Mathematical Models with Nonlocal Initial Conditions: An Exemplification from Quantum Mechanics

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Abstract: Nonlocal models are ubiquitous in all branches of science and engineering, with a rapidly expanding range of mathematical and computational applications due to the ability of such models to capture effects and phenomena that traditional models cannot. While spatial nonlocalities have received considerable attention in the research community, the same cannot be said about nonlocality in time, in particular when nonlocal initial conditions are present. This paper aims at filling this gap, providing an overview of the current status of nonlocal models and focusing on the mathematical treatment of such models when nonlocal initial conditions are at the heart of the problem. Specifically, our representative example is given for a nonlocal-in-time problem for the abstract Schrödinger equation. By exploiting the linear nature of nonlocal conditions, we derive an exact representation of the solution operator under assumptions that the spectrum of Hamiltonian is contained in the horizontal strip of the complex plane. The derived representation permits us to establish the necessary and sufficient conditions for the problem's well-posedness and the existence of its solution under different regularities. Furthermore, we present new sufficient conditions for the existence of the solution that extend the existing results in this field to the case when some nonlocal parameters are unbounded. Two further examples demonstrate the developed methodology and highlight the importance of its computer algebra component in the reduction procedures and parameter estimations for nonlocal models. Finally, a connection of the considered models and developed analysis is discussed in the context of other reduction techniques, concentrating on the most promising from the viewpoint of data-driven modelling environments, and providing directions for further generalizations.

Keywords: nonlocal problems; complex dynamic systems; time-dependent Schrödinger equations; well-posedness; Dunford–Cauchy formula; predictive multiscale modelling; model reductions and computer algebra; structure of space-time; coupled system-environment evolution; driven and dissipative systems; non-Hermitian operators; nonlocal regularization; data-driven dynamic environments

1. Introduction

The development of nonlocal mathematical models has a long history, with perhaps one of the most famous examples related to the de Broglie–Bohm theory as an interpretation of quantum mechanics [1], but rooted deeper in the concept of spacetime [2]. The importance of such models and a wide spectrum of their applicability have also been realized for a long time due to the fact that such models can capture effects and phenomena that traditional models cannot [3]. In quantum mechanics, the development of nonlocal models has been intrinsically interwoven with some of the most intriguing questions, paradoxes, and conceptual challenges, touching the very foundation of the discipline [4–6]. In a classical setting, the roots of this realization can be seen on an example of classical continuum mechanics. In a standard formulation, we think of a solid body as a set of idealized, infinitesimal material volumes, with the only interactions between them being

those described by conservation law equations, supplemented by constitutive relationships and boundary conditions, with a typical assumption on initial conditions as those given "precisely". At the same time, we realize that in reality such a solid body is not an ideal continuum and microstructural details are missing in such a continuum description. In order to account for such details, we should increase the "resolution" of our models, which leads us to a multiscale description of the material system, where we may need to combine our consideration at the macro, meso, micro, and eventually nano levels to account for size effects. However, even such a multiscale description has its limitation, because, on a small enough scale, any continuum description per se would no longer be adequate and would need to be replaced by a discrete model relying on quantum mechanical, and effectively discrete, approaches. What remains to be further appreciated is that whether we use classical or quantum models or their combination, infinitesimal material volumes, as well as particles, can interact nonlocally within spatiotemporal domains of interest.

To address the issue of spatial nonlocality, where interactions can occur at distance, various generalizations of continuum mechanics have been proposed (see, e.g., [7–9] and references therein). Such models play a prominent role in many problems involving fractures and damages of materials and structures, nonsmooth mechanics applications, and other areas. The significance of new developments in nonlocal mathematical models is not limited to the field of mechanics and materials science, as it includes a wide range of cutting-edge problems in biomedical, social, cosmological, and astrophysical sciences (e.g., [10–12]), among many other fields and disciplines where we have to deal with irregular solutions, involving non-differentiabilities, singularities, and discontinuities, and where spatial nonlocality comes naturally.

The situation with temporal nonlocality is strikingly different. While historically it has been connected with Young's type (double-slit) experiments and standard formalisms of quantum mechanics [13–16], overall, a very few works have addressed nonlocality-in-time with the vigor it deserves, and even less so the nonlocality which is present in initial conditions of complex dynamic systems. This paper aims at filling this gap. With this in mind, we organize the paper as follows.

In Section 2, we provide a review of approaches to account for nonlocal effects, in space and in time, and discuss their applications. In Section 3, we provide motivation for considering the evolution of quantum systems that are governed by Schrödinger's models with nonlocal initial conditions, as well as a mathematical formulation of such models. Section 4 provides necessary material related to the functional calculus of special type operators and their representations via the Danford–Cauchy technique. We also briefly review here other approaches, in particular those based on fractional calculus. Section 5 describes a reduction procedure for the nonlocal problem in hand, while Section 6 focuses on details of parameter estimations via computer algebra. Two examples are given in these sections in order to compare the derived conditions for solution existence with the ones already known. The discussion, presented in Section 7, is aimed at elucidating the applicability of the considered models in conjunction with data-driven techniques, as well as at throwing light on connections with stochastic modelling approaches. Possible generalizations and future directions are discussed in Section 8, with concluding Section 9 summarizing the main results of the paper.

2. Accounting for Nonlocality in Mathematical Models and Their Applications

Today, nonlocal models are used routinely in many areas of applications. The main reason for this rests on the fact that nonlocal models provide an improved predictive capability for such applications. For quite some time, this includes problems in contact, fracture, and damage mechanics, materials and structures, stochastic jump processes, subsurface flows, as well as various problems in image recognition, e.g., image deblurring/segmentation. Moreover, nonlocal models have become essential in capturing a broader spectrum of diffusion processes, including anomalous behaviors such as superdiffusion analyzed efficiently with fractional nonlocal models, in describing more accurately plasma and heat

conduction phenomena, and in getting better insight into complex multiscale systems with peridynamics models [7,9,17–20]. Recall also that nonlocal models have played a fundamental role in the analysis of pattern formations since the pioneering ideas that go back to the celebrated work of Alan Turing [21–23]. Their importance in biomedical sciences is well known, including genetics and neuroscience. Among others, such models as nonlocal Fisher-KPP (Kolmogorov–Petrovskii–Piskunov) and Lotka–Volterra are now firmly established as indispensable tool for modelling in these areas [24,25]. Additionally, other sources of nonlocal models are coming from convection-diffusion and reaction-diffusion systems of various types and their considerable range of applications in sciences and engineering [26], as well as from new applications in complex systems and dynamic networks [27–29]. This popularity is largely due to the fact that nonlocal models can handle complex systems involving nonsmooth and possible (discontinuous) singular solutions. As a matter of fact, nonlocal models have emerged as an important tool for simulating complex systems, dynamic networks, processes, and multiscale phenomena where model coupling and reductions are often necessary. The subject, which now also includes a range of far-reaching applications for coupled human-environment systems, such as those from climate challenges, control, AI, and decision-making processes, continues to grow [30–32].

In the study of quantum mechanical dynamic systems, most research carried out to date on nonlocal models has been limited to local initial conditions given "precisely". It has included dispersive and Schrödinger type models, as well as those with Parity-time (PT) symmetric nonlinearities [33–36]. Apart from initial conditions, among known modelling and numerical challenges specific to nonlocal models, we would also mention the prescription of nonlocal boundary conditions, as well as the treatment of nonlocal interfaces. In addition, some of the generic issues and challenges exist with unknown model parameters and nonlocal model identification, discretizations and their implementation, and designs of efficient scalable solvers. With increasing amounts of available data, new perspectives in this field are opening up with physics-informed machine learning approaches, nonlocal neural networks, and other data-driven techniques that would further increase the significance of nonlocal modelling. These issues we discuss in additional detail in Section 7. Now, before embarking on the challenge of nonlocal initial conditions (NICs), we will provide a brief overview of spatial and temporal nonlocalities.

