-operators.

We now show that the algebra preserving confined time-of-arrival operators are the Φ_l-representation of the Liouville time-of-arrival operator $\hat{T}$. First let us specify the momentum operator for the system, which determines the specific representation of $\hat{T}$. The momentum operator is determined by the condition that the Hamiltonian is purely kinetic in the non-interacting case. This condition projects the momentum operator $\hat{p}$ into the ring of momentum operators $\{\hat{p_\gamma} = -\mathrm{i}\hbar\partial_q, |\gamma| \leqslant \pi/2\}$, with $\hat{p}_\gamma$ having the domain consisting of absolutely continuous functions $\phi(q)$ in $\mathcal{H}_l = L^2[-l, l]$ with square integrable first derivatives, which further satisfy the boundary condition $\phi(-l) = \mathrm{e}^{-2\mathrm{i}\gamma}\phi(l)$. Since $\hat{T}$ depends on the momentum operator, the Φ_l-representation of $\hat{T}$ is then the set of operators $\{\hat{T}_\gamma\}$, with each $\hat{T}_\gamma$ corresponding to the momentum $\hat{p}_\gamma$.

To find $\hat{T}_\gamma$'s explicitly we need to have the explicit forms of the basis operators $\hat{T}_{-m,n}$ in $\mathcal{H}_l$ for every γ and for $m, n > 0$, in particular their kernels in coordinate Φ_l-representation. In coordinate Φ_l-representation, the operators $\hat{T}^\gamma_{-m,n}$ in $\mathcal{H}_l$ assume the integral form $\int_{-l}^{l} \langle q|\hat{T}^\gamma_{-m,n}|q'\rangle\varphi(q')\,\mathrm{d}q'$, where the kernels $\langle q|\hat{T}^\gamma_{-m,n}|q'\rangle$ are given by

$$\langle q|\hat{T}^{\gamma\neq0}_{-m,n}|q'\rangle = \frac{(-1)^{\frac{1}{2}(m-1)}(q-q')^{m-1}}{\sin\gamma\hbar^m(m-1)!}\frac{(q+q')^n}{2^{n+1}}(\mathrm{e}^{\mathrm{i}\gamma}H(q-q') + \mathrm{e}^{-\mathrm{i}\gamma}H(q'-q)) \tag{88}$$

$$\langle q|\hat{T}^{\gamma=0}_{-m,n}|q'\rangle = \frac{\mathrm{i}(-1)^{\frac{1}{2}(m-1)}}{\hbar^m}\frac{(q-q')^{m-1}}{(m-1)!}\frac{(q+q')^n}{2^{n+1}}\operatorname{sgn}(q-q') - \frac{\mathrm{i}}{l}\frac{(-1)^{\frac{1}{2}(m-1)}}{2\hbar^m}\frac{(q-q')^m}{(m-1)!}\frac{(q+q')^n}{2^n}. \tag{89}$$

We refer the reader to [35] for a detailed derivation of these expressions. Let us compare the kernel (59) in Φ-representation and the kernel (88) in Φ_l-representation of the $\hat{T}_{-m,n}$ basis operators. Observe that the following factors in the kernels,

$$\frac{\mu}{\mathrm{i}\hbar}\operatorname{sgn}(q-q') \longleftrightarrow -\frac{\mu}{\hbar\sin\gamma}(\mathrm{e}^{\mathrm{i}\gamma}H(q-q') + \mathrm{e}^{-\mathrm{i}\gamma}H(q'-q)),$$

have the common factors. Also let us compare the kernels (59) and (89). We find that the first term of (89) is equal to kernel (59), and the second term is just the integral of the factor of $\mu\operatorname{sgn}(q-q')/\mathrm{i}\hbar$ in $(q-q')$. These observations allow us now to write explicitly the operator $\hat{T}_\gamma$.

In coordinate representation, each $\hat{T}_\gamma$ is the integral operator $(\hat{T}_\gamma\varphi)(q) = \int_{-l}^{l}\langle q|\hat{T}_\gamma|q'\rangle\varphi(q')\,\mathrm{d}q'$ in the Hilbert space $\mathcal{H}_l = L^2[-l, l]$. Using the coordinate representation of the operators $\hat{T}_{-m,n}$ in $\mathcal{H}_l$ for a given γ, the kernel of $\hat{T}_\gamma$ can be shown to be given by

$$\langle q|\hat{T}_{\gamma\neq0}|q'\rangle = -\mu\frac{T(q,q')}{\hbar\sin\gamma}(\mathrm{e}^{\mathrm{i}\gamma}H(q-q') + \mathrm{e}^{-\mathrm{i}\gamma}H(q'-q)); \tag{90}$$

$$\langle q|\hat{T}_{\gamma=0}|q'\rangle = \frac{\mu}{\mathrm{i}\hbar}T(q,q')\,\mathrm{sgn}(q-q') - \frac{\mu}{\mathrm{i}l\hbar}\int_0^{(q-q')} T(u,v)\,\mathrm{d}v\bigg|_{u=q+q'}, \quad (91)$$

where $T(q,q')$ is the kernel factor and $T(u,v)$ is the kernel factor in uv-coordinates. (In [35] the variables $\zeta=(q-q')$ and $\eta=(q+q')/2$ are used in the second term of equation (91). They give the same results, however. Our present notation is more economical in that $T(u,v)$ is used directly.) These are just the APCTOA-operators that we have arrived at in [35] using the idea of supraquantization. In [35] the appearance of the second term in equation (91) is not clear; but its origin is now apparent.

