# Higher time derivatives in effective equations of canonical quantum systems

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# Higher time derivatives in effective equations of canonical quantum systems

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## Abstract

Quantum-corrected equations of motion generically contain higher time derivatives, computed here in the setting of canonically quantized systems. The main example in which detailed derivations are presented is a general anharmonic oscillator, but conclusions can be drawn also for systems in quantum gravity and cosmology.

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## I. INTRODUCTION

Quantum effects, generically, are non-local in time, captured in effective actions or equations [1, 2] by correction terms containing an asymptotic series of time derivatives of higher than second order. The path-integral formulation provides an intuitive explanation: entire paths connecting two points, not just a local neighborhood on a single trajectory, determine observable properties. In gravitational theories, one expects quantum corrections with higher time derivatives for an independent reason: The theory is interacting and therefore should receive non-trivial quantum corrections. The only generally covariant extension of the Einstein–Hilbert action by functionals of the metric is by higher powers and contractions of space-time curvature tensors, most of which introduce time derivatives of higher than second order in equations of motion. The presence of higher time derivatives should therefore be a generic feature of quantum theories of gravity, referring to perturbative quantizations as well as considerations of the semiclassical limit of non-perturbative theories. Our main motivation for this work is the latter situation, chiefly in the context of low-curvature phenomena of loop quantum gravity, a non-perturbative quantization of gravity. In cosmological models of this theory, effective equations have been derived, but the role of higher time derivatives has remained unclear and disputed. This situation will present the main physical example we have in mind throughout the paper, and to which we will come back in more detail in the concluding section.

Many properties of classical and quantum gravity are best described and analyzed in a canonical formulation, especially when gauge issues play a role. In canonical quantizations, however, it is not all too clear why and how corrections with higher time derivatives should result. Equations of motion with higher time derivatives imply additional degrees of freedom because more initial data must be provided compared to usual second-order ones. In a perturbative setting, the solution space does not increase in size because the surplus solutions are not analytic in the perturbation parameter that multiplies higher-derivative terms, and therefore must be discarded for self-consistency [3]. However, terms that contain higher time derivatives do modify the classical solutions of second-order equations and therefore the new degrees of freedom they come along with play an indirect role. In canonical quantizations, however, one replaces the classical phase space by a set of basic operators of the same number, without an obvious place for new quantum degrees of freedom. A clear identification of such variables together with a systematic procedure of deriving quantum corrections in which they appear is of general interest, not just in quantum-gravity research where higher-curvature corrections could be computed by such means.

Effective methods for canonical quantum systems do exist, using a systematic analysis of quantum back-reaction of fluctuations and higher moments of a state on the evolution of expectation values [2]. Applying this scheme to anharmonic oscillators with potential $V(q) = \frac{1}{2}m\omega^2 q^2 + U(q)$, it has been shown that results equivalent to those of path-integral based low-energy effective actions [1] are obtained. So far, these calculations, in [1] as well as [2], have been restricted to the first order in a semiclassical expansion by $\hbar$ and second order in an adiabatic expansion, analogous to a derivative expansion. To these orders, in

$$\Gamma_{\rm eff}[q(t)] = \int {\rm d}t \left( \frac{1}{2}\left( m + \frac{\hbar U'''(q)^2}{32m^2\omega^5\left(1+U''(q)/m\omega^2\right)^{5/2}} \right)\dot{q}^2 - \frac{1}{2}m\omega^2 q^2 - U(q) - \frac{\hbar\omega}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{1/2}\right) \tag{1}$$

one can see corrections by an effective quantum potential as well as a correction to the particle mass, but no higher time derivatives result.

Nevertheless, the scheme provides a natural candidate for quantum degrees of freedom analogous to new degrees of freedom in corrections with higher-time derivatives [4]: fluctuations and higher moments of a state. As in perturbative higher-derivative theories, these degrees of freedom play an indirect role when an adiabatic expansion is used, because their equations of motion can be solved and solutions can be inserted into equations for expectation values to determine quantum corrections. In this article, we push the required expansions to higher orders to compute several new correction terms for the same systems, general anharmonic oscillators, and confirm that higher time derivatives appear. These results are collected in Sec. III and put together in Sec. IV, after our review of canonical effective techniques in Sec. II.

Looking at the details of our analysis, we will also be able to draw several general conclusions about properties of effective canonical dynamics. These statements, together with a general discussion of the relevance of our findings for (loop) quantum cosmology, can be found in the concluding section V.

## II. ANHARMONIC OSCILLATORS

The classical Hamiltonian for an anharmonic oscillator is given by:

$$H(q,p) = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2 + U(q) \tag{2}$$

with the particle mass $m$, harmonic frequency $\omega$, and an arbitrary function $U(q)$ which, for many purposes such as quantum stability, is often restricted to be bounded from below. We will mainly be thinking of a polynomial $U(q)$ of higher than second order, whose total order is even if boundedness from below is required. (Our effective equations will be meaningful even when this condition is violated.) The frequency $\omega$ is uniquely determined only if one requires $U(q)$ to have no quadratic contribution.

The Hamiltonian (2) can straightforwardly be quantized, without factor ordering ambiguities. Quantum states $|\Psi\rangle(t)$ then satisfy the Schrödinger equation

$$i\hbar\frac{\partial|\Psi\rangle}{\partial t} = \hat{H}|\Psi\rangle = \frac{1}{2m}\hat{p}^2|\Psi\rangle + \frac{1}{2}m\omega^2\hat{q}^2|\Psi\rangle + U(\hat{q})|\Psi\rangle\,. \tag{3}$$

This equation takes the form of a differential equation when a representation of states, for instance as wave functions of $q$, is chosen. Effective equations, however, are independent of this representation choice. (There may be inequivalent representations not related unitarily, for instance on a non-separable Hilbert space [5]. In this case effective equations would depend on which representation is chosen; see the example [6] in quantum cosmology.)

Instead of representations of wave functions, we use the general evolution equation

$$\frac{\mathrm{d}\langle\hat{O}\rangle}{\mathrm{d}t} = \frac{\langle[\hat{O},\hat{H}]\rangle}{i\hbar} \tag{4}$$

for expectation values of observables $\hat{O}$. For a Hamiltonian as given here, (4) applied to $\hat{q}$ and $\hat{p}$ gives rise to Ehrenfest's equations

$$\frac{\mathrm{d}\langle\hat{q}\rangle}{\mathrm{d}t} = \frac{\langle\hat{p}\rangle}{m} \quad , \quad \frac{\mathrm{d}\langle\hat{p}\rangle}{\mathrm{d}t} = -\langle V'(\hat{q})\rangle\,, \tag{5}$$

resembling the classical ones but also exhibiting quantum corrections in the force term $-\langle V'(\hat{q})\rangle$ compared to $-V'(\langle\hat{q}\rangle)$. Canonical effective equations compute the difference of $-\langle V'(\hat{q})\rangle$ and $-V'(\langle\hat{q}\rangle)$ in a systematic way. (In [7], these equations are used to prove that quantum mechanics has the correct classical limit for $\hbar\to 0$.)

