Exponential unitary integrators for nonseparable quantum Hamiltonians

Maximilian Čirić,1,‡ Denys I. Bondar,2† and Ole Steuernagel1,‡

1Department of Physics, Astronomy and Mathematics, University of Hertfordshire, Hatfield, AL10 9AB, UK
2Tulane University, New Orleans, LA 70118, USA
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Quantum Hamiltonians containing nonseparable products of non-commuting operators, such as $\hat{x}^m\hat{p}^n$, are problematic for numerical studies using split-operator techniques since such products cannot be represented as a sum of separable terms, such as $T(\hat{p}) + V(\hat{x})$. In the case of classical physics, Chin [Phys. Rev. E 80, 037701 (2009)] developed a procedure to approximately represent nonseparable terms in terms of separable ones. We extend Chin’s idea to quantum systems. We demonstrate our findings by numerically evolving the Wigner distribution of a Kerr-type oscillator whose Hamiltonian contains the nonseparable term $\hat{x}\hat{p}^2 + \hat{p}\hat{x}^2$. The general applicability of Chin’s approach to any Hamiltonian of polynomial form is proven.

I. INTRODUCTION

Split-operator methods [1] are popular across many domains of physics because they combine the best of two worlds — simplicity of implementation and preservation of physical properties such as norm and energy. For the time evolution of Hamiltonian quantum systems (including those with nonlinearities [2]), unitary split-operator integrators [3] have emerged as reliable workhorses. However, such split-operator methods are currently restricted to Hamiltonians which are separable [4], i.e. those that are a sum of two terms $T(\hat{p})$ and $V(\hat{x})$, each depending only on $\hat{p}$ and $\hat{x}$ respectively (throughout, we denote all quantum operators in bold face).

Other recent approaches treating nonseparable classical Hamiltonians exist, including one that yields good long time behaviour for classical dynamics, but which does this at the resource-intensive price of doubling up the phase space, see [5] and references therein. In the case of quantum systems this is too high a price to pay.

Classical evolution is governed by Poisson-brackets, whose commutators Chin’s method [6] combines algebraically such that upon application of exponential split-operator integrators it extends to the treatment of nonseparable Hamiltonians. Whilst such classical evolution is phase space volume-conserving [7] quantum evolution is not [8], and its evolution is governed by Moyal brackets.

Therefore it remained unclear whether Chin’s approach can be adapted to quantum systems.

Here we show that Chin’s approach can be extended to quantum systems, see Sect. III such as Kerr-oscillators, see Sect. III. In Sect. VII we generalize its application to (nonseparable) Hamiltonians composed of polynomials. We use Wigner’s quantum phase space representation [9] and investigate its numerical performance in Secs. IV and V and then conclude in Sect. VII.

II. EXTENDING CHIN’S APPROACH TO QUANTUM EVOLUTION

A. From separable to nonseparable propagators

Separable Hamiltonians of the form $\hat{H} = T(\hat{p}) + V(\hat{x})$ allow for operator splitting. Here, we deal with classical and quantum operators as well as their eigenvalues. Following [4], we therefore adopt the following notation. Throughout, bold lettering $(\hat{x}, \hat{p})$ refers to quantum scalars whereas regular lettering $(x, p)$ refers to their classical counterparts or functions, such as $T$ or $V$. Hats $(\hat{p}, \hat{x})$ vs. $(\hat{p}, \hat{x})$ indicate their respective operators.

A state is propagated through a small time-step, $\varepsilon = -i\Delta t/\hbar$, by the unitary propagator $\hat{U}(\varepsilon)$. $\hat{U}$ can be split into the approximate form [3, 6]

\[
\hat{U}(\varepsilon) = e^{i\hat{H}} = e^{i(T+V)} \approx \prod_{i=1}^{N} e^{i\varepsilon T} e^{i\varepsilon V} = e^{i\hat{H}_{\Lambda}},
\]

(1)

here $\hat{T} = T(\hat{p})$ and $\hat{V} = V(\hat{x})$. $\hat{H}_{\Lambda}$ approximates $\hat{H}$; since $\hat{H}_{\Lambda}$ must be hermitian, it has to have an even-power expansion in $\varepsilon$. Here, all operator-products are meant to be from left to right: $\prod_{i=1}^{N} \hat{U}_i = \hat{U}_1 \hat{U}_2 \cdots \hat{U}_N$.