For completeness sake, let us give the quantized confined time-of-arrival operators. The QCTOA-operators are again integral operators $(\hat{T}_\gamma\varphi)(q)=\int_{-l}^{l}\langle q|\hat{T}_\gamma|q'\rangle\varphi(q')\,\mathrm{d}q'$ in the Hilbert space $\mathcal{H}_l=L^2[-l,l]$, whose kernels are given by

$$\langle q|\hat{T}_{\gamma\neq 0}|q'\rangle = -\mu\frac{T_0(q,q')}{\hbar\sin\gamma}(\mathrm{e}^{\mathrm{i}\gamma}H(q-q')+\mathrm{e}^{-\mathrm{i}\gamma}H(q'-q)),$$

$$\langle q|\hat{T}_{\gamma=0}|q'\rangle = \frac{\mu}{\mathrm{i}\hbar}T_0(q,q')\,\mathrm{sgn}(q-q') - \frac{\mu}{\mathrm{i}l\hbar}B_0(q,q'),$$

where

$$T_0(q,q') = \frac{1}{2}\int_0^{\eta}\mathrm{d}s\,{}_0F_1\left(;1;\frac{\mu}{2\hbar^2}\zeta^2\{V(\eta)-V(s)\}\right)$$

$$B_0(q,q') = \frac{\zeta}{2}\int_0^{\eta}\mathrm{d}s\,{}_1F_2\left(\frac{1}{2};1,\frac{3}{2};\frac{\mu}{2\hbar^2}\zeta^2\{V(\eta)-V(s)\}\right)$$

and ${}_pF_q$ is a specific hypergeometric function, with $\zeta=(q-q')$ and $\eta=(q+q')/2$. These can be extracted from the APCTOA-operators by retaining only the leading term in the kernel factor $T(q,q')$.

10.2. *The quartic oscillator CTOA-operator*

Let us illustrate the construction of confined time-of-arrival operators for the case of the quartic oscillator. Given the explicit form of the time-of-arrival operator for the quartic oscillator, we get the following kernel for $\gamma\neq 0$:

$$\begin{aligned}\langle q|\hat{T}_{\gamma\neq 0}|q'\rangle &= -\sum_{k=0}^{\infty}(-1)^k\beta^k\mu^{k+1}\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\langle q|\hat{T}^{\gamma\neq 0}_{-2k-2j-1,4k-2j+1}|q'\rangle\\ &= -\frac{\mu}{\hbar\sin\gamma}\left[\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k\sum_{j=0}^{k}4^j c_{k,j}(q+q')^{4k-2j+1}\frac{(q-q')^{2k+2j}}{(2k+2j)!}\right]\\ &\quad\times(\mathrm{e}^{\mathrm{i}\gamma}H(q-q')+\mathrm{e}^{-\mathrm{i}\gamma}H(q'-q))\\ &= -\frac{\mu}{\hbar\sin\gamma}T_{qo}(q,q')(\mathrm{e}^{\mathrm{i}\gamma}H(q-q')+\mathrm{e}^{-\mathrm{i}\gamma}H(q'-q)),\end{aligned}$$

where the second line follows from the identification that the bracketed quantity in the first line is the kernel factor, and $T_{qo}(q,q')$ is the quartic oscillator kernel factor. This kernel agrees with equation (90).

Now for $\gamma=0$, we get the corresponding kernel after appropriate substitutions and simplifications,

$$\langle q|\hat{T}_{\gamma=0}|q'\rangle = -\sum_{k=0}^{\infty}(-1)^k\beta^k\mu^{k+1}\sum_{j=0}^{k}(-1)^j\hbar^{2j}c_{k,j}\langle q|\hat{T}^{\gamma=0}_{-2k-2j-1,4k-2j+1}|q'\rangle$$

$$
\begin{aligned}
&= \frac{\mu}{\mathrm{i}\hbar}\left[\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k \sum_{j=0}^{k} 4^j c_{k,j}(q+q')^{4k-2j+1}\frac{(q-q')^{2k+2j}}{(2k+2j)!}\right]\operatorname{sgn}(q-q') \\
&\quad - \frac{\mu}{i l\hbar}\left[\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k \sum_{j=0}^{k} 4^j c_{k,j}(q+q')^{4k-2j+1}\frac{(q-q')^{2k+2j+1}}{(2k+2j+1)!}\right] \\
&= \frac{\mu}{\mathrm{i}\hbar} T_{qo}(q,q')\operatorname{sgn}(q-q') \\
&\quad - \frac{\mu}{i l\hbar}\int_0^{(q-q')} \mathrm{d}v \left[\frac{1}{4}\sum_{k=0}^{\infty}\left(\frac{\beta\mu}{16\hbar^2}\right)^k \sum_{j=0}^{k} 4^j c_{k,j}(q+q')^{4k-2j+1}\frac{v^{2k+2j}}{(2k+2j)!}\right] \\
&= \frac{\mu}{\mathrm{i}\hbar} T_{qo}(q,q')\operatorname{sgn}(q-q') - \frac{\mu}{\mathrm{i}l\hbar}\int_0^{(q-q')} T_{qo}(u,v)\,\mathrm{d}v\bigg|_{u=q+q'},
\end{aligned}
$$

where the last line follows immediately from the known form of the kernel factor for the quartic oscillator. This kernel agrees with equations (91).