Unless the potential is at most quadratic, Eqs. (5) do not provide a closed set of equations that could be solved for the expectation values, starting from some initial values. A cubic term $\lambda q^3$ in the potential, for instance, gives rise to $-3\lambda\langle\hat{q}^2\rangle = -3\lambda(\langle\hat{q}\rangle^2+(\Delta q)^2)$. The second term is a quantum correction to the classical force $-3\lambda q^2$, but it depends on the position fluctuation $\Delta q$ which is independent of the expectation value $\langle\hat{q}\rangle$. Ehrenfest's equations therefore cannot be solved in this case, unless one already knows how the quantum state or at least its position fluctuation evolves.

To provide a complete set of equations, effective techniques enlarge the set of Ehrenfest's equations by deriving differential equations for fluctuations and all moments

$$\tilde{G}^{a,n} := \left\langle (\hat{q} - \langle\hat{q}\rangle)^{n-a}(\hat{p} - \langle\hat{p}\rangle)^a \right\rangle_{\text{Weyl}} \tag{6}$$

where the subscript "Weyl" indicates Weyl (or totally symmetric) ordering. Since these variables are defined by expectation values, equations of motion for them can be derived from the same equation (4) as used earlier. Moreover, these variables provide infinitely many quantum degrees of freedom independent of expectation values, just the degrees of freedom which, at least qualitatively, should be related to implications of higher time derivatives.

Unlike expectation values, moments cannot take arbitrary values. For $n = 2$, they must satisfy the familiar uncertainty relation

$$\tilde{G}^{0,2}\tilde{G}^{2,2} - (\tilde{G}^{1,2})^2 \geq \frac{\hbar^2}{4} \tag{7}$$

and there are analogous, but less familiar relations at higher orders. All these inequalities follow from the Schwarz inequality. Only if they are obeyed can the moments correspond to a state. If they are, the state may be pure or mixed; if a selection of pure states is required, additional conditions must be imposed. (See also the examples in [8].)

Instead of calculating all the commutators required for equations of motion (4) of moments, it is usually more straightforward to take a phase-space point of view. We first consider the right-hand side of (4), which in classical mechanics would be the Poisson bracket of $O$ with the Hamiltonian $H$. This comparison motivates the definition of a Poisson bracket between expectation values of arbitrary operators,

$$\{\langle\hat{A}\rangle, \langle\hat{B}\rangle\} := \frac{\langle[\hat{A}, \hat{B}]\rangle}{i\hbar}\,. \tag{8}$$

This bracket is antisymmetric, linear and satisfies the Jacobi identity by virtue of those properties realized for the commutator. If we extend it to products of expectation values by using the Leibniz rule, we obtain a well-defined Poisson bracket on the quantum phase space, whose elements are states parameterized by their expectation values of $\hat{q}$ and $\hat{p}$ together with all moments. (The quantum phase space is symplectic. However, in effective equations one truncates the system at finite orders of $\hbar$, which translates to finite orders of the moments. The Poisson tensor remains well-defined on these subspaces, but in general is no longer invertible. Effective equations therefore cannot be described by symplectic techniques.)

Combining (4) and (8), the Schrödinger flow is described equivalently by a Hamiltonian flow on the quantum phase space, generated by the quantum Hamiltonian $H_Q(\langle\hat{q}\rangle, \langle\hat{p}\rangle, \tilde{G}^{a,n}) := \langle\hat{H}\rangle_{\langle\hat{q}\rangle,\langle\hat{p}\rangle,\tilde{G}^{a,n}}$. The subscript indicates that the expectation value is taken in a state characterized by the values $\langle\hat{q}\rangle, \langle\hat{p}\rangle, \tilde{G}^{a,n}$; the result then defines the value of the quantum Hamiltonian at the quantum phase-space point corresponding to the same state.

As a function of expectation values and moments, quantum Hamiltonians can be computed by writing $\langle H(\hat{q},\hat{p})\rangle = \langle H(\langle\hat{q}\rangle+(\hat{q}-\langle\hat{q}\rangle), \langle\hat{p}\rangle+(\hat{p}-\langle\hat{p}\rangle))\rangle$ and expanding in the "small" quantities $\hat{q}-\langle\hat{q}\rangle$ and $\hat{p}-\langle\hat{p}\rangle$. This formal expansion is a shortcut for a direct computation of the expectation value. Inserting a Taylor expansion and assuming $H(\hat{q},\hat{p})$ to be Weyl ordered (in case there is any factor-ordering choice), we obtain

$$H_Q := \langle H(\hat{q},\hat{p})\rangle = \sum_{n=0}^{\infty}\sum_{a=0}^{n}\frac{1}{n!}\left(\binom{n}{a}\right)\frac{\partial^n H(q,p)}{\partial p^a \partial q^{n-a}}\tilde{G}^{a,n} \tag{9}$$

with the moments (6). (Here and from now on we identify $q := \langle\hat{q}\rangle$ and $p := \langle\hat{p}\rangle$ to simplify our notation.)

The moments may be written in dimensionless form as $G^{a,n} = \hbar^{-n/2}(m\omega)^{n/2-a}\tilde{G}^{a,n}$ to facilitate future expansions. In terms of these dimensionless variables, we obtain, for the given anharmonic oscillator, the quantum Hamiltonian as:

$$H_Q = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2 + U(q) + \frac{\hbar\omega}{2}(G^{0,2}+G^{2,2}) + \sum_{n=2}^{\infty}\frac{1}{n!}(\hbar/m\omega)^{n/2}U^{(n)}(q)G^{0,n}\,. \tag{10}$$

The first quantum correction, depending only on fluctuations but not on expectation values, is a zero-point energy. The sum, on the other hand, contains products of expectation values and moments if there is an anharmonic potential, and therefore describes the coupling between quantum variables and expectation values, or quantum back-reaction. (Note that the moments vanish identically if $n = 1$. The sum therefore starts at $n = 2$.)