2.1. Spatial Nonlocality

As far as spatial nonlocality concerns, there are a number of well-developed approaches in modelling. One of them has originally grown from continuum mechanics [37], with developed extensions that include now a range of different spatial scales and their interactions, all the way down to the nanoscale. This approach is based on extensions of classical field theory with generalizations of point responses by functionals rather than functions, within the medium of interest. Starting initially from theory of elasticity, it covers today various fields theories such as nonlocal electromagnetic theory, a wealth of problems in science and engineering, including nanoscience and nanotechnology, hydrodynamic-type modelling and its applications, ranging from semiconductors to challenges of climate, as well as cell engineering and other biological applications [38–47]. The latter applications include also such coupled complex systems as the human brain where nonlocal models are becoming increasingly important not only in our better understanding of information processing but also in revealing the onset and development of neurodegenerative diseases, for instance, Alzheimer's and Parkinson's to name just a few, as well as in addressing a challenge of the human behaviour in socially-interacting systems [23,48–51]. Naturally that at a basic level of physics, much research has been centered around various versions of the Bell test, as well as scenarios with corresponding Bell inequalities, and non-classical correlations [52–55]. Such research is critical for further development of quantum information theory, including quantum communication, cryptography, and quantum computation [56,57], with some recent results hinting at possible extensions of entanglement-based quantum communication conventions to relativistic regimes [58]. An-

other approach that has attracted an increasing attention of the researchers, with its direct relevance to nonlocal models, is based on fractional calculus, which allows us to deal with differentiation and integration of arbitrary order, and associated fractional derivatives. It arises in a natural way in a multitude of areas of applied science and engineering, including continuum mechanics and electromagnetic theory, physics and chemistry, biology and ecology, economics and finance, control theory, signal and image processing, rheology and viscoelasticity, aerodynamics, complex systems and media, experimental data fitting and identification problems [59–61]. While singular kernels have been used predominantly in this field, the development of methodologies with non-singular kernels, such as approximations of the Caputo-Fabrizio type, has also been under way during recent years for problems in both classical and quantum settings [62,63], not without certain controversy [64]. At the fractional operator level, a comparison of such kernels with the classical Mittag–Leffler kernel has been recently carried out [65,66] which may result in the development of new numerical-analytical methods useful for applications of nonlocal models. Even though the analysis of nonlocal models based on nonlinear parabolic PDEs in various blow-up and heat localization regimes has been a subject on interest for a long time [67,68], more recently this area has been revitalized in the context of fractional differential models [69,70].

A critically important step forward in this field was the realization of the importance of nonlocal boundary conditions. Although the idea of such conditions can be traced back at least to the works of Hilb [71], it took several decades before the interest to such problems has been reignited due to new arising applications and theoretical challenges [72–75]. Albeit such considerations are often more realistic, it should be noted that so far most attention in this context has been paid to closed systems. Moreover, with a few exceptions [76–79], non-conservative systems fall out from such considerations. At the same time, a large class of nonlocal models has been motivated by dissipative systems which are themodynamically open, exchanging energy and matter with their environments. This class should become an important consideration in recent developments in biological evolution and unifying principles in complex systems dynamics in other disciplines [50,80,81]. Unlocking the full potential of nonlocality can be done if we look not only in space but in time as well. That is what we address next.

2.2. Nonlocality in Time

While the first efforts in this direction go back to the work of great minds of ancient civilizations, which included works of Greek philosophers [82,83], it was Einstein's general theory of relativity that pointed out at space and time as soft, malleable entities, with a consequence for time not being able to extend back indefinitely, as discovered in the 1960-ies by Hawking and Penrose [84,85]. Even though the interest to temporal nonlocality has been growing steadily since then, the theory is in a great need of new developments. In the context of quantum mechanics, some authors distinguish also dynamic nonlocality [86], specific to the quantum equations of motion for the Aharanov–Bohm effect [87]. In the meantime, temporal nonlocality in this context is understood as the ability to impose independent initial and final boundary conditions on the evolution of a quantum system. Both cases are quite different to what we discussed in the previous section. The latter case, in particular, has also been discussed in the context of several quantum paradoxes (e.g., the Quantum Cheshire Cat and the Quantum violations of the pigeonhole principle [88–90]), dealt with by the technique known as pre- and post-selections [91]. Clearly, the importance of temporal nonlocality is not limited to quantum physical systems and the idea that the "flow" of time is the result of correlations between "subsequent" moments of time which are entangled (or correlated) in non-local manner has been re-surging in different forms on many different occasions (e.g., [5,83,92,93] and references therein). This importance touches the foundation of several currently well-accepted theories. For example, if we take a theory of dynamical systems, it relies heavily on the initial conditions of the system we are dealing with, whereas the lack of precision in their choice can lead to instabilities and chaos. The

latter has its routes in the deterministic viewpoint (regardless of the actual mathematical model used) in a sense that it arises from practical inability to know (precisely) the initial conditions of the system. Naturally, a number of proposals have been put forward to mitigate the influence of (imprecise definition of) initial conditions, some of which have been developed in the context of nonholonomic systems, including controlled systems with nonholonomic constraints [94,95]. An approach advocated by some authors is based on avoiding discretization until the last possible moment and, in the context of control problems, on asking the controllability question before discretization [96,97]. While this approach has also been applied to stochastic models, it addresses neither the determinism of initial conditions in such models, nor more subtle questions of nonlocality and the structure of space-time with corresponding frameworks used for it. The latter is the topic of discussions, new proposals, and continuous debates that are seen often in the domain of quantum mechanics [98–104].

A fundamentally different viewpoint comes with the acceptance of complexity and its blend with uncertainty, with new states being interwoven which are inherent in the system because of emergence, the concept known from the time of Aristotle [50,82]. Along this viewpoint, there are several different proposals, leading to possible couplings of the initial conditions with the system in a nonlocal manner, rather than at a single point (e.g., at $t_0 = 0$) as it is conventionally done. These couplings have to be implemented from the beginning of and alongside with the model development, not a posteriori. Based on the idea of ramifications from initial conditions given approximately (RICA), this approach was developed in a series of earlier papers, offering also a new generalized framework for control problems [105–109]. Another attempt along this direction has been labeled as MOND, the Modified Newtonian Dynamics approach [110–112], which is also time-nonlocal.

Time-nonlocal models have been receiving an increasing interest in the physics and engineering communities [113–115] which also generated renewed attention to nonconservative and dissipative systems already mentioned in Section 2.1. Some of the developed approaches, such as the nonlocal-in-time kinetic energy proposal [116], in addition to its numerous applications [117–119], may also be useful in shedding further light into the relationship between classical and quantum mechanics. Another source of applications of such models is due to time-fractional order derivatives (TFODs) and operators such as Caputo's TFODs used in modelling various relaxation and anomalous processes, as well as crossover regimes [30,120,121], with new possible applications to nanoscience and nanotechnology [122]. Naturally, much of the development in this area has been pertinent to open systems [50,123], that is the systems with external interactions as oppose to thermodynamic systems enclosed by rigid immovable walls where certain boundary conditions are assumed, usually disallowing energy (closed systems) or energy and matter (idealized, isolated systems) to enter or leave the system. The challenge here is well known since first advances in quantum mechanics, given that in the general case time cannot be represented by a selfadjoint operator [124–126], and yet this challenge has not been addressed with the vigor it deserves.

In the reminder of this section, we will highlight the development of theory and applications of nonlocal initial conditions, starting from works of L. Byszewski [74,127], who largely pioneered and popularized this topic in the mathematics community. Driven by applications, the interest to NICs has been also continuously fueled in the context of parabolic PDEs, the theory of diffusion and heat conduction, as well as functional differential equations [128–130]. Note also that motivated by mathematical models in such areas as fluids dynamics and geophysics, a number of theoretical results were also obtained for the ultraparabolic and second order evolution equations [131–134]. Other classes of motivational models for NICs have traditionally been integro-differential and dynamic inclusions on time scales [135–138], along with delay differential equations and reaction-diffusion systems [139]. While we were already mentioning fractional diffusion problems as one of the key motivations in this field, it is also worthwhile to point out

that fractional mathematical models with NICs have been a subject of interest [140] where one of the tools for the analysis of their well-posedness relies on Mittag–Leffler functions, traditionally useful in nonlocal models [141,142].

Finally, we also mention that several noticeable examples of non-trivial initial conditions have been discussed in the literature (e.g., such as those with superoscillatory Aharonov–Berry initial data [143–145]), but very little has been done in the context of the NICs for quantum mechanical problems, which is a reason for us to choose our main exemplification from that area and to fill the existing gap.

3. Time-Dependent Non-Homogeneous Schrödinger Equations

Our main exemplification concerns evolutionary models based on non-homogeneous Schrödinger equations. In the abstract setting the evolution of quantum system is governed by differential equation

$$i\psi'_t - H\psi = f(t), \quad t \in [0, T], \tag{1}$$

which is called time-dependent non-homogeneous Schrödinger equation with driving force $f(t)$. Standard axiomatic approach to the quantum mechanics ensures that the state of the system described by a wave function $\psi(t) \in X$, is uniquely determined by (1) and a given initial state ψ_0

$$\psi(0) = \psi_0. \tag{2}$$

This is achieved by requiring that the linear operator (Hamiltonian) $H : X \to X$ is self-adjoint in the Hilbert space X and its domain $D(H) \subseteq X$ is dense. Stone's theorem states that in such a case there exists a strongly continuous unitary group $U(t) = e^{-iHt}$ with generator iH [146]. The function $\psi(t)$ is called a mild solution of (1), (2), if it satisfies the equation

$$\psi(t) = U(t)\psi(0) + \int_0^t U(t-s)v(s)ds, \quad t \in [0, T]. \tag{3}$$

The term $v(t)$ in (3) is defined through the driving force $f(t) = iv(t)$ and can also be thought as a term emerging from an approximation of a more general form of the time-dependent Schrödinger equation or other related models (e.g., [147–149]). Substitution of the initial data from (2) into this general solution representation leads us to the usual propagator formula $\psi(t) = U(t)\psi_0$ for the solution of (1), (2) with $v(t) \equiv 0$.

