

Resolution of the singularity of the ODE $x'=x^2$ when the initial x has uncertainties

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Abstract

We show that the classical initial value problem $x'=x^2$ has a continuous solution for all time, when the initial x has any finite amount of uncertainties (which is unavoidable in engineering). This is in stark contrast with the singular solution when x has no uncertainties.

General picture

Consider a sample space defined by the real line. Since we can always define a wave-function by taking the square-root of the probability measure, the Koopman-von Neumann version of classical statistical mechanics[1][2][3][4] defines classical statistical mechanics as a particular case of quantum mechanics where the algebra of observable operators is necessarily commutative (because the time-evolution is deterministic).

However, it is well known that for two unbounded self-adjoint operators, the fact that they commute does not imply that their corresponding spectral measures commute[5], then we would say that they *strongly* commute. Thus in principle, it is possible to have a classical dynamical system defined by an *ordinary differential equation* where the unitary time-evolution is non-deterministic, that is, the algebra of observable operators is non-commutative. We will not study this possibility here, this is consistent with the fact that in a continuous standard probability space we can not neglect uncertainties, for that we would need to work in the larger space of finitely additive measures[6], which has very different properties than a standard probability space. Note that such solutions non-deterministic solutions do not appear if at the initial time, there is a joint probability distribution for all the random variables appearing in the ordinary differential equation, which is a common assumption.

Since the real line is a simply connected group (for addition), then by Bargmann's theorem any strongly continuous projective representation of the real line is induced by some strongly continuous representation of the real line on the corresponding Hilbert space[7][8]. Then, Stone's theorem implies that such representation on the Hilbert space is the exponential of a time-independent Hamiltonian[7][8]. Thus, if there is a solution in a standard probability space of a differential equation without singularities for all times (including negative times), then there is a quantum Hamiltonian corresponding to such solution which is time-independent. Moreover, if such solution is deterministic then the fact that there are more Hamiltonians that generate the same differential equation does not change the unique solution, up to initial conditions: suppose that $x(t) = U(t)x(0)U^\dagger(t)$ is a deterministic solution to the differential equation, then $x(t) = f(x(0),t)$ is a

measurable function of $x(0)$ and it can be rewritten as $c(t) = U_2^\dagger(t)x(t)U_2(t) = U_2^\dagger(t)f(x(0), t)U_2(t)$. It verifies $\dot{c} = U_2^\dagger(t)[H - H_2, f(x(0), t)]U_2(t) = 0$, because the difference between Hamiltonians must preserve the differential equation. Thus $x_2(t) = U_2(t)x(0)U_2^\dagger(t) = U_2(t)c(t)U_2^\dagger(t) = x(t)$. Then, $x(t) = U(t)x(0)U^\dagger(t)$ is the unique solution, up to initial conditions.

Moreover, any solution in a standard probability space is given by a time-dependent self-adjoint Hamiltonian in a larger probability space, then the singularities in a standard probability space are consequence of a time-dependent Hamiltonian which is non-integrable. But since any time-dependent Hamiltonian can be converted into a time-independent Hamiltonian in an even larger sample space, then we can always resolve the singularities in a larger sample space which better defines the dynamical system. Thus, solutions without singularities for all times (including negative times) defined by time-independent Hamiltonians are expressive enough, even to deal with singularities at the cost of choosing a larger sample space.

State-of-the-art

Consider the differential equation: $\dot{x} = x^2$. The general solution without uncertainties is:

$$x(t) = \frac{x(0)}{1 - t x(0)} \quad (1)$$

The general solution has a singularity at $t = \frac{1}{x(0)}$. There are no solutions without singularities, when the uncertainty is neglected[9].

When considering uncertainties, if we assume that the solution Equation 1 exists for some $t > 0$, then there is an isometry $T(t)$ such that $x(t) = T^\dagger(t)x(0)T(t)$ is a real number for all eigenvalues of $x(t)$, since the total probability must be conserved and the solution is deterministic. The eigenvalues of the operator $x(0)$ such that $x(0) > \frac{1}{t}$ have no corresponding $x(t)$ which is a real number given by the isometry in agreement with the solution Equation 1, because the deterministic solution becomes ill-defined for $t \geq \frac{1}{x(0)}$. We can repeat the same reasoning for $t \leq 0$. Thus, we conclude that the solution Equation 1 is implemented by a non-unitary isometry when working with probability measures, for all $t \neq 0$. This is a time-dependent restriction on the allowed initial probability measures, for instance any initial Gaussian distribution is not allowed for any $t \neq 0$. The solution Equation 1 can also be implemented by a unitary operator at the cost of choosing a larger sample space, which we will do in the following.