If we look at the equations of motion for expectation values and moments generated by the quantum Hamiltonian [2],

$$\begin{aligned}
\dot{q} &= \{q, H_Q\} = \frac{p}{m} \\
\dot{p} &= \{p, H_Q\} = -m\omega^2 q - U'(q) - \sum_{n=2}^{\infty} \frac{1}{n!}(\hbar/m\omega)^{n/2} U^{(n+1)}(q) G^{0,n} \qquad (11)
\end{aligned}$$

$$\begin{aligned}
\dot{G}^{a,n} &= -a\omega G^{a-1,n} + (n-a)\omega G^{a+1,n} - \frac{U''(q)a}{m\omega} G^{a-1,n} \qquad (12) \\
&\quad + \frac{\sqrt{\hbar} a U'''(q)}{2(m\omega)^{3/2}} G^{a-1,n-1} G^{0,2} + \frac{\hbar a U''''(q)}{3!(m\omega)^2} G^{a-1,n-1} G^{0,3} \\
&\quad - \frac{a}{2} \left( \frac{\sqrt{\hbar} U'''(q)}{(m\omega)^{3/2}} G^{a-1,n+1} + \frac{\hbar U''''(q)}{3(m\omega)^2} G^{a-1,n+2} \right) + \cdots
\end{aligned}$$

(not all terms are written in the last equation) we can already see that moments are related to higher time derivatives: Eq. (11) can be interpreted as identifying an infinite linear combination of moments with the second derivative of $q$, in a way that also depends on $q$ itself. Taking further time derivatives of the whole equation (11) and inserting (12) relates different combinations of the $G^{a,n}$ (no longer linear) to time derivatives of $q$ of higher than second order. It is therefore clear that moments in the canonical setting play the role of higher time derivatives in a Lagrangian one. But so far the identification is not very direct, and the equations we obtain for higher time derivatives in terms of moments are difficult to invert. In the rest of this paper, we work out a systematic method, using two expansions as in [2], to write (11) as an equation corrected by higher-derivative terms, eliminating the moments.

## III. SEMICLASSICAL AND ADIABATIC EXPANSIONS

Our first expansion is a semiclassical one. In a semiclassical state, the moments by definition obey the $\hbar$ierarchy $\tilde{G}^{a,n} = O(\hbar^{n/2})$ so that an expansion by $\hbar$ to a given finite order makes use of only finitely many moments. Thanks to the definition of dimensionless variables $G^{a,n} = \hbar^{-n/2}(m\omega)^{n/2-a}\tilde{G}^{a,n}$, suitable powers of $\hbar$ already appear as factors in equations of motion such as (11), and we only need to truncate the sum.

Although the leading order of $\hbar$ is split off the moments when using dimensionless variables, each moment, as a solution of (12), could still have higher-order corrections in $\hbar$. For full generality, we therefore make these terms explicit by expanding by powers of $\sqrt{\hbar}$:

$G^{a,n} = \sum_e G_e^{a,n}\hbar^{e/2}$. The coefficients $G_e^{a,n}$ are then independent of $\hbar$. Some features of this expansion may look unfamiliar, which we explain by two comments:

- As written explicitly, we should expect half-integer orders in $\hbar$ because a moment of order $n$ behaves as $O(\hbar^{n/2})$. If all odd-order moments vanish, which is the case in a large subclass of semiclassical states, only integer orders appear, as naively expected. Such an assumption can always be made for an initial state, but non-trivial quantum back-reaction can easily generate non-vanishing odd-order moments. (See for instance the example in [9].)

- Since $\hbar$ has non-trivial dimensions, the coefficients $G_e^{a,n}$ have different dimensions for different $e$. If this feature is unwanted, one can use coefficients or parameters in the anharmonicity potential $U(q)$, together with $m$ and $\omega$, to define a parameter $L$ of the same dimensions as $\hbar$ and expand by $\sqrt{\hbar/L}$. The parameters of the harmonic-oscillator Hamiltonian have already been used to absorb the dimensions of $\tilde{G}^{a,n}$, and they do not allow a combination with the dimensions of $\hbar$. In the harmonic case, an expansion by $\sqrt{\hbar/L}$ cannot be done, and it is not necessary because the equations of motion for moments can then be solved exactly, showing that each moment $\tilde{G}^{a,n}$ is exactly proportional to $\hbar^{n/2}$ and stays so at all times. This property is no longer realized for anharmonic oscillators, but then there are additional parameters in the potential that can be used to define a suitable $L$. We refrain from doing so here because we work with a general anharmonicity $U(q)$. Its derivatives then provide the correct dimensions.

With the semiclassical expansion in $\hbar$, the equations of motion for the moments partially decouple. At $O(\hbar^0)$ and $O(\hbar^{1/2})$, we have

$$\dot{G}_0^{a,n} = -a\omega G_0^{a-1,n} + (n-a)\omega G_0^{a+1,n} - \frac{U''(q)a}{m\omega} G_0^{a-1,n} \tag{13}$$

$$\begin{aligned}\dot{G}_1^{a,n} &= -a\omega G_1^{a-1,n} + (n-a)\omega G_1^{a+1,n} - \frac{U''(q)a}{m\omega} G_1^{a-1,n} + \frac{U'''(q)a}{2(m\omega)^{3/2}} G_0^{0,2} G_0^{a-1,n-1} \\ &\quad - \frac{U'''(q)a}{2(m\omega)^{3/2}} \left( G_0^{a-1,n+1} - \frac{(a-1)(a-2)}{12} G_0^{a-3,n-3} \right)\end{aligned} \tag{14}$$

which we could try to solve order by order. The equations for $G_0^{a,n}$ couple only the $n+1$ moments at fixed order $n$ and are linear in the moments. The equations for $G_1^{a,n}$ (and similarly for higher orders in $\hbar$) are inhomogeneous but also contain only moments $G_1^{a,n}$ of the same order $n$, as well as non-linear inhomogeneous terms of different orders.

By the semiclassical expansion, the infinitely coupled original system has been reduced to finitely coupled subsets. In principle one could solve this system order by order, but since coefficients of the differential equations also depend on $q$ for a non-trivial anharmonicity, they are difficult to solve explicitly. We therefore make use of a second expansion, an adiabatic one, which reduces the differential equations to algebraic ones. This approximation will also be crucial to bring out the nature of moments as higher time derivatives. (In the conclusions we will comment on the nature of moments in regimes in which no adiabatic expansion is possible.)