Following [6], we will only consider symmetric factorisation schemes for [1] such that the weighting coefficients are either $t_i = 0$ and $v_i = v_{N-i+1}$, $t_{i+1} = t_{N-i+1}$, or $v_{N} = 0$ and $v_i = v_{N-i}$, $t_i = t_{N-i+1}$.

Then, according to the Baker-Campbell-Hausdorff formula [8], $\hat{H}_{\Lambda}$ has the form

\[
\hat{H}_{\Lambda} = e_{\tau} \hat{T} + e_{\nu} \hat{V} + \varepsilon^2 e_{\tau\tau\nu} [\hat{T}\hat{T}\hat{V}] + O(\varepsilon^4),
\]

(2)

where condensed commutator brackets $[\hat{T}\hat{T}\hat{V}] = [\hat{T}, [\hat{T}, \hat{V}]]$, $[\hat{T}\hat{V}\hat{V}] = [\hat{T}, [\hat{V}, [\hat{T}, \hat{V}]]]$, etc., are used. The coefficients $e_{\tau}$, $e_{\nu\tau\nu}$, etc., are functions of $\{t_i\}$ and $\{v_j\}$.

By choosing $\{t_i\}$ and $\{v_j\}$ such that $\sum_i t_i = 0 = \sum_j v_j$, we impose that

\[
e_{\tau} = e_{\nu} = 0.
\]

(3)
If we also impose that $e_{VT} = 0$, or $e_{VT} = 0$, then the approximate propagator $[\hat{T}]$ codes for nonseparable Hamiltonians $\hat{H}_A$, either of the form
\[ \hat{H}_A \approx H_{TTV} \propto [TTV], \text{ or } \hat{H}_A \approx H_{VT} \propto [VT]. \]

To summarise, combined separable terms in Eq. (4) can emulate specific nonseparable operator products $[\hat{\gamma}]$.

Chin showed in 6 that the specific symmetric product of nine exponentials 7, with coefficients $v_0 = -2(v_1 + v_2)$, $v_1 = -v_2$, $v_2 = -\frac{1}{2}v_1$ and $v_1 = \frac{1}{2}v_2$, enables us to remove the third order term $[VT^2]$ and is therefore the harmonic oscillator squared and is is of the form
\[ \hat{H}_A \approx H_{TTV} \propto [TTV], \text{ or } \hat{H}_A \approx H_{VT} \propto [VT]. \]

To summarise, combined separable terms in Eq. (4) can emulate specific nonseparable operator products $[\hat{\gamma}]$.

The single-mode Kerr oscillator, in its simplest form, has the energy of the harmonic oscillator squared and is therefore analytically fully solvable. Explicitly, its Hamiltonian has the form
\[ \hat{H}_{\text{Kerr}} = \left( \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} \right)^2 = \frac{\hat{p}^4}{4} + \frac{[\hat{p}^2, \hat{x}^2]_+}{4} + \frac{\hat{x}^4}{4}, \]

where we used the anti-commutator $[\hat{a}, \hat{b}]_+ \equiv \hat{a}\hat{b} + \hat{b}\hat{a}$. The quantum Kerr effect comes about due to the self-interaction of photons in nonlinear media 10. Its dynamics is non-trivial and periodic with a recurrence time of $\tau = \frac{\pi}{\lambda}$; its phase space current follows circles 11.

We now show that its nonseparable terms $[\hat{p}^2, \hat{x}^2]_+$ can be cast into the shape of $\hat{H}_A$ in Eq. (2). To first order in the time step $\varepsilon = -\hat{\alpha} \Delta t/\hbar$, the Moyal bracket 3 8 of quantum phase space dynamics agrees with the classical Poisson bracket 5 8. We therefore have to hope that the commutator $[TTV]$ in Eq. (5) behaves similarly to the classical Poisson bracket–based Lie operators analysed by Chin 6.