We could think that a unitary time-evolution is somehow too demanding, that only with restrictions to the allowed initial probability measures we can find all solutions to the differential equation defined above. But as a matter of principle that should not be correct since we always work with such restrictions under the assumption that we will somehow be able to recover a corresponding result in the space of probability measures, otherwise such result cannot be tested experimentally or even in most numerical simulations (due to approximation uncertainties). Indeed, if we consider the space $L^2(\mathbb{R}^2)$ and the complex number $z(t) = x(t) + iy(t)$ satisfying $\dot{z}(t) = z^2(t)$ then the singularity condition $t \rightarrow \frac{1}{z(0)}$ cannot be satisfied except in a set of null measure where $y(0) = 0$, thus there is no singularity in $L^2(\mathbb{R}^2)$. But $y(0)$ can be as concentrated around zero as we want, so this unitary solution in a larger sample space recovers the corresponding non-unitary solution in the original sample space.

Changing the sample space, effectively changes the equation, since $y(0) = 0$ strictly is not possible in $L^2(\mathbb{R}^2)$. This has been the approach so far to resolve the singularities: modify the equation until no singularities exist up to some large finite time for some interval of interest for the initial value. For instance, the 3D Euler's equations appear to be appropriate for many problems, however since there is evidence that they have finite-time singularities[10] then we can instead use the more general 3D Navier-Stokes equations in the hope that they don't have singularities for the parameters of interest. That is why it is so important to find out whether or not the 3D Navier-Stokes equations have singularities[10], because then we may need yet another set of equations. But this approach does not work in most real-world cases because it is very hard to predict whether or not a differential equation has singularities for the parameters of interest in a specific real-world problem[10]. So, in each specific real-world problem, engineers have to test and modify differential equations several times until they find one that fits their specific needs, which severely diminishes the predictive power of the calculations. In this article we propose a different approach without the need to change many differential equations, by using the uncertainties in x .

Resolution of the singularity using the uncertainties in x

The quantum Hamiltonian operator corresponding to $\dot{x} = x^2$ is $H = \frac{1}{2}(px^2 + x^2p) = (-ix + x^2p)$ (such that the commutator $[x, p] = i$ and the domain is the dense set of smooth functions with compact support), can be proved to be essentially self-adjoint[11][12] (using H^2 as a positive auxiliary operator in Corollary 1.1 of [11]), meaning that the unitary time-evolution $U(t)$ is uniquely defined. Even if $x(t) = U(t)x(0)U^\dagger(t)$ would commute with $x(0)$, these are unbounded self-adjoint operators so the relevant question is whether or not they *strongly* commute for all times. If they *strongly* commute for all times, then they can be simultaneously diagonalized and there is a deterministic solution without singularities. This would be in stark contrast with the fact that there are no deterministic solutions without singularities, when the uncertainty is neglected[9].

The unitary operator:

$$U(x, p) = \frac{e^{-i\frac{p}{x}}}{\sqrt{2\pi x}} \quad (2)$$

It diagonalizes the Hamiltonian, that is $H U(x, p) = p U(x, p)$. Then, the time evolution operator is given by:

$$\begin{aligned} e^{-iHt}\{\psi\}(x) &= \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dy U(x, p) e^{-ipt} U^*(y, p) \psi(y) \\ &= \int_{-\infty}^{+\infty} \frac{dy}{2\pi xy} 2\pi \delta\left(t + \frac{1}{x} - \frac{1}{y}\right) \psi(y) \\ &= \int_{-\infty}^{+\infty} \frac{dw}{xw} \delta\left(t + \frac{1}{x} - w\right) \psi\left(\frac{1}{w}\right) = \frac{1}{xt+1} \psi\left(\frac{x}{xt+1}\right) \end{aligned} \quad (3)$$

Where we did the change of variables $y \rightarrow \frac{1}{w}$. Given a self-adjoint operator ρ diagonal in the x basis (for instance, a probability measure):

$$\begin{aligned}
\rho\{\psi\}(x) &= \rho(x)\psi(x) \\
(e^{-iHt}\rho e^{iHt})\{\psi\}(x) &= \\
&= \frac{1}{xt+1} \int_{-\infty}^{+\infty} \frac{dy}{1-yt} \delta\left(\frac{x}{xt+1} - y\right) \rho(y)\psi\left(\frac{y}{1-yt}\right) = \\
&= \rho\left(\frac{x}{xt+1}\right)\psi(x)
\end{aligned} \tag{4}$$

A singularity at finite-time in the time-evolution of an initial value problem defined by an ordinary differential equation implies that the derivative in time of the corresponding wave-function diverges. In the case of $x'=x^2$, the coordinate goes instantly from $+\infty$ to $-\infty$ at some time, this is concerning but we need to consider a finite amount of uncertainties which allows us to define a wave-function.

Since the derivative in time corresponds to the Hamiltonian (whose spectral measure is conserved by the time-evolution) then if the initial condition only involves eigenfunctions corresponding to a spectrum up to some maximum absolute value, there is no way in which the time-evolution will produce a divergent derivative in time of the wave-function. Such initial condition also makes sense from a physics point of view, where we usually have limited energy available when we apply physical transformations to a system; it also makes sense from the point of view of numerical calculations[13], where the Krylov subspace methods for computations of matrix exponentials are only guaranteed to converge if the spectrum of the matrix (in this case the Hamiltonian) is bounded, otherwise the well known phenomenon aliasing may occur.