In this work we consider a nonlocal generalization of condition (2):

$$\psi(0) + \sum_{k=1}^n \alpha_k \psi(t_k) = \psi_1. \tag{4}$$

For the fixed state $\psi_1 \in X$ this condition is determined by the set of parameters $0 < t_1 < t_2 < \ldots < t_n \leq T$, $\alpha_k \in \mathbb{C}$ which will be called the *parameters of nonlocal condition*. Aside from the standard initial condition (2) it generalizes other important types of conditions, such as periodic $\psi(0) = \psi(t_1)$ and Bitsadze–Samarskii conditions $\psi(0) + \alpha_1 \psi(t_1) = \alpha_2 \psi(t_2)$ (e.g., [150]). Formula (4) can be also viewed as approximation to a more general nonlinear condition $\psi(0) + g(t_1, \ldots t_k, \psi(\cdot)) = 0$ for a suitably defined function $g(t_1, \ldots t_k, \cdot) : X \to X$. Among other applications, nonlocal problem (1), (4) is important for the theory of driven quantum systems, where one is interested in a way to recapture specific nonlocal behavior of solution $\psi(0) = \alpha_1 \psi(t_1) + \psi_1$ by changing the properties of driving potential $p(t)$ from the Hamiltonian $H = H_0 + p(t)$ (this may also be of interest in the context of Hamiltonian identification and inverse problems [151–153], Section 6). To stay within the classical formulation (1), (2) this theory routinely operates upon assumption that $p(t)$ is periodic [154–156]. Then, a predictable nonlocal-in-time behavior of the system follows from the Floquet theorem [157]. The case of non-periodic $p(t)$ is much harder to treat, since the Floquet theory can not be applied. Generally, the nonlocal formulation can be viewed as a viable alternative to other proposed generalizations of

periodic quantum driving discussed in the literature (e.g., [158,159]). The above mentioned two-point nonlocal condition with $\psi_1 \neq 0$ can also be thought of as a certain generalization of the renowned Rabi problem [160,161] used in the modern quantum computing for state preparation and information processing [162]. The study of Bose–Einstein condensates was behind the motivation for the analysis of a nonlinear Schrödinger system under nonlocal conditions in [163]. Other motivational examples have been provided in Section 2.

In spite of the increasing importance, a surprisingly little is known about the solution of (1), (4). This type of problems was studied in [164], using the Hilbert space methods. For the self-adjoint H it was proved that the condition

$$\sum_{k=1}^{n} |\alpha_k| < 1$$

is sufficient for the existence of solution to (1), (4), when ψ_1 is a smooth enough vector with respect to H (see [164] for details). The same type condition appeared even earlier in [165], where a more general nonlocal problem for the first order equation with sectorial operator coefficient in a Banach space was considered. Inspired by the subsequent development of this direction (see, e.g., [166]), in the current work we focus on the following generalization of the condition from [164,165]:

$$\sum_{k=1}^{n} |\alpha_k| e^{dt_k} \leq 1. \tag{5}$$

Here d is a half-height of the strip containing the spectrum of operator H defined in the Banach space X. In the course of the work we show that inequality (5) represents only a fraction of the parameter space where problem (1), (4) is well-posed and have a mild solution defined by (3). More generally, we establish new necessary and sufficient conditions for the existence of solution to (1), (4) which can be verified for any given set of α_k, t_k from (4). In addition to that, we derive several versions of sufficient conditions for the solvability of the given nonlocal problem which extend the region of admissible α_k outside the manifold governed by (5).

In what follows, first we will introduce a notion of strip-type operators H acting on Banach space X with the aim to specify the class H such that the propagator $U(t)$ is well-defined and can be represented via the Dunford–Cauchy formula. Then, we will carry out the analysis of solution existence, starting with the reduction of nonlocal problem (1), (4) to a Cauchy problem. Next, the operator calculus will be applied to study the obtained solution operator of nonlocal problem. Theorem 1 of this paper will give the necessary and sufficient conditions for the existence and uniqueness of mild solution to (1), (4). Corollaries 2 and 3 will concern the existence of strong solution and the well-posedness of the given problem. The conditions on parameters α_k, t_k, mentioned in Theorem 1, are verifiable once the values of these nonlocal parameters are specified. When suited with the properly chosen conformal mapping (adjusted to the spectral-strip parameter d), by following the ideas of [167], we will develop the technique which will permit us to reduce the question of solution's existence to the question about the location of roots for a certain polynomial associated with the nonlocal condition. This, in turn, will enable us to obtain the conditions for the existence and uniqueness of the solution to (1), (4) stated in terms of the constraints on t_k, α_k (Theorems 2 and 3 of this paper). Finally, we will compare newly derived conditions against (5), using the three-point nonlocal problem as a model example.

4. Fractional and Functional Calculi in Handling Nonlocality

While fractional calculus is useful in handling nonlocality in space (see Section 2.1), in dealing with nonlocality in time we use some of the key ideas from the functional calculus [168], specifically pertinent to strip-type operators.

With intent to study problem (1), (4) in a Banach space setting, in this section, we review necessary facts from the holomorphic functional calculus for operators with the

spectrum in a horizontal strip [169]. A densely defined closed linear operator H with the domain $D(H) \subseteq X$, whose spectrum belongs to the set

$$\Sigma_d = \{z = x + iy | \ x, y \in \mathbb{R}, \ |y| \le d\}, \tag{6}$$

and the resolvent $R(z, H) \equiv (zI - H)^{-1}$ satisfies

$$\|R(z, H)\| \le \frac{M}{|\Im z| - d}, \quad z \in \Omega \setminus \Sigma, \ \Sigma \subset \Omega, \tag{7}$$

is called a strip-type operator of the height $2d > 0$. The class of such strip-operators goes beyond traditional considerations of classical Hermitian operators and is of major interest for open quantum systems driven away from equilibrium (see Section 8 for further details).

Next, we define the rule to interpret operator functions. Let $f(z)$ be a complex valued function analytic in the neighborhood Ω of the spectrum $\Sigma(H) \subset \mathbb{C}$ and $|f(z)| < c_f(1 + |z|)^{-1-\delta}$, for $\delta > 0$. Suppose that there exists a closed set $\Phi \subset \Omega$ with the boundary Γ consisting of a finite number of rectifying Jordan curves, then the operator function $f(H)$ can be defined as follows

$$f(H)x = \frac{1}{2\pi i} \int_{\Gamma} f(z) R(z, H) x \, dz. \tag{8}$$

This formula yields an algebra homomorphism between the mentioned class of holomorphic functions and the algebra of bounded operators on X, besides any two valid functions of the same operator commute.

Unfortunately, Dunford–Cauchy integral (8) can not be used straight away to define the propagator, because $|e^{-iz}|$ will not vanish as $z \to \infty$ on Γ. Assume that there exists a so-called *regularizer* function $e(z)$ such that both $e(H)$ and $ef(H)$ are well defined in terms of (8) and $e(H)$ is injective. Then the formula

$$f(H) = e^{-1}(H) ef(H) \tag{9}$$

is used to define $f(H)$ for a class of functions wider than the natural function calculus defined by (8) alone. By setting $e(z) = (\lambda - z)^{-1-\delta}$ with $|\Im \lambda| > d$ we ensure that $f(H)x$ is well defined and bounded, whenever $f(z)$ is bounded in Ω and $e^{-1}(H)x$ exists. In other words, the propagator $U(t)$ is bounded linear operator with the domain $x \in D(H^{1+\delta})$. By using the closed graph theorem [170], $U(t)$, $t \in \mathbb{R}$ can be extended to the bounded operator on X when the set $D(H^{1+\delta})$ is dense in X. For more details on the construction and properties of the functional calculus for strip-type operators we direct the reader to the relevant literature (e.g., [168]).