Following Ref. 5, we therefore try the ansatz of a second order polynomial for $\hat{T}$ and a fourth order polynomial for $\hat{V}$. The choices $\hat{T} = \frac{c_T}{2} \frac{\hat{p}^2}{\hbar}$ and $\hat{V} = \frac{c_V}{12} \hat{x}^4$ yield $[TTV] = \frac{c_T^2 c_V}{96} (\hat{x}^4 \hat{p}^4 + \hat{p}^4 \hat{x}^4 - 2 \hat{p}^2 \hat{x}^4 \hat{p}^2)$. With $c_T = 1 = c_V$ and using Heisenberg’s commutation relation $[\hat{p}, \hat{x}] = \frac{i}{\hbar}$ this simplifies (we used Mathematica 12) to
\[ [TTV] = -\frac{\hbar^4}{4} - \frac{\hbar^2}{4} [\hat{p}^2, \hat{x}^2]_+, \]

with a real-valued constant term which gives rise to a global phase that can be ignored or subtracted out.

Alternatively, one can, for example, use $\hat{T} = \frac{\hat{p}^4}{2\pi} + \frac{\hat{p}^2}{2\pi^2}$ and $\hat{V} = \frac{\hat{x}^2}{2\pi^2}$ while swapping $\hat{V} \leftrightarrow \hat{T}$ in expression (5), the formal result is the same (8), but numerical performance can differ slightly 13.

We have thus established that a propagator using the separable terms $\hat{T}$ and $\hat{V}$ in $\hat{U}$, in Eq. (1), can generate a propagator featuring the product term $[\hat{p}^2, \hat{x}^2]_+$, which represents the nonseparable middle term of the Kerr Hamiltonian in Eq. (7).

IV. PROPAGATION OF MIXED STATES USING WIGNER’S PHASE SPACE APPROACH

Instead of limiting ourselves to pure states propagated in the Schrödinger picture, as in Sect. IV B, we now study the time evolution of general quantum states $W(x, p, t)$, in Wigner’s phase space representation.

We employ Wigner’s representation for the following four reasons: firstly, many dissipative systems use coupling terms of product form, so Chin’s approach allows us to avoid iterations such as those as used in Eqs. (63) and (64) of 4. Secondly, the Wigner representation describes mixed systems which result from such dissipative couplings. Thirdly, it can be efficiently implemented (in Schrödinger equation-like form, see below and 4). Finally, comparison of the quantum with Chin’s classical description becomes transparent when using the Wigner representation since it describes $W$’s dynamics using Moyal brackets 13, the quantum analogue of Poisson brackets:
\[ \frac{\partial W}{\partial t} = \{ H, W \} = \frac{1}{i\hbar} \hat{G}[W]. \]

Here, the Hamiltonian $H$, is given by the Wigner transform 15 of $\hat{H}$, which in the case of the Kerr Hamiltonian 4 is $H = \left( \frac{\hat{p}^2}{2} + \frac{\hat{x}^2}{2} \right)^2 - \frac{\hbar^2}{4}$. The generator of
motion $\hat{\mathcal{G}}$ is the Lie superoperator associated with the Moyal bracket $\mathcal{G}$, namely

$$\{f, g\} = \frac{f \star g - g \star f}{i\hbar} = \frac{2}{\hbar} f(x, p) \sin \left[ \frac{\hbar}{2} \left( \frac{\partial^2}{\partial x \partial p} - \frac{\partial^2}{\partial p \partial x} \right) \right] g(x, p),$$

(10)

where $\star$ denotes the Groenewold-Moyal product $\mathcal{G}$.

Taylor’s expansion of Moyal’s bracket (10) yields

$$\{f, g\} = \{f, g\} + \mathcal{O} \left( \hbar^n \text{[derivatives]} \right) \quad \left( n \geq 2 \right).$$

(13)

To lowest order, this gives us Poisson’s bracket $\{f, g\} = \partial_f g / \partial_p - \partial_f g / \partial_p$ of classical mechanics. We see that in Wigner’s representation the time evolution is formally similar to that in the classical case treated by Chin $\mathcal{G}$. We mention in passing that sending $\hbar \downarrow 0$, for instance in Eq. (16), (also numerically) implements a classical propagator. Wigner’s representation is additionally of interest, because it can be treated efficiently numerically since Moyal’s equation of motion $\mathcal{G}$ can be cast into the form of a Schrödinger equation $\mathcal{G}$, see next Sect. V.