Thus, the sample space of our initial system is usually not the coordinate space, since it verifies an energy limit. We can relate such initial sample space to the coordinate space through a physical transformation, which is only hypothetical, because it would require the availability of an arbitrarily large amount of energy. That is, we can only guess what the coordinate x would be (with an uncertainty) if we would do the necessary transformation, but never really do such transformation and thus never measure the coordinate.

The time-evolution would be deterministic in the coordinate space, but it is non-deterministic in the sample space which verifies an energy limit.

Note that the claim that limiting the energy of the initial condition suffices to solve the singularity is not by itself in conflict with the special relativity, because special relativity is expressed in Quantum Mechanics through an Hamiltonian that verifies extra conditions. By limiting the energy (Hamiltonian's spectrum) of the initial condition we do not break such extra conditions, because the spectrum of the Hamiltonian verifies the same extra conditions as the Hamiltonian itself.

Conjecture

We can easily see that for instance, all time-independent polynomial quantum Hamiltonians such that the domain is the dense set of smooth functions with compact support, can be proved to be essentially self-adjoint[11][12], using H^2 as a positive auxiliary operator in Corollary 1.1 of reference [11]. Thus, the conclusions apply to many more differential equations with would-be singularities and we can find

non-deterministic solutions instead.

References

- [1] Sudarshan, E. C. G. 1976. “Interaction Between Classical and Quantum Systems and the Measurement of Quantum Observables.” *Pramana* 6 (3): 117–26. <https://www.ias.ac.in/article/fulltext/pram/006/03/0117-0126>.
- [2] Joseph, Ilon. 2020. “Koopman–von Neumann Approach to Quantum Simulation of Nonlinear Classical Dynamics.” *Phys. Rev. Research* 2 (4): 043102. <https://doi.org/10.1103/PhysRevResearch.2.043102>.
- [3] Mezic, Igor. 2005. “Spectral Properties of Dynamical Systems, Model Reduction and Decompositions.” *Nonlinear Dynamics* 41 (August): 309–25. https://www.researchgate.net/publication/226501509_Spectral_Properties_of_Dynamical_Systems_Model_Reduction_and_Decompositions.
- [4] Bevanda, Petar, Stefan Sosnowski, and Sandra Hirche. 2021. “Koopman Operator Dynamical Models: Learning, Analysis and Control.” *Annual Reviews in Control* 52: 197–212. <https://doi.org/10.48550/arXiv.2102.02522>.
- [5] Schmüdgen, K. 2012. *Unbounded Self-Adjoint Operators on Hilbert Space*. Graduate Texts in Mathematics. Springer Netherlands.
- [6] Toland, John. 2020. *The Dual of $L^\infty(X, L, \lambda)$, Finitely Additive Measures and Weak Convergence: A Primer*. Springer International Publishing. <https://doi.org/10.1007/978-3-030-34732-1>.
- [7] Cassinelli, G., E. Vito, A. Leviero, and P.J. Lahti. 2004. *The Theory of Symmetry Actions in Quantum Mechanics: With an Application to the Galilei Group*. Lecture Notes in Physics. Springer Berlin Heidelberg.
- [8] Simms, D.J. 1971. “A Short Proof of Bargmann’s Criterion for the Lifting of Projective Representations of Lie Groups.” *Reports on Mathematical Physics* 2 (4): 283–87. [https://doi.org/10.1016/0034-4877\(71\)90011-5](https://doi.org/10.1016/0034-4877(71)90011-5).
- [9] Goriely, Alain, and Craig Hyde. 2000. “Necessary and Sufficient Conditions for Finite Time Singularities in Ordinary Differential Equations.” *Journal of Differential Equations* 161 (2): 422–48. <https://doi.org/10.1006/jdeq.1999.3688>.
- [10] Chen, Jiajie, and Thomas Y. Hou. 2022. “Stable Nearly Self-Similar Blowup of the 2D Boussinesq and 3D Euler Equations with Smooth Data.” arXiv. <https://doi.org/10.48550/ARXIV.2210.07191>.
- [11] Faris, William G., and Richard B. Lavine. 1974. “Commutators and Self-Adjointness of Hamiltonian Operators.” *Communications in Mathematical Physics* 35 (1): 39–48. <https://projecteuclid.org/journals/communications-in-mathematical-physics/volume-35/issue-1/Commutators-and-self-adjointness-of-Hamiltonian-operators/cmp/1103859517.pdf>.
- [12] Faris, William G. 2006. *Self-Adjoint Operators*. Vol. 433. Springer.

- [13] Wang, Hao, and Qiang Ye. 2017. “Error Bounds for the Krylov Subspace Methods for Computations of Matrix Exponentials.” *SIAM Journal on Matrix Analysis and Applications* 38 (1): 155–87. <https://doi.org/10.48550/arXiv.1603.07358>.