In conclusion of this section, we note that time-fractional mathematical models are gaining popularity too. For example, new versions of fractional Schrödinger equations can be constructed from path integral based on the notions of fractional velocity and the concept of fractional action-like variational approach motivated from fractal arguments (e.g., [171]). However, it is not clear if the methodology that is being developed in that context can potentially be applied to nonlocal initial conditions which are in the focus of our study (see Section 2.2).

5. Reduction of Nonlocal Models

In this section, we focus on a reduction methodology for the time-dependent nonlocal model formulated in Section 3. The development of such reduction procedures is important for both theory and applications of nonlocal modelling [172,173]. When it comes to time-dependent problems, one of the most powerful methodologies for this is provided by computer algebra which has been efficiently used for other complex dynamic systems (e.g., [174–177]). In what follows we demonstrate how to reduce the nonlocal problem (1), (4) to a Cauchy problem.

We depart from the general solution Formula (3), with $\psi(0)$ supplied by (4)

$$\psi(t) = U(t)\left(\psi_1 - \sum_{k=1}^{n} \alpha_k \psi(t_k)\right) + \int_0^t U(t-s)v(s)ds, \tag{10}$$

that is valid for the strip-type operator H under assumptions of Section 4. To get the exact representation for $\psi(t)$ one needs to factor out the unknown $\psi(t_k)$, $k = \overline{1,n}$ from the above formula. We define $w \equiv \sum_{k=1}^{n} \alpha_k \psi(t_k)$ and then formally evaluate this expression by using (10) as a representation for $\psi(t)$. It leads to the equation

$$w = -\sum_{i=1}^{n} \alpha_i U(t_i)w + \sum_{i=1}^{n} \alpha_i U(t_i)\psi_1 + \sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds.$$

By denoting $B = I + \sum_{i=1}^{n} \alpha_i U(t_i)$ we rewrite this equation as follows

$$Bw = B\psi_1 - \psi_1 + \sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds. \tag{11}$$

At this point it is clear that Equation (11) can be solved for w with any combination of ψ_1 and $v(t)$ if and only if the operator function B posses the inverse B^{-1}. In such a case the substitution

$$w = \psi_1 - B^{-1}\psi_1 + B^{-1}\sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds \tag{12}$$

into (10) yields a representation of the general (mild) solution to nonlocal problem (1), (4)

$$\psi(t) = U(t)\left(B^{-1}\psi_1 - B^{-1}\sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds\right) + \int_0^t U(t-s)v(s)ds. \tag{13}$$

Now we can formalize our previous analysis as a theorem.

Theorem 1. *Let H be a strip-type operator with the spectrum Σ, having nonempty point-spectrum component, and the domain $D(H^\delta)$ is dense in X for some $\delta > 1$. The mild solution of nonlocal problem (1), (4) exists and is unique for any $\psi_1 \in X$, $v \in L^1((0;T), X)$ if and only if all the zeros of the entire function*

$$b(z) = 1 + \sum_{k=1}^{n} \alpha_k e^{(-it_k z)}, \tag{14}$$

associated with (4), are contained in the interior of the set $\mathbb{C}\backslash\Sigma$.

Proof. We prove necessity first. A solution to the given nonlocal problem satisfies differential Equation (1), hence general representation (3) is valid for such solution with any given combination of $\psi(0)$, $v(t)$. Upon setting $v(t) = 0$ in this representation, we substitute it into (4) to get the equation

$$B\psi(0) = \psi_1 \tag{15}$$

with respect to $\psi(0)$. Suppose that the function $b(z)$ has a root $z_0 \in \Sigma$ which belongs to the point spectrum of H, with $\varphi \neq 0$ being the corresponding eigenstate. Now, we pick a bounded sequence $\{\psi_{1k}\}_{k=1}^{\infty}$, so that $\psi_{1k} \in D(H^\delta)$, $\psi_{1k} \neq \varphi$ and $\psi_{1k} \to \varphi$ strongly. Such sequence always exists since the domain $D(H^\delta)$ is dense in X. By the theorem's premise,

for any ψ_1 there should exist a corresponding bounded state $\psi(0)$ satisfying (15). To show that this is not true for $\psi_1 = \varphi$, we first evaluate $B\varphi$ via the Dunford–Cauchy integral

$$B\varphi = \frac{1}{2\pi i} \int_\Gamma b(z) R(z, H)\varphi dz = \frac{1}{2\pi i} \int_\Gamma \frac{b(z)}{z - z_0} \varphi dz = b(z_0) = 0,$$

and then apply the general inequality $\|B^{-1}\| \geq \frac{1}{\|B\|}$ to $B^{-1}\psi_{1k}$:

$$\lim_{k\to\infty} \|B^{-1}\psi_{1k}\| \geq \lim_{k\to\infty} \frac{1}{\|B\psi_{1k}\|} = \infty.$$

Next, we prove sufficiency. Assume that all the zeros of $b(z)$ belong to the interior of $\mathbb{C}\backslash\Sigma$. By using the operator function calculus from Section 4 we define

$$B^{-1}\varphi = \frac{1}{2\pi i} \int_\Gamma \frac{1}{b(z)} R(z, H)\varphi dz, \tag{16}$$

for any $\varphi \in X$. The contour Γ satisfying the requirements of (8) exists, since $1/b(z)$ is holomorphic in the neighborhood of Σ. Formula (16), the condition $v \in L^1((0;T), X)$ and Lemma 5.2 from [146] guarantee that the state ψ_0 given by

$$\psi_0 = B^{-1}\psi_1 - B^{-1} \sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds, \tag{17}$$

is well-defined for any combination of $v(t)$ and ψ_1 fulfilling the theorem's assumptions. That, in turn, implies a well-definiteness of $\psi(t)$ given by Formula (13). To prove that $\psi(t)$ is a solution to nonlocal problem (1), (4) we need to check if it satisfies (10). This is trivially done, since (13) is transformed into (10) via the direct manipulation with initial state (17) using (12):

$$\psi_0 = \psi_1 - \psi_1 + \psi_0 = \psi_1 - w = \psi_1 - \sum_{k=1}^{n} \alpha_k \psi(t_k).$$

The uniqueness of solution (13) to the given nonlocal problem follows from the linear nature of both differential Equation (1) and nonlocal condition (4) as well as from the fact that $\psi(t) \equiv 0$ when ψ_1 and $v(t)$ are equal to zero simultaneously. $\quad\square$

We note that the proof of sufficiency relies only on the assumptions needed for the existence of operator function $B(H)\psi$ for any $\psi \in X$. These assumptions do not include the requirement for H having at least one eigenvector, which is essential to prove the necessity of Theorem 1. The theorem concerns the existence and uniqueness of the solution for any possible combination of ψ_1 and $v(t)$. It does not discount the existence of solutions other than (13) for some specific combination of ψ_1 and $v(t)$. Namely, if the nonzero initial data $\psi_1, v(t)$ is chosen in such a way that the right-hand side of

$$B\psi(0) = \psi_1 - \sum_{i=1}^{n} \alpha_i \int_0^{t_i} U(t_i - s)v(s)ds \tag{18}$$

is zero and there is a non-empty intersection between the set of roots of $b(z)$ and the spectrum of H, then one can construct a whole family of non-trivial solutions to (1), (4). Indeed, as we have shown in the proof, every eigenstate of H for which the corresponding eigenvalue coincides with the root of $b(z)$, will satisfy (18) with the zero right-hand side.

It should also be noted, that by its structure, Formula (13) resembles representation (3) of the solution to classical Cauchy problem (1), (2). More precisely, the following is true.

Corollary 1. *Assume that the requirements of Theorem 1 are fulfilled, then the mild solution of nonlocal problem* (1), (4) *is equivalent to the solution of classical Cauchy problem* (1), (2) *represented by* (3), *with the initial state ψ_0 defined by* (17).

The correspondence between the solution of the nonlocal problem and the solution of the classical Cauchy problem permits us to establish other important properties of (1), (4).

Corollary 2. *Assume that in addition to the requirements of Theorem 1 on H, both $b(z)$, ψ_1 belong to $D(H)$ and either one of the following two conditions is satisfied:*

(a) $v(t) \in D(H)$ and $v(t)$, $Hv(t)$ are continuous on $[0,T]$, or

(b) $v(t)$ is continuously differentiable on $[0,T]$.

Then (13) *is a strong (genuine) solution of nonlocal problem* (1), (4).