The adiabatic expansion is defined by replacing all time derivatives in equations of motion for moments ($q$ and $p$ are not assumed to change just adiabatically) by $\mathrm{d}/\mathrm{d}t \to \lambda \mathrm{d}/\mathrm{d}t$, expanding all coefficients $G_e^{a,n} = \sum_{i=1}^{\infty} G_{e,i}^{a,n} \lambda^i$ in $\lambda$, solving equations order by order in $\lambda$, and setting $\lambda = 1$ in the end. The expansion is formal because there is no guarantee that the series converges for $\lambda = 1$. Moreover, the parameter $\lambda$, unlike $\hbar$ in the semiclassical expansion, has no physical meaning. As we will see later, the procedure rather serves as a systematic way of organizing the appearance of derivatives of different orders.

At zeroth order of the adiabatic approximation of $\dot{G}^{a,n} = \{G^{a,n}, H_Q\}$, we have equations

$$0 = \{G_{e,0}^{a,n}, H_Q\} \tag{15}$$

which are algebraic rather than differential. At higher orders,

$$\dot{G}_{e,i}^{a,n} = \{G_{e,i+1}^{a,n}, H_Q\} \tag{16}$$

contains time derivatives, but if we proceed order by order, we can assume that $G_{e,i}^{a,n}$ has already been solved for, starting with the algebraic equation for $G_{e,0}^{a,n}$. With the time dependence on the left-hand side of (16) known, the equation again reduces to an algebraic one for $G_{e,i+1}^{a,n}$. Proceeding order by order, the main equations to be solved are algebraic. (Some differential consistency conditions also arise, as we will see explicitly.)

Combining both expansions, our moments read

$$G^{a,n} = \sum_e \sum_i G_{e,i}^{a,n} \hbar^{e/2} \lambda^i \,. \tag{17}$$

Equations to be solved for the coefficients $G_{e,i}^{a,n}$ show both advantages noted above: They split into finitely coupled sets, and are algebraic.

We now proceed to computing explicit solutions to several orders. But first we interject a comment on our designation of $\hbar$-orders to avoid confusion. For most of this paper, we will be looking at the moment equations (12) and their solutions, and therefore speak of the $O(\hbar^0)$-order when all $\hbar$-terms are dropped, of the $O(\hbar^{1/2})$-order when terms linear in $\sqrt{\hbar}$ are kept, and so on. These orders give us the relevant information about state properties at the corresponding orders. However, if we use these moment solutions to compute correction terms for effective equations of expectation values, inserting the moments in (11) as we will do in the end, the $\hbar$-orders shift because (11) contains explicit factors of $\hbar$. Somewhat counter-intuitively, even the $O(\hbar^0)$-order in the moments will then contribute to non-trivial quantum corrections. This intermingling of the orders cannot be avoided because equations of motion for different variables — expectation values or moments of different orders $n$ — have their own arrangements of $\hbar$-terms.

### A. Adiabatic Approximation at $O(\hbar^0)$ in the Moments

At zeroth order in the adiabatic approximation, we can ignore all time dependence: $\{G^{a,n}_{e,0}, H_Q\} = 0$. At zeroth order also in the $\sqrt{\hbar}$ expansion, we have from (13)

$$0 = -a\omega G^{a-1,n}_{0,0} + (n-a)\omega G^{a+1,n}_{0,0} - \frac{U''(q)a}{m\omega} G^{a-1,n}_{0,0} \tag{18}$$

for $0 \leq a \leq n$, which gives a solution of the form

$$G^{a,n}_{0,0} = C_n \frac{(n-a)!a!}{((n-a)/2)!(a/2)!} \left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n)/4} \tag{19}$$

with some coefficients $C_n$ if both $n$ and $a$ are even. Otherwise, $G^{a,n}_{0,0} = 0$. (For odd $a$, Eq. (18) used with $a = 0$ implies that $G^{1,n}_{0,0} = 0$, which upon recurrence to $a = 2k+1$ with integer $k$ implies that $G^{a,n}_{0,0} = 0$ for odd $a$, no matter whether $n$ is even or odd. For $n$ odd and $a$ even in $G^{a,n}_{0,0}$, Eq. (18) evaluated for $a = n$ is meaningful, with a zero value implied for $G^{n+1,n}_{0,0}$, only if all $G^{a,n}_{0,0}$ with odd $n$ and even $a$ vanish.)

Only the values (19) with even $n$ and $a$ can be non-zero. Based on the zeroth-order equation (13) alone, the $C_n$ could depend on $q$ as well, but this possibility is ruled out by a consistency condition obtained at first adiabatic order [2, 4]. The values of $C_n$ in general effective equations remain free (provided the resulting moments satisfy the uncertainty relation) and parameterize different choices of adiabatic states. A prominent choice is the anharmonic vacuum, whose values can be obtained by requiring that the harmonic limit $U(q)=0$ provides the known moments of the harmonic-oscillator ground state. The $C_n = 2^{-n}$ [2] are then fixed, and we have

$$G^{a,n}_{0,0} = \frac{(n-a)!a!}{2^n((n-a)/2)!(a/2)!}\left(1+\frac{U''(q)}{m\omega^2}\right)^{(2a-n)/4} \tag{20}$$

for even $a$ and $n$.

As recalled here, the derivation of (20) with its precise coefficient requires additional assumptions about the initial values of the moments, or about the kind of states whose evolution is considered. General effective equations are not unique owing to the dependence on classes of states described by them. The usual low-energy effective action (1) is parameter-free only because it refers to a specific regime of states near the interacting vacuum, as indicated by the qualifier "low-energy." The underlying conditions are tantamount to requiring the moments to agree with those of the harmonic-oscillator ground state when $U(q)=0$, and indeed canonical effective equations with this choice are equivalent to equations of motion that follow from the low-energy effective action [2]. The solutions for moments then amount to expanding around the adiabatic vacuum state of the anharmonic system. Since our results build on (20), we will be dealing with the same states, but to higher orders in the semiclassical and adiabatic expansions.