Equation (17) connects the Wigner transform $\mathcal{G}$ of non-commutative Hilbert space operator products $f(\hat{x}, \hat{p}) \cdot g(\hat{x}, \hat{p})$ with non-commutative $\star$-products $f(x, p) \star g(x, p)$ on phase space:

$$f(x, p) \star g(x, p) \Leftrightarrow f(\hat{x}, \hat{p}) \cdot g(\hat{x}, \hat{p}),$$

(14)

$$\{f(x, p), g(x, p)\} \Leftrightarrow \{f(\hat{x}, \hat{p}), g(\hat{x}, \hat{p})\}.$$  

(15)

V. NUMERICAL CONSIDERATIONS

In Wigner-Weyl transformed variables, we can give $\mathcal{G}$ of Eq. (9) the explicit form $\mathcal{G}$

$$\mathcal{G} = H \left( \hat{x} - \frac{\hbar}{2} \hat{\theta}, \hat{\theta} + \frac{\hbar}{2} \hat{\lambda} \right) - H \left( \hat{x} + \frac{\hbar}{2} \hat{\theta}, \hat{\theta} - \frac{\hbar}{2} \hat{\lambda} \right)$$

$$\equiv \hat{H}_{-,+} - \hat{H}_{+, -}, \quad (16)$$

with the commutation relations $\mathcal{G} [18]$

$$[\hat{x}, \hat{p}]_\mathcal{G} = 0, \quad [\hat{x}, \hat{\lambda}]_\mathcal{G} = i, \quad [\hat{p}, \hat{\theta}]_\mathcal{G} = i, \quad [\hat{\lambda}, \hat{\theta}]_\mathcal{G} = 0,$$

(18)

which span a suitable Wigner-Weyl ‘Hilbert phase space’ $\mathcal{G}$

Hence,

$$\hat{U} = \exp \left( \varepsilon \left( \hat{H}_{-,+} - \hat{H}_{+, -} \right) \right),$$

(19)

and for time-independent Hamiltonians

$$W(t) = \exp \left( -i \frac{t - t_0}{\hbar} \mathcal{G} \right) [W(t_0)] = \hat{U} [W(t_0)].$$

(20)

We emphasise that in choosing the $(x, \theta)$-representation $\mathcal{G}$, for Eq. (18), using suitable Bopp operators $\mathcal{G}$

$$\hat{x} = x, \quad \hat{p} = i \frac{\partial}{\partial \theta}, \quad \hat{\lambda} = -i \frac{\partial}{\partial x}, \quad \text{and} \quad \hat{\theta} = \theta,$$

(21)

Eq. (9) becomes Schrödinger equation-like, making it possible to apply efficient numerical propagation employing fast Fourier transform methods $\mathcal{G}$ [17, 20, 21]. This is very useful for systems that cannot be modelled as pure states, such as in the presence of decoherence.

Using $\hat{P}_\pm \equiv \hat{p} \pm \frac{\hbar}{2} \hat{\lambda}$ and $\hat{X}_\pm \equiv \hat{x} \pm \frac{\hbar}{2} \hat{\theta}$, we can express $\hat{U}$ (19) for the Kerr Hamiltonian (7) as

$$\hat{U}_{\text{Kerr}} = \exp \left[ \frac{\varepsilon}{4} \left( \hat{P}_-^2 - \hat{P}_+^2 + \left[ \hat{P}_+^2 \hat{X}_-^2 - \hat{P}_-^2 \hat{X}_+^2 + \hat{X}_-^2 \hat{P}_+^2 - \hat{X}_+^2 \hat{P}_-^2 \right] + \hat{X}_-^4 - \hat{X}_+^4 \right) \right]$$

$$= \exp \left[ \frac{\varepsilon}{4} \left( \hat{P}_-^2 - \hat{P}_+^2 \right) \right] \exp \left[ \frac{\varepsilon}{4} \left( [\hat{P}_-^2, \hat{X}_-^2]_\mathcal{G} - [\hat{P}_-^2, \hat{X}_+^2]_\mathcal{G} + \hat{X}_-^4 - \hat{X}_+^4 \right) \right] + \mathcal{O}(\varepsilon^2).$$

(22a)

$$\hat{U}_{\text{Kerr}}^2 = \exp \left[ \frac{\varepsilon}{4} \left( \hat{P}_+^2 - \hat{P}_-^2 + \left[ \hat{P}_-^2 \hat{X}_-^2 + \hat{X}_-^2 \hat{P}_-^2 \right] + \hat{X}_-^4 - \hat{X}_+^4 \right) \right]$$

(22b)

According to Eq. [8], the appearance of anti-commutators in the middle exponential of expression (22b) allows us to express the contribution from the central product term in the Kerr Hamiltonian (7) as a single product of form (5); for an efficient implementation in Python see $\mathcal{G}$.