11. But are they meaningful in the first place?

A question that naturally arises is what exactly is the physical content of the operators that we have constructed. They satisfy the required commutation relation with their respective Hamiltonians and they reduce to the classical local time of arrival. These properties hint that these operators are the quantum versions of the classical time-of-arrival observable. But we need more than these properties to appreciate the substance of these operators or to justify our calling them quantum first time-of-arrival operators. Our recent investigations on the confined time-of-arrival operators give the first intimations that these operators are more than just formal constructs.

For continuous potentials, the CTOA-operators are compact and self-adjoint operators in $\mathcal{H}_l = L^2[-l,l]$; that implies that they possess complete sets of square integrable eigenfunctions with discrete spectra. Numerical simulations for the non-interacting [33, 34] and interacting cases [35] show that the CTOA-eigenfunctions evolve according to Schrödinger's equation such that the *event of the position expectation value assuming the arrival point*, and the *event of the position uncertainty being minimum* occur at the same instant of time equal to their corresponding eigenvalues. We have referred to this dynamical behavior of the CTOA-eigenfunctions as unitary arrival at the given arrival point. Since the eigenvalues are the first times of unitary arrivals of the eigenfunctions, the confined time-of-arrival operators are quantum first time-of-arrival operators, as what we have intended them to be. This demonstrates that the earlier reservations on the quantization of the classical time of arrival is unwarranted. This in turn builds more our confidence on the plausibility that the theory of quantum first time-of-arrival operators based on Liouville time-of-arrival operators can correctly describe quantum first time of arrivals.

Indeed, in [40] one of us developed a theory of quantum first time of arrival based on the operators constructed herein. The theory allows us to compute for the first time-of-arrival distribution for an arbitrary arrival point and for an arbitrary interacting potential. But more than the distribution that can be computed from theory is the insight it provides on the connection between quantum time-of-arrival measurements and the problem of the spatial collapse of the wavefunction on the appearance of particle. It suggests that the appearance of particle arises as a combination of the collapse of the initial wavefunction into one of the eigefunctions of the time-of-arrival operator, followed by the unitary Schrödinger evolution of the eigenfunction. We refer the reader to [40] for a detailed discussion.

12. Conclusion

In this paper, we have constructed representation-free time-of-arrival operators for arbitrary analytic potentials in one dimension. With this we are able to accomplish several things. Foremost, we have been able to show that supraquantized local time of arrival in the entire configuration space and the confined time-of-arrival operators are two distinct representations of one and the same abstract time-of-arrival operator. Moreover, the quantized local time-of-arrival operators are naturally subsumed in the construction, and they can be extracted from the Liouville time-of-arrival operator by setting $\hbar$ infinitesimal. The paper then affectively unites several aspects of quantum time-of-arrival operators into a coherent theory of a single quantum time-of-arrival operator. Moreover, our results endow Bender–Dunne's minimal solution an interpretation beyond Bender and Dunne's original intentions. Our results on the confined time-of-arrival operators give us confidence on the substance of our time-of-arrival operators. That is the quantum first time-of-arrival operators can be given unambiguous physical interpretation within the confines of standard single Hilbert space formulation of quantum mechanics.

However, several problems remain open. For now we are only able to investigate the dynamics of the quantized confined time-of-arrival operator, because of our inability to solve the time kernel equation for nonlinear systems. While in principle we can solve the time kernel equation to give exact results like those we have here, the results are not useful because they cannot be used in solving the eigenvalue problem because of their intractable form. However, due to the non-standard nature of the boundary conditions of the time kernel equation there is still no available algorithm to solve the differential equation numerically; only then that we can fully investigate the effects of the quantum corrections to the classical equations of motion. A more pressing issue is the question of whether the projection of the Liouville time-of-arrival operator in the Hilbert space for the entire configuration space exists or not. In this paper and in earlier papers the projection is only for the operator to act from a set of test functions into its dual space. Their status as a Hilbert space operator is currently not clear, in contrast to the confined time-of-arrival operators which are well-defined self-adjoint Hilbert space operators. Also we have shown that for non-analytic potentials no solution can be found in the Bender–Dunne space. It is possible that a separate theory for non-analytic potentials maybe needed, and it may turn out to be completely different from what we have developed here and elsewhere. Addressing these issues may very well bring us more understanding of the quantum nature of time.

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