Proof. We proceed by reducing the proof to the corresponding results on the genuine solution of the classical Cauchy problem ([146], Lemma 5.1). In order to achieve that it is enough to show that the theorem's assumptions imply $\psi_0 \in D(H)$ or, which is equivalent, that $H\psi_0$ is well defined. We depart from (17) and use the above-mentioned properties of functional calculus for strip-type operators:

$$
\begin{aligned}
H\psi_0 &= HB^{-1}\left(\psi_1 - \sum_{i=1}^{n}\alpha_i\int_0^{t_i}U(t_i-s)v(s)ds\right) \\
&= B^{-1}H\psi_1 - B^{-1}\sum_{i=1}^{n}\alpha_i\int_0^{t_i}U(t_i-s)Hv(s)ds.
\end{aligned}
$$

The first term in the last formula is well defined because $\psi_1 \in D(H)$ and there always exists a sequence of states from $D(H^\delta)$ with ψ_1 as a limit, such that $B^{-1}H$ is bounded on the elements of that sequence. By the same token, we can show the well-definiteness of the second term, under the assumption that *(a)* is true. The case of *(b)*, as well as the rest of the proof, follows the proof of the mentioned Lemma 5.1 from [146], and thus will be omitted here. □

The conditions necessary for the existence of the strong solution are closely related to the well-posedness of (1), (4). The evolution problem is called uniformly well-posed in $t \in [0,T]$ (see Section 1.2 of [146]), if and only if the strong solution exists for a dense subspace of the initial data and the solution operator is uniformly bounded in t on compact subsets of $[0,T]$.

Corollary 3. *Let H be an operator satisfying the assumptions of Theorem 1. The nonlocal problem* (1), (4) *is uniformly well-posed in $t \in \mathbb{R}$ for any bounded $t_k \in [0,T]$, $\alpha_k \in \mathbb{C}$ if, and only if, all the zeros of $b(z)$ defined by* (14) *are separated from Σ.*

Proof. In Corollary 2, we have already identified the dense subset $D(H)$ of X such that for any $\psi_1 \in D(H)$ there exists a genuine solution of (1), (4). Assumptions on the parameters of nonlocal conditions imply the boundedness of B^{-1}. In Section 4, we mentioned that $U(t)$ is bounded as well, thus the solution operator from (13) is bounded. To conclude the proof we recall that the propagator $U(t)$ forms the group for $t \in \mathbb{R}$, hence the bounded solution operator is also uniformly bounded ([146], Theorem 2.1). □

Example 1. *Let us consider a two point version of nonlocal problem* (1), (4). *In such simple case, nonlocal condition* (4) *takes the form*

$$
u(0) + \alpha_1 u(t_1) = u_0, \quad t_1 > 0. \tag{19}
$$

Here we assume that H has all the properties mentioned in Theorem 1. To determine the location of zeros of $b(z)$ we need to solve the equation

$$1 + \alpha_1 e^{-zit_1} = 0,$$

assuming that $\alpha_1 \in \mathbb{C}$ and $t_1 \in [0, T]$ are given. It has an infinite number of solutions z_m

$$
\begin{aligned}
z_m &= -\frac{1}{it_1} \ln\left(-\frac{1}{\alpha_1}\right) = \\
&= \frac{1}{t_1}\left[\operatorname{Arg}\left(\frac{1}{\alpha_1}\right) + 2\pi m + i\ln\left|\frac{1}{\alpha_1}\right|\right], \quad m \in \mathbb{Z}.
\end{aligned}
\tag{20}
$$

Here $\operatorname{Arg}(\cdot)$ stands for a principal value of the argument of complex number. The zeros z_m are situated on the line, where the imaginary part $\Im z = \ln|1/\alpha_1|/t_1$ is constant. They will belong to $\mathbb{C} \setminus \Sigma$ if $|\Im z|$ is greater than the half-height d of the spectrum Σ defined by (6). Consequently, the solution of (1), (19) exists if and only if

$$|\alpha_1| < e^{-t_1 d}, \quad \text{or} \quad |\alpha_1| > e^{t_1 d}. \tag{21}$$

The given nonlocal problem is well-defined for any $\alpha_1 \in \mathbb{C}$, except for the complex numbers lying in the annulus $e^{-t_1 d} \le |\alpha_1| \le e^{t_1 d}$.

It is important to note that constraints (21) enforce $|\alpha_1| \ne 1$. That requirement can be relaxed for some $\psi_1, v(t)$ if the spectrum of H is disjoint in the neighborhood of $\mathbb{R}$. Another unique feature of the two-point problem (1), (19) is expressed by one's ability to write the closed-form solution (20), without specifying α_1 beforehand. It becomes impossible for the general case of multi-point nonlocal condition (4), where one must rely on the numerical procedures to solve $b(z) = 0$ and for that reason predefine the parameters of nonlocal condition. For many applications of (1), (4) with $n > 1$ this is not enough as one still would like to have some a priori information about the admissible set of α_k rather than simply check the existence of solution for a fixed sequence $\alpha_k, k = \overline{1, n}$.

6. Parameter Estimations via Computer Algebra

In the general case, zeros of $b(z)$ from Section 5 (see Theorem 1) present a challenge to calculate. To find a way around this challenge (and given the fact that $b(z) = 0$ is not amenable to analytical solution for $n > 1$ and arbitrary α_k, t_k), we start with a general observation suggested by Example 1. Specifically, in the previous section we have shown that under some natural assumptions the question of the well-possedness of (1), (4) can be reduced to the question about the zeros of transcendental function $b(z)$ given by (14) and associated with the parameters α_k, t_k of nonlocal condition (4). In this section, we will show how to estimate nonlocal parameters by using polynomial root finding methods. In particular, we will describe an efficient procedure on how roots of $b(z)$ can be reliably found and, more importantly, how the position of these roots can be characterized in terms of the constraints on $\alpha_k, t_k, 1 \le k \le n$.

The function $b(z)$ can be arbitrary closely approximated by a periodic function $b^\star(z) \equiv 1 + \sum_{k=1}^n \alpha_k e^{(-it_k^\star z)}$, where each $t_k^\star$ is the rational approximation to the corresponding real number $t_k, k = \overline{1, n}$. The function $b^\star(z)$ better suits our needs than $b(z)$, because the equation $b^\star(z) = 0$ can always be reduced to the polynomial root finding problem.

Let

$$t_k = \frac{\lambda_k}{\mu_k}, \quad \lambda_k \in \mathbb{Z}, \quad \mu_k \in \mathbb{N},$$

we set $c_k = \frac{Q\lambda_k}{\mu_k}$, where

$$Q = \frac{\operatorname{LCM}(\mu_1, \mu_2, \ldots, \mu_n)}{\operatorname{GCD}(\lambda_1, \lambda_2, \ldots, \lambda_n)}.$$

is the ratio of the least common multiple (LCM) and the greatest common divisor (GCD) of the numerators and denominators of t_k correspondingly. A substitution

$$\Phi: \ u = \exp\left(-iz/Q\right) \tag{22}$$

transforms the original problem about the location of zeros of $b(z)$ in $\mathbb{C} \setminus \Sigma$ into the problem about the location of zeros of a polynomial

$$r(u) = 1 + \sum_{k=1}^{n} \alpha_k u^{c_k} \tag{23}$$

in the exterior of an annulus

$$\mathrm{Y}: \quad e^{-d/Q} \le |u| \le e^{d/Q}, \quad u \in \mathbb{C}.$$

Now, suppose that we can show that under some conditions the zeros of $r(u)$ (23) belong to $\mathbb{C} \setminus \mathrm{Y}$. This would guarantee that the zeros of the corresponding $b(z)$ belong to the set $\Phi^{-1}(\mathbb{C} \setminus \mathrm{Y}) = \mathbb{C} \setminus \Sigma$ which is our goal. The technique based on the use of transformation $b(z) \to r(u)$ was first applied in [167,178] to the case of abstract nonlocal parabolic problems. Observe, however, that unlike previous works, including [167], the function Φ here transforms the boundary of Σ directly onto the boundary of Y. This allows us to get considerably stronger results regarding the solvability of the given problem than have been previously known (compare, for example, necessary and sufficient conditions of Theorem 3 below versus sufficient conditions of [167]).

The polynomial root finding problem for $r(u) = 0$ has been extensively studied (see, e.g., [179,180] in particular, as well as more generic works and overviews [181–183] and references therein). Polynomial $r(u)$ has exactly c_n roots u_k over $\mathbb{C}$. Their closed form representation exists for $c_n \le 4$. So, now we technically can write the exact solvability conditions for (1), (4) in terms of α_k for k up to 4. More importantly, it is possible to avoid the full solution of $r(u) = 0$ altogether whilst checking $u_k \in \mathbb{C} \setminus \mathrm{Y}$:

$$|u_k| < e^{-d/Q} \vee |u_k| > e^{d/Q}, \quad k = \overline{1, c_n}. \tag{24}$$

The shape of Y suggests that we should narrow our focus on a subclass of available root finding methods with results stated in the form of bounds on roots u_k having satisfied (24). Among those, we choose three effective complex root bounds for $P(u) = \sum_{k=0}^{N} a_k u^k$ (see [178,184–186] for the discussion and comparisons). We have ordered them by the increasing computational complexity. Each of the following bounds has been reformulated as a double estimate to better fit (24).