A. Error Scaling for Kerr System

In the following, we set $\hbar = 1$ and use coherent states

$$W(x, p, t = 0) = \frac{1}{\pi} \exp \left( - (x - x_0)^2 - (p - p_0)^2 \right).$$

(23)
Using exponential propagators (whose action is time-reversible), we confirmed that Chin’s approach preserves the state’s norm at machine precision.

We checked for energy and phase stability, varying the time step $\Delta t$. In the case of a classical system with similar structure Chin reports [9], in accord with Eq. 5, scaling with order $O(\epsilon^5)/O(\epsilon^3) \sim O(\Delta t^{2/3})$; this is roughly what we observed here, in the quantum Kerr case, as well.

The period of our Kerr system is $\pi$, see Fig. 1 (c). As a proxy for phase drift, associated with this algorithm, we determine the wave function overlap at recurrence times $\tau = \pi$ and find that $1 - |\langle W_{\text{exact}}(0)|W(\tau)\rangle| \sim O(\Delta t^{1/2})$, a scaling better than that of the energy fluctuations (we distinguish between $W_{\text{exact}}$ and the numerically propagated distribution $W$). For this we could not find a quantitative explanation. We also numerically propagated $\psi$ and confirmed that $1 - |\langle \psi_{\text{exact}}(0)|\psi(\pi)\rangle|^2 \sim O(\Delta t^{1/2})$ follows the same scaling as the Wigner function propagator. To make sure there is nothing special about one complete revolution we also checked for $\tau = \pi/2$, $1 - |\langle W_{\text{exact}}(\pi/2)|W(\tau)\rangle| \sim O(\Delta t^{1/2})$, the behaviour is the same. Alternatively, $\langle W_{\text{exact}}(0) - W(\tau)\rangle/\sqrt{\langle W_{\text{exact}}(0) - W(\tau)\rangle^2}$, used as overlap measures, yield error scaling $\sim O(\Delta t^{2/3})$ and, again, behave the same whether running for one complete revolution or otherwise. For details see Ref. [13].

B. Modification of Chin’s expression

In the Kerr-case studied here, it is possible to modify Chin’s expression [9] by removing first and last terms yielding the approximation

\[ \hat{U}_7(\varepsilon) = e^{e t_1 T} e^{e t_1 V} e^{e t_1 T} e^{e t_1 V} e^{e t_1 T} e^{e t_1 V} e^{e t_1 T} \] (24a)

\[ = \hat{U}_9(\varepsilon) - \frac{\varepsilon^3}{t_2} [\hat{V} \hat{V} T] + O(\varepsilon^5). \] (24b)

We use the modified coefficients $v_0 = -2t_1$, $t_1 = -t_2$, $v_1 = \frac{1}{t_2}$, and again $T = \frac{\varepsilon^2}{\sqrt{2} \hbar^2} \hat{p}^2$ and $V = \frac{\varepsilon^2}{\sqrt{2} \hbar^2} \hat{x}^2$, with the final result [12]

\[ \hat{U}_7(\varepsilon) = 1 + \varepsilon^3 \left( -\frac{\hbar^4}{4} - \frac{\hbar^2}{4} \hat{p}^2, \hat{x}^2 \right] + \frac{\hbar^2}{9\sqrt{2} \epsilon t_2^3} \hat{x}^6 \right) + O(\varepsilon^5). \] (25)

This is similar to result [8]. We have to compensate for the unwanted term in $\hat{x}^6$, by subtracting $\frac{\hbar^2}{9\sqrt{2} \epsilon t_2^3} \hat{x}^6$ from potential terms in Eqs. [9] and [22], but gain the advantage of having to numerically calculate fewer terms.