### 1. *Solutions at zeroth and first adiabatic order*

Using zeroth-order solutions in $\dot{G}^{a,n}_{0,0} = \{G^{a,n}_{0,1}, H_Q\}$, the equation of motion at first order in $\lambda$ and zeroth order in $\sqrt{\hbar}$, we have, for odd $a$ or $n$,

$$\dot{G}^{a,n}_{0,0} = 0 = -a\omega G^{a-1,n}_{0,1} + (n-a)\omega G^{a+1,n}_{0,1} - \frac{U''(q)a}{m\omega} G^{a-1,n}_{0,1} \tag{21}$$

But this equation is identical to (18), so we have the same solution, namely zero, for odd $n$. This pattern continues to all orders in the adiabatic approximation:

$$G^{a,n}_{0,i} = 0 \ \text{ for odd } n. \tag{22}$$

For even $n$, however, solutions change with progressing adiabatic order. We can still use (21) for $a$ odd and $n$ even, describing solutions $G^{a,n}_{0,1}$ with even $a$ and $n$. Again, the equation is identical to (18), solved by (19) with new coefficients $C'_n$ instead of $C_n$. If we match with the harmonic-oscillator ground state, we must require its values for the moments $G^{a,n}_{0,0}+G^{a,n}_{0,1}$ to the present order, so that $C_n+C'_n=2^{-n}$. Only this combination of $C_n$ and $C'_n$ appears in equations of motion to first adiabatic order, and therefore it is not necessary (nor possible) to determine both coefficients independently. Since we already fixed $C_n$, we keep this value as well as $G^{a,n}_{0,0}$ as in (20). This choice implies $C'_n=0$ and therefore

$$G^{a,n}_{0,1}=0 \quad \text{for even } a \text{ and } n\,. \tag{23}$$

For moments of odd $a$ and even $n$, finally, the solution of (21) (with odd $a$ inserted) is different. In this case, the time derivative of (20) becomes the left-hand side of the first-order adiabatic equation of motion:

$$\frac{(n-a)!a!}{2^n((n-a)/2)!(a/2)!}\frac{2a-n}{4}\frac{U'''(q)\dot{q}}{m\omega^2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{(2a-n-4)/4} = -a\omega G^{a-1,n}_{0,1}+(n-a)\omega G^{a+1,n}_{0,1}-\frac{U''(q)a}{m\omega}G^{a-1,n}_{0,1} \tag{24}$$

We can solve this immediately for $a=n$, and then substitute the result in to solve for the case $a=n-2$, and so on. The general solution is

$$G^{a,n}_{0,1}=C_{a,n}\frac{U'''(q)\dot{q}}{m\omega^3}\left(1+\frac{U''(q)}{m\omega^2}\right)^{(2a-n-6)/4} \tag{25}$$

for odd $a$ and even $n$, where the $C_{a,n}$ are dimensionless prefactors. In particular, while the zeroth adiabatic order does not allow quantum correlations, they may appear at first adiabatic order, for instance by $G^{1,2}\neq 0$.

In the harmonic limit, (25) vanishes identically, and therefore the $C_{a,n}$ are not restricted by the requirement of perturbing around the harmonic ground state. Instead, the $C_{a,n}$ are fully determined by the adiabatic equations. For $a=n$ in (24), we have $C_{n-1,n}=-2^{-(n+2)}n!/(n/2)!$. Plugging (25) into (24) we find

$$C_{a-1,n}=\frac{n-a}{a}C_{a+1,n}-\frac{(n-a)!(a-1)!}{2^{n+2}((n-a)/2)!(a/2)!}(2a-n)\,, \tag{26}$$

a recurrence relation solved by the general expression

$$\begin{aligned} C_{a-1,n} \;=\; & -\frac{(n-a)!(a-1)!}{2^{n+2}((n-a)/2)!(a/2)!}(2a-n) \\ & -2^{-n-2}\sum_{b=0}^{(n-a-2)/2}\left[\prod_{c=0}^{b}\frac{n-(a+2c)}{a+2c}\right]\frac{(n-a'_b)!(a'_b-1)!}{((n-a'_b)/2)!(a'_b/2)!}(2a'_b-n) \end{aligned} \tag{27}$$

for even $a$, where $a'_b = a + 2(b+1)$.

To summarize, at first adiabatic order only moments with odd $a$ and even $n$ change, depending on the time derivative of $q$ in (25).

### 2. Second Adiabatic Order

At second order in $\lambda$ and zeroth order in $\hbar$, the equation of motion is

$$\dot{G}^{a,n}_{0,1} = -a\omega\left(1 + \frac{U''(q)}{m\omega^2}\right) G^{a-1,n}_{0,2} + (n-a)\omega G^{a+1,n}_{0,2}\,. \tag{28}$$

For odd $n$ the solution is zero by (22), and even $a$ and $n$ in the equation of motion leads to $G^{a,n}_{0,2}$ of the form (19) for odd $a$ and even $n$, again with new coefficients $C_n$. For these moments to vanish in the harmonic limit, we have $G^{a,n}_{0,2} = 0$ for odd $a$.

For odd $a$ and even $n$, the left-hand side is given by the time derivative of equation (25). Substituting in this result and rearranging slightly, we have

$$\begin{aligned} G^{a+1,n}_{0,2} = \quad & \frac{a}{n-a}\left(1 + \frac{U''(q)}{m\omega^2}\right) G^{a-1,n}_{0,2} \\ & + \frac{C_{a,n}}{(n-a)m\omega^4}\left( (U'''(q)\ddot{q} + U''''(q)\dot{q}^2)\left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n-6)/4} \right. \\ & \left. + (U'''(q)\dot{q})^2 \frac{2a-n-6}{4m\omega^2}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n-10)/4} \right). \end{aligned} \tag{29}$$

The form of this equation suggests an ansatz

$$\begin{aligned} G^{a,n}_{0,2} \quad & = A_{a,n}\left( \frac{1}{m\omega^4}(U'''(q)\ddot{q} + U''''(q)\dot{q}^2)\left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n-8)/4} \right) \\ & + B_{a,n}\left( \frac{1}{4m^2\omega^6}(U'''(q)\dot{q})^2\left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n-12)/4} \right) \\ & + \binom{n/2}{a/2}\binom{n}{a}^{-1}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{a/2} G^{0,n}_{0,2} \end{aligned} \tag{30}$$

where $A_{a,n}$ and $B_{a,n}$ are dimensionless coefficients determined by $a$ and $n$, and the final term is motivated by the solution at zeroth order in $\lambda$, generated by the first term in (29). Using this ansatz in (29), we find recursion relations for $A_{a,n}$ and $B_{a,n}$:

$$A_{a+1,n} = \frac{C_{a,n}}{n-a} + \frac{a}{n-a}A_{a-1,n} \tag{31}$$

$$B_{a+1,n} = \frac{C_{a,n}(2a-n-6)}{n-a} + \frac{a}{n-a}B_{a-1,n} \tag{32}$$

for odd $a$. Consistency of (30) requires that $A_{0,n} = B_{0,n} = 0$, which gives $A_{2,n} = \frac{C_{1,n}}{n-1}$ and $B_{2,n} = -\frac{n+4}{n-1}C_{1,n}$. The recursion relations, with these initial values, give

$$A_{a+1,n} = \frac{C_{a,n}}{n-a} + \sum_{b=0}^{(a-3)/2} \left( \prod_{c=0}^{b} \frac{a-2c}{n-(a-2c)} \right) \frac{C_{a-2(b+1),n}}{n-(a-2(b+1))} \tag{33}$$

for odd $a \geq 3$, where the $C_{a,n}$ are given in (26). The expression for the $B_{a,n}$ is similar, the only change being that $C_{a,n}$ is replaced by $(2a-n-6)C_{a,n}$ in each term.