Lemma 1. *([179], Theorem 2.4) The zeros of $P(u)$ satisfy the following inequalities:*

$$|u| \le \left(1 + \left(\frac{M_s}{|a_N|}\right)^q\right)^{1/q}, \quad |u| \ge \frac{|a_0|}{\left(|a_0| + M_s^q\right)^{1/q}},$$

$$M_s = \left(\sum_{k=1}^{N} |a_k|^s\right)^{1/s}, \quad s, q \in \mathbb{R}_{>1}, \quad \frac{1}{s} + \frac{1}{q} = 1.$$

The next estimate is due to M. Fujiwara [187]. It is the nearly optimal homogeneous bound in the space of polynomials [185]:

Lemma 2. *All zeros of $P(u)$ satisfy the inequalities*

$$|u| \leq 2 \max \left\{ \left| \frac{a_0}{2a_N} \right|^{1/N}, \left| \frac{a_1}{a_N} \right|^{1/(N-1)}, \dots, \left| \frac{a_{N-1}}{a_N} \right| \right\},$$

$$|u| \geq \frac{1}{2} \min \left\{ \left| \frac{2a_N}{a_0} \right|^{1/N}, \left| \frac{a_N}{a_1} \right|^{1/(N-1)}, \dots, \left| \frac{a_N}{a_{N-1}} \right| \right\},$$

where $1/0 = +\infty$.

The third estimate, originally proved by H. Linden [188] and developed further in [178] in the form covering the situation here, gives bounds on the real and imaginary parts of zeros separately.

Lemma 3. *All zeros of $P(u)$ satisfy the double estimate $\max\{V_1^{-1}, V_2^{-1}\} \leq |u| \leq \min\{V_1', V_2'\}$, where*

$$V_1 = \cos \frac{\pi}{N+1} + \frac{|\alpha_N|}{2|\alpha_0|} \left(\left| \frac{\alpha_1}{\alpha_N} \right| + \sqrt{1 + \sum_{k=1}^{N-1} \left| \frac{\alpha_k}{\alpha_N} \right|^2} \right),$$

$$V_2 = \frac{1}{2} \left(\left| \frac{\alpha_1}{\alpha_0} \right| + \cos \frac{\pi}{N} \right) + \frac{1}{2} \left[\left(\left| \frac{\alpha_1}{\alpha_0} \right| - \cos \frac{\pi}{N} \right)^2 + \left(1 + \left| \frac{\alpha_N}{\alpha_0} \right| \sqrt{1 + \sum_{k=2}^{N-1} \left| \frac{\alpha_k}{\alpha_N} \right|^2} \right)^2 \right]^{1/2},$$

and V_i' is obtained from V_i by the substitution $a_k = a_{N-k}$, $k = \overline{0, N}$, $i = 1, 2$.

Now we are in the position to formulate our next result.

Theorem 2. *Suppose that operator H from (1) satisfies the assumptions of Theorem 1 and all t_k in (4) are rational numbers. If at least one bound from Lemmas 1–3 for polynomial (23) induces (24), then the nonlocal problem (1), (4) has the following properties:*

1. *it is uniformly well-posed in $t \in \mathbb{R}$;*
2. *for any $\psi_1 \in X$, $v \in L^1((0; T), X)$ there exists mild solution (13) with the characteristics mentioned in Theorem 1;*
3. *solution (13) will also be strong if $\psi, v(t)$ satisfy either of the requirements, (a) or (b), from Corollary 2.*

Proof. If the zeros u_k of (23) obey (24), their images,

$$z_k = \Phi^{-1}(u_k) = Q[\text{Arg}(u_k) + 2\pi m + i \ln |u_k|],$$

are clearly in the interior of $\mathbb{C} \setminus \Sigma$ no matter what is the value of $m \in \mathbb{Z}$. The application of Theorem 1 and Corollaries 2 and 3 concludes the proof. □

The result of Theorem 2 can be turned into criteria by enforcing the necessary and sufficient conditions for the validity of (24) derived via the Schur–Cohn algorithm ([181], p. 493). For a given polynomial $r(u)$ the algorithm produces a set of up to $2c_n$ inequalities, that are polynomial in α_k, $k = \overline{1, n}$. These inequalities need to be valid simultaneously in order for the Schur–Cohn test to pass ([181], Thm. 6.8b). The precise result is stated as follows.

Theorem 3. *Suppose that operator H from (1) satisfies the assumptions of Theorem 1 and all t_k in (4) are rational numbers. Nonlocal problem (1), (4) has properties 1–3 of Theorem 2 if and only if the polynomials $b(e^{d/Q}u)$, $u^{c_n}b(e^{-d/Q}u)$ pass the Schur–Cohn test for the given set of parameters $\alpha_k \in \mathbb{C}$, $k = \overline{1, n}$ from (4).*

Proof. The substitution $u = e^{d/Q} u'$ ($u = u'^{c_n} b(e^{-d/Q} u')$) transforms right (left) inequality from (24) into the inequality $u'_k > 1$. In both cases the validity of the last inequality is checked by the Schur–Cohn test ([181], Thm. 6.8b). "If" clause of Theorem 1 along with Corollaries 2 and 3 assures the sufficiency. Mapping Φ is a bijection of the vertical strip $|\Im z| \le \pi \frac{\text{GCD}(\mu_1, \mu_2, \dots, \mu_n)}{\text{LCM}(\lambda_1, \lambda_2, \dots, \lambda_n)}$ onto $\mathbb{C}$. The strip's height equals to the period of $b(z)$. This fact guaranties the necessity via application of the "only if" clause of Theorem 1 and Corollaries 2 and 3. $\square$

The following question remains unanswered: what happens when some of t_k are irrational? Consider an approximation $b^\star(z)$ of $b(z)$ mentioned above. If $t_k^\star \to t_k$, $k = \overline{1, n}$ the function $b^\star(z)$ uniformly converges to $b(z)$ on the compact subsets of the open set containing Σ. Hurwitz theorem ([181], Corollary 4.10f) provides the means to claim that all zeros of $b(z)$ lies in the interior of $\mathbb{C} \setminus \Sigma$, if that is true for $b^\star(z) : t_k^\star \to t_k$. The degree of polynomial $r^\star(u)$ corresponding to $b^\star(z)$ grows to ∞ when $t_k^\star \to t_k$ and this t_k is irrational. However, its coefficients α_k are not affected by the increase of $c_n^\star$. This keeps the root estimates from Lemmas 1–3 meaningful. As a result, we have arrived at the following corollary.

Corollary 4. *Assume that for every $k = 1, \dots, n$ the sequence of rational numbers $\left\{ t_{kl}^\star \right\}_{l=1}^\infty$ is such that $\lim_{l \to \infty} t_{kl}^\star = t_k$. If the conditions of Theorem 2 regarding the roots of $r_l^\star(u)$ associated with $t_{kl}^\star$, $k = \overline{1, n}$ are fulfilled for all $l > 0$, then the rest of theorem's statement remains valid for $t_k \in \mathbb{R}$.*

One observation that is worthwhile to note regarding $b(z)$ is that the terms $\alpha_k e^{(-it_k z)}$ from its representation are analytic functions of $t \in [0, T]$. Moreover, for any $\alpha_k < \infty$ these terms remain bounded in an arbitrarily chosen bounded complex neighborhood of the interval $[0, T]$. As a result, in addition to the problem with condition (4), studied in this work, it is also meaningful to consider its modification with an integral nonlocal condition

$$\psi(0) + \int_0^T \psi(s)\beta(s)ds = \psi_1. \tag{25}$$

This condition can even be interpreted as a more general condition, compared to (4), since the latter can be thought as an approximation obtained from (25) by the application of some quadrature formula with the weight function $w(s)$, $\alpha_k = \beta(t_k)w(t_k)$, $\beta(0) > 0$. Problems of type (1), (25) might be more natural than (1), (4) in the situations where only time-averaged knowledge about system's states is available. If $\beta(t_k)$ admits an analytic extension in the neighborhood of $[0, T]$, then the appropriately chosen quadrature will converge to the integral in (25). This would allows us to study (1), (25) by means of the technique developed in Sections 5 and 6 with modifications that would account for an approximation error introduced by the quadrature. Hence, the results for such nonlocal integral conditions are readily obtainable, where the existence conditions for (1), (25), that would imitate (5), can be established following the ideas of earlier works (see, e.g., [189,190]). In other areas, the interest to nonlocal integral initial conditions and their modified versions is also motivated by mathematical models based on fractional differential equations and inclusions, as well as by problems involving dynamic control with state-dependent requirements [191,192]. They include also stochastic and nonlinear formulations, as well as problems with terminal time conditions, arising naturally in various applications [142,193–195].