Whether a form like (24a) that is as useful as (25) can be found in the general case, we do not know at this stage. We emphasise that $U_7$ has fewer product terms and runs a little faster but also performs worse than $U_9$ of Eq. 5 in absolute terms, see Fig. 1. The errors in energy and phase both scale roughly with $O(\Delta t^{2/3})$, similarly to and worse than in the case of $U_9$, respectively.

For more details consult our code [13], further discussions of such questions is beyond the scope of this work.

VI. CHIN’S APPROACH IS GENERAL

In order to show that Chin’s approach is generally applicable, let us prove

**Theorem 1.** Any polynomial $\hat{P}(\hat{x}, \hat{p})$ of $\hat{x}$ and $\hat{p}$ can be written as a finite linear combination of $[\hat{x}^n, [\hat{x}^n, \hat{p}^m]] \equiv [\hat{x}^n, [\hat{x}^n, \hat{p}^m]]$ and $[\hat{p}^m, [\hat{x}^n, \hat{p}^m]] \equiv [\hat{p}^m, [\hat{x}^n, \hat{p}^m]]$.

**Proof.** Let us provide a constructive proof. A polynomial $\hat{P}(\hat{x}, \hat{p})$ is Weyl-transformed [15] to $P(x, p)$ in phase space, according to Eq. (14). Assume $x^N p^M$ is its leading term, namely, $P(x, p)$ is a polynomial of order $(N, M)$.

Via Eq. (15), a double commutator $[\hat{x}^n, [\hat{x}^n, \hat{p}^m]]$ corresponds to $\{x^n, \{x^n, p^m\}\}$. In fact, the latter are polynomials because the Moyal bracket (10) is obtained by differentiating its arguments. According to Eq. (13), the leading term of the polynomial $\{x^n, p^m\}$ is $x^{n-2} p^{m-2}$; hence, the leading term of $\{x^n, \{x^n, p^m\}\}$ is $x^{n-2} p^{m-2}$. Likewise, a double commutator $[\hat{p}^m, [\hat{x}^n, \hat{p}^m]]$ corresponds to the polynomial $\{p^m, [x^n, p^m]\}$ with the leading term of order $x^{n-2} p^{m-2}$.

The set of polynomials

\[ \{x^n, \{x^n, p^m\}\}, \{p^m, [x^n, p^m]\} \] (26)

is linearly independent and large enough to span the set of polynomials of order $(N, M)$, including $P(x, p)$. \qed

We observe that in the above proof all Moyal brackets $\{\ldots\}$ can be substituted by Poisson brackets $\{\ldots\}$ whilst leaving the argument intact: Chin’s approach applies to polynomial classical hamiltonians as well.

Theorem 1 prescribes how any polynomial quantum Hamiltonian can be decomposed into the Hamiltonians of the form (4). Hence, Chin’s algorithm is very general.

VII. CONCLUSION

We have shown that Chin’s method [9] for the propagation of classical nonseparable Hamiltonians can be adopted to quantum systems. Chin’s method is general, and therefore allows for the universal treatment of non-separable Hamiltonians using split-operator techniques. Chin’s method should be especially well suited for numerical simulations of large open quantum systems using stochastic Schrödinger equations [23] since their errors scale poorly.
FIG. 1. Kerr system \( \text{(a)} \) evolves an initial coherent state \( |\psi(0)\rangle \) with amplitude ‘3’ \( |\psi(0)\rangle = \frac{3}{\sqrt{2}}, p_0 = \frac{3}{\sqrt{2}} \) using timesteps \( \Delta t = 0.0001 \) in columns (a) to (c) and \( \Delta t = 0.0015 \) in column (d). We observe that the initial state recurs at the system’s recurrence time \( \tau = \pi \) columns (c) and (d) and fractional revivals of the initial states with approximate three-fold symmetry \( \text{[22–24]} \) form at times \( \tau/3 \) and \( 2\tau/4 \), see columns (a) and (b), respectively. The same parameters are used in top and bottom row, except that the top row employs the more accurate propagator \( \hat{U}_{\gamma} \) of Eq. (5) whereas the bottom row uses \( \hat{U} \) of Eq. (24a), the numerical errors become more pronounced with both, increasing propagation time and increasing timesteps.

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DATA AVAILABILITY STATEMENT

The codes developed for the current study are available at [13].

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