To fully determine the moments, which are thus far given in terms of $G^{0,n}_{0,2}$, we need a condition from third order. Since we are still at $O(\hbar^0)$, the third-order equation of motion has the same form, so the condition is given by [4]

$$\sum_{\text{even } a} \binom{n/2}{a/2} \left(1 + \frac{U''(q)}{m\omega^2}\right)^{(n-a)/2} \dot{G}^{a,n}_{0,2} = 0 \tag{34}$$

for even $n$. From (30) we see that this is a complicated differential equation for $G^{0,n}_{0,2}$. Given (30), this condition suggests an ansatz for $G^{0,n}_{0,2}$ of the form

$$G^{0,n}_{0,2} = A'_n \frac{1}{m\omega^4}(U'''(q)\ddot{q} + U''''(q)\dot{q}^2) \left(1 + \frac{U''(q)}{m\omega^2}\right)^r + B'_n \frac{1}{4m^2\omega^6}(U'''(q)\dot{q})^2 \left(1 + \frac{U''(q)}{m\omega^2}\right)^s \tag{35}$$

where $r$, $s$, $A'_n$, and $B'_n$ are some undetermined constants. (Given a differential equation (34), we expect one free parameter, which would be multiplying all $G^{a,n}_{0,2}$. However, since we are also solving the recurrence relation (30), whose first two terms are fixed, imposing the consistency condition (34) will not leave any free parameters.)

Substituting (30) into (34) with (35), differentiating, and moving things around a bit, we have that

$$\begin{aligned}
&\frac{1}{m\omega^4} \sum_a \Bigg\{ \binom{n/2}{a/2} A_{a,n} \left[ \frac{\mathrm{d}\left(U'''\ddot{q} + U''''\dot{q}^2\right)}{\mathrm{d}t} X^{\frac{n-8}{4}} + \frac{2a-n-8}{4} \frac{U'''\dot{q}}{m\omega^2} \left(U'''\ddot{q} + U''''\dot{q}^2\right) X^{\frac{n-12}{4}} \right] \\
&+ A'_n \binom{n/2}{a/2}^2 \binom{n}{a}^{-1} \left[ \frac{\mathrm{d}\left(U'''\ddot{q} + U''''\dot{q}^2\right)}{\mathrm{d}t} X^{r+\frac{n}{2}} + \left(r + \frac{a}{2}\right) \frac{U'''\dot{q}}{m\omega^2} \left(U'''\ddot{q} + U''''\dot{q}^2\right) X^{r+\frac{n}{2}-1} \right] \Bigg\} \\
&+ \frac{1}{4m^2\omega^6} \sum_a \Bigg\{ \binom{n/2}{a/2} B_{a,n} \left[ 2U'''\dot{q}\left(U'''\ddot{q} + U''''\dot{q}^2\right) X^{\frac{n-12}{4}} + \frac{2a-n-12}{4} \frac{U'''\dot{q}}{m\omega^2} \left(U'''\dot{q}\right)^2 X^{\frac{n-16}{4}} \right] \\
&+ B'_n \binom{n/2}{a/2}^2 \binom{n}{a}^{-1} \left[ 2U'''\dot{q}\left(U'''\ddot{q} + U''''\dot{q}^2\right) X^{s+\frac{n}{2}} + \left(s + \frac{a}{2}\right) \frac{U'''\dot{q}}{m\omega^2} \left(U'''\dot{q}\right)^2 X^{s+\frac{n}{2}-1} \right] \Bigg\}
\end{aligned} \tag{36}$$

must vanish, where $X = 1 + U''/m\omega^2$. By inspection, we see that for $r = -(n+8)/4$ and $s = -(n+12)/4$, terms involving the same expressions with $q$ and its derivatives also have the same power of $X$. This leaves only the numerical coefficients to be fixed. Only the first terms in the first two lines are proportional to $X^{(n-8)/4}\mathrm{d}(U'''\ddot{q}+U''''\dot{q}^2)/\mathrm{d}t$; generically, these terms must add to zero separately, which allows us to solve for

$$A'_n = -\frac{\sum_a \binom{n/2}{a/2} A_{a,n}}{\sum_a \binom{n/2}{a/2}^2 \binom{n}{a}^{-1}} \,. \tag{37}$$

Similarly, only the last terms in the last two lines are proportional to $(U'''\dot{q})^3 X^{(n-16)/4}$, the remaining terms being proportional to $U'''\dot{q}\,(U'''\ddot{q}+U''''\dot{q}^2)\,X^{(n-12)/4}$, so we can solve for $B'_n$ in similar fashion:

$$B'_n = -\frac{\sum_a \binom{n/2}{a/2} B_{a,n}(2a-n-12)}{\sum_a \binom{n/2}{a/2}^2 \binom{n}{a}^{-1}(2a-n-12)} \,. \tag{38}$$

To confirm that these expressions are indeed valid, we need to check that the remaining terms in (36) vanish. Substituting in our expressions for $A'_n$ and $B'_n$, factoring out common quantities, and making use of the fact that $\sum_a \binom{n/2}{a/2}^2 \binom{n}{a}^{-1}(2a-n) = 0$, we find that

$$\text{remaining terms} \;\propto\; \sum_a \binom{n/2}{a/2}(2a-n)\,(6A_{a,n}+B_{a,n}) \,. \tag{39}$$

We have checked that this expression vanishes for $n = 2, 4, 6$, confirming the solution

$$\begin{aligned} G^{0,n}_{0,2} \;=\; & \frac{A'_n}{m\omega^4}(U'''(q)\ddot{q}+U''''(q)\dot{q}^2)\left(1+\frac{U''(q)}{m\omega^2}\right)^{-(n+8)/4} \\ & +\frac{B'_n}{4m^2\omega^6}(U'''(q)\dot{q})^2\left(1+\frac{U''(q)}{m\omega^2}\right)^{-(n+12)/4} \end{aligned} \tag{40}$$

at least to these orders, where $A'_n$ and $B'_n$ are given above. This expression also reduces to the solution for $G^{0,2}_{0,2}$ given in [4], with the correct coefficients $A'_2 = 1/16$ and $B'_2 = -5/16$, which can be checked using the earlier expressions for $A_{a,n}$, $B_{a,n}$, and $C_{a,n}$. The solution for $G^{0,n}_{0,2}$ does not modify the ground-state condition for $C_n$ in (19) because it automatically vanishes in the harmonic limit $U(q) = 0$. Instead, the coefficients $A'_n$ and $B'_n$ are completely fixed without a choice of state.