Now, we would like to demonstrate the application of the presented results on an example of the problem with three-point nonlocal condition and compare the constraints on nonlocal parameters $\alpha_1, \alpha_2 \in \mathbb{R}$ obtained with help of Theorems 2 and 3 against the previously known sufficient condition stated by (5).

Example 2. *Let us consider a version of problem (1), (4) with the strip-type operator having its spectrum Σ_d defined by (6) and three-point nonlocal condition*

$$u(0) + \alpha_1 u(t_1) + \alpha_2 u(t_2) = 0, \quad t_1, t_2 > 0. \tag{26}$$

For simplicity we set $t_1 = 1$, $t_2 = 2$ and consider the non-zero spectral half-height $d = \pi/40$. Then, the equation $b(z) = 0$ is reduced to $1 + \alpha_1 u + \alpha_2 u^2 = 0$. As shown in Figure 1b), the exact conditions on α_1, α_2 calculated by Theorem 3 (the Schur–Cohn algorithm)

$$\begin{bmatrix} \begin{cases} |a_2|^2 < e^{-4d}, \\ e^{4d}|a_1|^2|a_2|^2 - e^{6d}|a_2|^4 - 2e^{4d}|a_2|(|a_1|^2 - |a_2|) + |a_1|^2 < e^{-2d} \\ \begin{cases} |a_2|^2 > e^{4d}, \\ e^{-4d}|a_1|^2|a_2|^2 - e^{-6d}|a_2|^4 - 2e^{-2d}|a_2|(|a_1|^2 - |a_2|) + |a_1|^2 > e^{2d} \end{cases} \end{cases} \end{bmatrix} \tag{27}$$

lead to a considerably wider class of admissible pairs (α_1, α_2) than those obtained by (5).

In fact, the second system of inequalities from (27) gives rise to the unbounded region (union of two unbounded sets depicted in Figure 1b) in the space of parameters $\alpha_1, \alpha_2 \in \mathbb{R}$, meanwhile the solutions of (5) are strictly bounded in $|\alpha_1|, |\alpha_2|$ (the interior of the rhombic region in Figure 1b). They lay within the isosceles triangle which acts as graphical solution of the first system of inequalities in (27). The gap between this triangle and the two other regions containing the solutions of (27) shortens when $d \to 0$, and in the limit is described by $|\alpha_2| = 1$. Comparison of generalized condition (5) from [164,165] and the sufficient conditions provided by Theorem 2 (depicted in Figure 1a) unveils that (5) performs better than the inner circle estimates of Lemmas 1–3 (the part $\mathbb{C} \setminus Y$ defined by the first inequality in (24)). Therefore, when it comes to the a priori estimates on the parameters of nonlocal condition, we advice to use the combination of (5) and the part of Theorem 2 which implies $|u_k| > e^{d/Q}$.
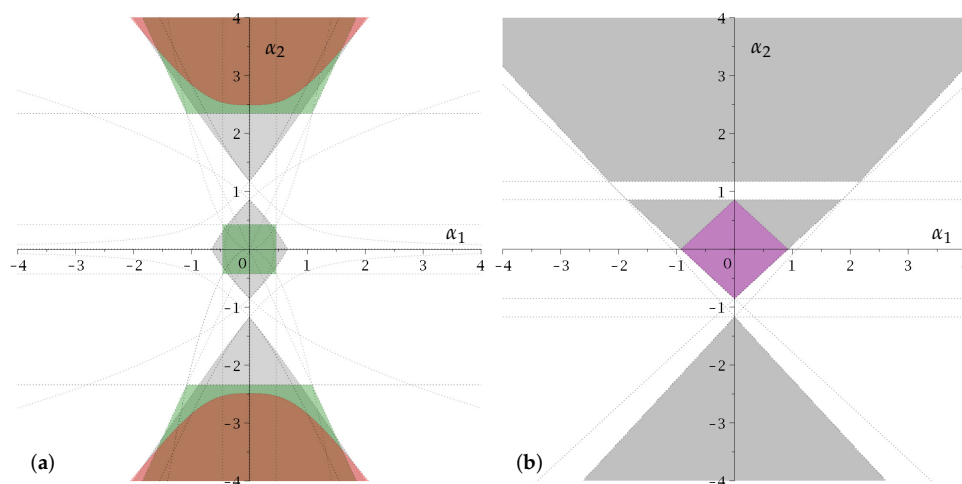

Figure 1. The regions (filled) in the space of parameters $\alpha_1, \alpha_2 \in \mathbb{R}$ from (4) where problem (1), (4) is well-posed, $d = \pi/40$, $t_1 = 1, t_2 = 2$ (color online). (**a**) Application of Theorem 2 and root estimates from: Lemma 1 with $s = q = 2$—dark gray (red); Lemma 2—middle gray (green); Lemma 3—light gray; (**b**) The complete set of feasible (α_1, α_2) via the application of Theorem 3—gray, and set of pairs based on the estimate (5)—dark grey (violet).

We would like to point out that the ability to prove the well-posedness of (1), (4) for a set of nonlocal parameters α_k under condition that some α_k may become unbounded (see Figure 1b) is not a trivial matter. It is, in fact, essential for certain types of applications

of nonlocal problem (1), (4). In this context, we would like to mention problems with quasi-reversibility condition

$$\sum_{k=1}^{n} \alpha_k \psi(t_k) = \psi_1, \tag{28}$$

that, in the simplest case, can be reduced to the terminal-time value problems which we already mentioned earlier in this section. This leads to well-known difficulties connected with non-uniqueness in solving parabolic equations backward in time (e.g., [196]). From a practical perspective, such problems can be coupled with noisy and/or incomplete data and are typical of ill-posed time-reversed systems [197]. Moreover, the source can be driven by a stochastic process, which can be approximated in some cases by classical or fractional Brownian motions [198]. A number of regularization and quasi-reversibility approaches have been developed to solve the resulting inverse problems, including convexification techniques and the construction of Tikhonov-type functionals weighted by a Carleman function [199–201]. The approach we take in this context, which we call the method of nonlocal regularization with quasi-reversibility perturbation (NRQRP), stems from earlier works (e.g., [202,203]), where the associated problems were considered in the form of abstract parabolic equations. Multiple versions of the nonlocal regularization and general regularization techniques have been proposed in the past [204–206], many in the context of image reconstructions and inverse scattering problems, and optimality issues of nonlocal regularization operators from certain classes have recently been studied in [207]. However, as seen in the previous sections, our approach is different as it exploits the nature of nonlocal conditions, where an assumption that the spectrum of Hamiltonian is contained in the horizontal strip of the complex plane plays an important role. This proposal has allowed us to develop an efficient methodology of regularization based on the nonlocal condition at hand. Moreover, the algoritmization of this methodology is amenable to parallelization, which can be a salient feature for more complex problems, including inverse designs of nanostructures and other data-driven applications [208]. It follows the main idea of the numerical technique from [203]. Specifically, in order to regularize problem (1), (28), we perturb the quasi-reversibility condition with a term $\varepsilon\psi(0)$ which, then, transforms to

$$\psi(0) + \frac{1}{\varepsilon} \sum_{k=1}^{n} \alpha_k \psi(t_k) = \frac{1}{\varepsilon} \psi_1. \tag{29}$$

One can approximate the solution of (1), (28) by the solution of problem (1), (29) with small ε, provided that it is well-defined for such ε and, in the limit $\varepsilon \to 0$, converges to the solution of unperturbed problem. Observe that in this scenario the coefficients of nonlocal condition (29) become unbounded and, moreover, one has to know the region of admissible α_k a priori. The approach presented in this paper has these properties and, hence, can be used to analyse quasi-reversible problems.

In the analysis and simulation of complex systems besides those discussed here, computer algebra tools, such as Reduce [175,177,209], provide an efficient way to implement steps similar to those described in the last two sections, as well as to deal with more general situations. The codes for the presented here exemplification from quantum mechanics were written in Maplesoft Maple [210], a standard and easily accessible tool of Computer Algebra Systems.

7. Modelling with Nonlocality in Data-Driven Environments

In this section, we will highlight additional features and challenges connected with the development of mathematical models in the presence of nonlocality, focusing on problems of parameter identification in data-driven environments.

Firstly, it is well known that in its general setting, parametric identification for nonlocal mathematical models leads to an inverse problem [211–213]. In solving inverse problems based on differential and integro-differential equations in data-driven environments, with possible noise, as well unstructured and multi-fidelity data, we can use physics-informed

neural networks (known as pINNs [214]). The growing amount of literature is devoted to inverse problems of parameter identification, including inverse scattering, with new methodologies based on machine learning and deep learning schemes [215] which can potentially be extended to nonlocal mathematical models.

Secondly, in the model development under various situations, e.g., when additional couplings need to be included, the issue of model closure becomes important. This has to be done in a dynamic manner, and one of the possible routes for completing this task lies through a reformulation of the problem as a supervised machine learning (SML) process [216]. In this context, we would like to mention the Nakajima–Zwanzig equation which belongs to the Mori–Zwanzig theory within the statistical mechanics of irreversible processes. By means of a projection operator, the dynamics is split into a slow, collective part (often most relevant part) and a rapidly fluctuating (often irrelevant) part. The goal is to develop dynamic equations for the collective part, and the Nakajima–Zwanzig integral equation has been originally considered as the one describing the time evolution of the "relevant" part of a quantum-mechanical system. It is formulated in the density matrix formalism and can be regarded as a generalization of the master equation. This approach has been popular in the community of mixed quantum-classical dynamics, including problems of nonadiabatic quantum dynamics (beyond the Born–Oppenheimer approximation) and coupling classical and quantum degrees of freedom, where various approximations to the quantum-classical Liouville equation can also be derived [217]. Starting from generalized versions of the master equation, one has to construct an efficient procedure for calculating memory kernels, including non-Markovian cases [218]. Nonperturbative approaches [219–222] can provide here superior efficiency and accuracy improvements, see, e.g., [223] where they were tested on the Fenna–Matthews–Olson (FMO) light-harvesting complexes important in the analysis of photosynthetic systems [224–227]. The problems of reductions of Mori–Zwanzig theory models (not limited to their quantum-classical versions) have been a topic of discussion which included also relevant computational complexity issues [228].

Various extensions of the Nakajima–Zwanzig operator technique [229] and the Mori-Zwanzig representation of a projected dynamical system have been proposed in the literature [230]. The idea of coupling the system with a heat bath, conventionally used in many classical settings, such as molecular dynamics, faces new challenges in the context of these problems. In particular, it is the case when open systems are considered such that dissipation processes have to be accounted for in the underlying system-environment evolution. While the Nakajima–Zwanzig methodology has been used extensively within the mathematical framework of dynamical systems [231] (see Section 2 for limitations of the corresponding models), several new promising formalisms have been proposed to unify this commonly used Nakajima–Zwanzig approach for reduced density matrix dynamics with the more versatile Mori theory in the context of nonequilibrium dynamics, allowing also to accurately calculate equilibrium time correlation functions of many-body quantum systems [232,233]. With the advance of data-driven models, new reduction methodologies have been under active developments in this field [234].

In the meantime, the issue of coupling is coming at the forefront of research in these areas since the coupling of quantum systems to some external degrees of freedom can barely be neglected, not only due to fundamental theoretical reasons but also due to restrictions imposed by the implementation of leading-edge quantum technologies [235]. In developing plausible approaches here, one should take into account nonlocality. A possible way to do so would be to explore a connection between the local (time-convolutionless) and nonlocal descriptions of open quantum system dynamics, as has been done in the above-quoted paper [235]. While main results were presented for semi-Markovian evolution, these ideas might also be useful in the non-Markovian regimes.

Nonlocal models have become increasingly important in many stochastic applications where nonlocal initial conditions have also been considered. Some of the well-known examples with nonlocal initial conditions for quantum systems include the analysis of

the von Neumann entanglement entropy via reduced density evolution operators [236]. Clearly, this interest has not been limited to just quantum systems with recent developments included a relationship between stochastic processes and nonlocal versions of classical models [237], as well as new probabilistic approaches to known nonlocal models [238]. Based on the Stochastic Variational Inference technique, Bayesian learning coarse-grained methodologies with probabilistic state-space have also been receiving attention in the analysis of complex systems dynamics in data-driven environments [239] which could present interest for nonlocal models. Many parameterization methods related to the Mori-Zwanzig formalism have been a natural development of control-theoretical ideas such as Kalman-filtering which allowed the construction of reduced models for both classical and quantum systems, including those based on Schrödinger equations [240]. With the ready availability of data, it is often necessary to deal with non-Markovian character of such data sets which can be done with new reduction approaches based in their core on the Mori–Zwanzig theory, as discussed above, and certain projection techniques, e.g., Nakajima–Zwanzig, Wiener, etc. [234,241].

8. Discussion and Generalizations

Nonlocal problems have become ubiquitous in the modelling of many real-world systems, processes, and phenomena. Inverse and control problems provide a rich source of such problems, which is particularly true in the era of big data. For example, as mentioned earlier, they arise naturally in inverse scattering problems [242], where the presence of measured scatted data nonlocal boundary conditions are typical, and advanced data-based methodologies, such as deep learning schemes [215], may be required. Other substantial sources are provided by open driven systems, and in particular driven quantum systems [50,158,243–245], including those for Floquet engineering [246], quantum information control with quantum computing applications [247], as well as various nonlinear problems such as those described by Rabi's models, providing, among other things, new perspectives on the entanglement via the von Neumann entropy [248,249]. It is envisaged that in dealing with such systems, communication complexity will play a progressively growing role. One of the challenges lies with the development of efficient algorithms to discriminate between local and non-local correlations, a task, which in its generality, maybe intractable [52,250]. Moreover, while experiments on quantum systems are typically divided into the preparation of states and the registration of observables, it is well-known that, based on traditional mathematical methods, it is not possible to distinguish between observables and states [251,252], which stimulates the development of new approaches in this field, some of which are based on the ideas discussed in this paper.

Clearly, dissipative quantum systems of nonequilibrium physics are at the forefront of many motivations behind nonlocal models [246]. Therefore, as an intriguing direction for generalizations of some of the ideas presented in this paper, we would like to point out to time-dependent models of non-Hermitian quantum mechanics [253–255], as well as to non-Hermitian operators in general, given their prominent role in the study of dissipative systems, not just limiting to quantum mechanics [256,257]. It is interesting to note that pseudospectra, known for their non-trivial behavior even in relatively simple cases [258], have been considered to be playing a central role in mechanics with non-Hermitian operators [259]. It has been known for quite some time that such operators are omnipresent in the problems where we have to couple a system under the study to a generic dissipative environment [260–263]. In addition to that, new powerful stimuli to the development in this field have been coming from the works on non-Hermitian Hamiltonians having PT symmetry. Pioneered by Bender and Boettcher with the demonstration of real spectra of such operators (see, e.g., [264] and references therein), we have been witnessing new experimental results and applications that have appeared in this field during recent years [265], including the works on PT-symmetry breaking non-Hermitian operators which are relevant to both classical and quantum regimes [266,267].

9. Conclusions

The paper has provided an overview of the current state-of-the-art in nonlocal modelling, in both space and time. While both classical and quantum systems have been considered, special attention has been given to nonlocal initial conditions with the main focus on and exemplification from quantum mechanics. Specifically, we have analyzed a nonlocal-in-time problem for the abstract Schrödinger equation. We have established the dependence of the solution to this problem on the parameters of nonlocal conditions, derived well-posedness criteria, and proved the theorems concerning the existence of the solution under different regularities. The conditions on the existence of the solution to the given nonlocal problem obtained here generalize other results available in the literature (beyond the case of α_k bounded by (5)). To demonstrate the developed methodology for the analysis of nonlocal models, the obtained results have been applied to the general two- and three-point nonlocal problems. For each model problem, we have been able to describe analytically the entire manifold of admissible parameters of the corresponding nonlocal condition.

The technique used to prove the main results of Sections 5 and 6 of this paper relies on the linear nature of the problem and the existence of exact representation for the solution operator via the Dunford–Cauchy formula. The results of the paper can be generalized in a fairly straightforward manner to several other classes of nonlocal problems for Schrödinger-type equations. Other generalizations are less trivial, and they have been discussed in further detail in the paper. In addition to the case of a classical Schrödinger operator, the developed methodology for the analysis of nonlocal models can be applied to the situations where this operator may be non-Hermitian. Among other possibilities, covering both quantum and classical dissipative systems, the latter situations occur frequently in the modeling of open quantum systems, where the anti-Hermitian part of the Hamiltonian describes the interaction of the quantum systems with its dissipative interfaces and surroundings. Such possible generalizations have been also discussed, along with a connection of the considered models and developed analysis in the context of novel reduction techniques and their applications in data-driven modelling environments.

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