### B. Adiabatic Approximation at $O(\sqrt{\hbar})$ in the Moments

Starting with the first order in $\sqrt{\hbar}$, we need to consider different adiabatic orders in separation.

### 1. *Zeroth Adiabatic Order*

At leading order in the adiabatic approximation, $\{G_{e,0}^{a,n}, H_Q\} = 0$. At $O(\sqrt{\hbar})$, that is, $e = 1$, this gives (from Eq. (14))

$$\begin{aligned} 0 &= -a\omega G_{1,0}^{a-1,n} + (n-a)\omega G_{1,0}^{a+1,n} - \frac{U''(q)a}{m\omega} G_{1,0}^{a-1,n} + \frac{U'''(q)a}{2(m\omega)^{3/2}} G_{0,0}^{0,2} G_{0,0}^{a-1,n-1} \\ &\quad - \frac{U'''(q)a}{2(m\omega)^{3/2}} \left( G_{0,0}^{a-1,n+1} - \frac{(a-1)(a-2)}{12} G_{0,0}^{a-3,n-3} \right) . \end{aligned} \tag{41}$$

The solutions at $O(\hbar^0)$ are given by (20) for even $a$ and $n$, and $G_{0,0}^{a,n} = 0$ for odd $a$ or $n$. We can use this result in (41) to obtain solutions for the $G_{1,0}^{a,n}$. For even $a$ or $n$ in (41), all the $G_{0,0}$ terms vanish, and the equation is identical to (18), giving the same solution for the moments involved:

$$G_{1,0}^{a,n} = 0 \text{ for odd } a \tag{42}$$

$$G_{1,0}^{a,n} = C''_n \frac{(n-a)!a!}{((n-a)/2)!(a/2)!} \left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n)/4} \quad \text{for even } a \text{ and } n \tag{43}$$

As before at first adiabatic order, we implement the ground-state condition by requiring $G_{0,0}^{a,n} + \sqrt{\hbar} G_{1,0}^{a,n}$ to agree with the known harmonic values when $U(q) = 0$; thus, $C_n + \sqrt{\hbar} C''_n = 2^{-n}$ ($C''_n$ is not dimensionless). Again keeping $G_{0,0}^{a,n}$ unchanged compared to (20), we have $C''_n = 0$ and therefore $G_{1,0}^{a,n} = 0$ for even $a$ and $n$.

For odd $a$ and $n$ in (41), the $G_{0,0}$ terms do not vanish. Substituting (20) into (41) and simplifying the resulting expression, we have

$$\begin{aligned} 0 &= (n-a)G_{1,0}^{a+1,n} - a\left(1 + \frac{U''(q)}{m\omega^2}\right) G_{1,0}^{a-1,n} \\ &\quad + \frac{U'''(q)a}{m^{3/2}\omega^{5/2}} \frac{4a-3n-1}{12\pi} \Gamma\left(\frac{a}{2}\right) \Gamma\left(\frac{n-a+1}{2}\right) \left(1 + \frac{U''(q)}{m\omega^2}\right)^{(2a-n-3)/4} . \end{aligned} \tag{44}$$

For the case $a = n$, this gives

$$G_{1,0}^{n-1,n} = \frac{U'''(q)a}{m^{3/2}\omega^{5/2}} \frac{n-1}{12\pi} \Gamma\left(\frac{n}{2}\right) \Gamma\left(\frac{1}{2}\right) \left(1 + \frac{U''(q)}{m\omega^2}\right)^{(n-7)/4} . \tag{45}$$

We can plug this solution into the $a = n-2$ equation to solve for $G_{1,0}^{n-3,n}$, and so on. In general,

$$G_{1,0}^{a-1,n} = \frac{n-a}{a}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-1} G_{1,0}^{a+1,n}$$
$$+\frac{U'''(q)}{m^{3/2}\omega^{5/2}}\frac{4a-3n-1}{12\pi}\Gamma\left(\frac{a}{2}\right)\Gamma\left(\frac{n-a+1}{2}\right)\left(1+\frac{U''(q)}{m\omega^2}\right)^{(2a-n-7)/4} . \quad (46)$$

From (45), we see that the two terms have the same power in $1+U''(q)/m\omega^2$, which allows us to write the solution as

$$G_{1,0}^{a,n} = D_{a,n}\frac{U'''(q)}{m^{3/2}\omega^{5/2}}\left(1+\frac{U''(q)}{m\omega^2}\right)^{(2a-n-5)/4} \quad \text{for even } a \text{ and odd } n, \quad (47)$$

where

$$D_{a,n} = \frac{(-1)^b\Gamma\left(\frac{n}{2}\right)}{12\pi(1-\frac{n}{2})_b}\left((n-1)b!\sqrt{\pi}+(n-8b-1)\Gamma\left(b+\frac{1}{2}\right)\right.$$
$$\left.-\sum_{c=0}^{b-2}(-1)^c(n-8(b-c-1)-1)\Gamma\left(b-c-\frac{1}{2}\right)(-b)_{c+1}\right) \quad (48)$$

if $n \geq 5$ and $b \geq 2$, and

$$D_{a,n} = \begin{cases} \frac{n-1}{12\pi}\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{1}{2}\right) & \text{if } n\geq 3,\ b=0 \\ \frac{3n-11}{12\pi(n-2)}\Gamma\left(\frac{n}{2}\right)\Gamma\left(\frac{1}{2}\right) & \text{if } n\geq 3,\ b=1 \end{cases} \quad (49)$$

is a dimensionless prefactor that depends on $a$ and $n$. In the above expression, $b=(n-a-1)/2$ and $(x)_n = x(x+1)\cdots(x+n-1)$ is the Pochhammer symbol. Comparing to (20), we see that for odd $n$ and even $a$,

$$G_{1,0}^{a,n} \propto \left(1+\frac{U''(q)}{m\omega^2}\right)^{-1} G_{0,0}^{a,n+1} . \quad (50)$$

The additional dimensionful factor of $U'''/m^{3/2}\omega^{5/3}$ in (47) provides the correct dimension of $\hbar^{-1/2}$.

### *2. First Adiabatic Order*

At first order in the adiabatic approximation and at $O(\sqrt{\hbar})$, the equation of motion is

$$\dot{G}_{1,0}^{a,n} = (n-a)\omega G_{1,1}^{a+1,n} - a\omega\left(1+\frac{U''(q)}{m\omega^2}\right)G_{1,1}^{a-1,n} + \frac{U'''(q)a}{2(m\omega)^{3/2}}\left(G_{0,0}^{0,2}G_{0,1}^{a-1,n-1}\right.$$
$$\left.+G_{0,1}^{0,2}G_{0,0}^{a-1,n-1} - G_{0,1}^{a-1,n+1} + \frac{(a-1)(a-2)}{12}G_{0,1}^{a-3,n-3}\right) . \quad (51)$$

If $a$ is odd, we see from (42) that the left-hand side is zero. If $n$ is even, we see from (22) that the last four terms on the right-hand side vanish. Let us consider the simplest case first: odd $a$ and even $n$. In this case the equation is identical to (18), giving the same solution (19) for the moments involved, with a new (and dimensionfull) $C_n$. Recalling that the $O(\hbar^{1/2}\lambda^0)$ and $O(\hbar^0\lambda)$ solutions (43) and (23) were also the same, we can write

$$G^{a,n}_{1,1} \propto G^{a,n}_{0,1} \propto G^{a,n}_{1,0} \propto G^{a,n}_{0,0}$$

Now requiring $G^{a,n}_{0,0}+G^{a,n}_{0,1}+\sqrt{\hbar}(G^{a,n}_{1,0}+G^{a,n}_{1,1})$ to agree with the known ground-state moments in the harmonic limit and keeping $G^{a,n}_{0,0}$ as in (20), we have

$$G^{a,n}_{1,1} = G^{a,n}_{0,1} = G^{a,n}_{1,0} = 0 \quad \text{for even } a \text{ and } n\,. \tag{52}$$

In these equalities we have made use of another relation. It turns out that the simplification of the equation of motion observed here is by itself not sufficient to guarantee the same solution, because the equation does not fully determine all the moments. As in the zeroth-order approximation in both $\sqrt{\hbar}$ and $\lambda$, a constraint (34) is needed from the next adiabatic order in order to determine $G^{0,n}$ [4]. (More specifically, the constraint shows that $C_n$ does not depend on $q$.) Here, the second-order adiabatic equation of motion at $O(\sqrt{\hbar})$ is

$$\begin{aligned}\dot{G}^{a,n}_{1,1} &= (n-a)\omega G^{a+1,n}_{1,2} - a\omega\left(1+\frac{U''(q)}{m\omega^2}\right)G^{a-1,n}_{1,2} + \frac{U'''(q)a}{2(m\omega)^{3/2}}\Bigg(G^{0,2}_{0,0}G^{a-1,n-1}_{0,2}\\ &+G^{0,2}_{0,1}G^{a-1,n-1}_{0,1} + G^{0,2}_{0,2}G^{a-1,n-1}_{0,0} - G^{a-1,n+1}_{0,2} + \frac{(a-1)(a-2)}{12}G^{a-3,n-3}_{0,2}\Bigg)\end{aligned} \tag{53}$$

But $n$ is still even, so the last five terms vanish, again due to (22). The right-hand side once again is the same for all cases considered for now, so the same condition on the left-hand side follows as in [4], and (52) is indeed correct. We note, however, that not all these equalities between the moments will be valid at second order in $\lambda$ because $\dot{G}^{a,n}_{1,1}$, appearing at the left-hand side of the equation of motion (53), will no longer be zero for odd $a$ and even $n$.

Now let us consider the case where $a$ and $n$ in (51) are both even. The extra terms on the right-hand side vanish, but the left-hand side is given by the time derivative of $G^{a,n}_{1,0}$. The resulting equation, which describes moments with odd $a$ and even $n$, is identical to (24), the corresponding equation at $O(\hbar^0)$ — except that the coefficient $2^{-n}$ is the $C_n$ belonging to $G^{a,n}_{1,0}$, with $G^{a,n}_{1,0}=0$ for even $a$ and $n$. In this case the equation of motion fully determines all the moments; no constraint from the next order references to harmonic states are needed.

Consequently, the solution is

$$G^{a,n}_{1,1} = 0 \;\text{ for odd } a \text{ and even } n. \tag{54}$$

For odd $n$, the solutions are not the same as the $O(\hbar^0)$ solutions (22), which are zero. In the case where $a$ and $n$ are both odd in (51), the extra terms remain, but the left-hand side is zero. If we compare (51) to (41) and recall (52), we see that the additional terms are identical, except that the $G^{0,2}G^{a-1,n-1}$ term in (41) effectively occurs twice in (51). This has the effect of replacing the factor of $4a-3n-1$ in (44) with $4a-3n+2$, so the solution is the same up to a change in the prefactor in (47).

The final case, where $a$ is even and $n$ is odd in (51) is more difficult. The left-hand side is nonzero and given by the time derivative of (47), and the extra terms on the right-hand side involve the expression given in (25). Here we will not attempt to find a general solution.

### C. Adiabatic Approximation for $n = 2$-moments at $O(\hbar)$

At second order in $\sqrt{\hbar}$, the equations again get more complicated. We will restrict ourselves here to deriving a relation for solutions of second-order moments ($n = 2$) as needed for the leading correction in the equation of motion (11). Our considerations in this section only illustrate the procedure but do not provide complete solutions.

The $n = 2$-moments, which are the same at $O(\hbar^0)$ and $O(\hbar^{1/2})$, are different at $O(\hbar)$. The $O(\hbar)$ equation of motion for the moments is given by [2]

$$\begin{aligned}
\dot{G}^{a,n}_2 \;=\;& -a\omega G^{a-1,n}_2 + (n-a)\omega G^{a+1,n}_2 - \frac{U''(q)a}{m\omega}G^{a-1,n}_2 \\
&+\frac{U'''(q)a}{2(m\omega)^{3/2}}\left(G^{0,2}_1 G^{a-1,n-1}_0 + G^{0,2}_0 G^{a-1,n-1}_1\right) \\
&-\frac{U'''(q)a}{2(m\omega)^{3/2}}\left(G^{a-1,n+1}_1 - \frac{(a-1)(a-2)}{12}G^{a-3,n-3}_1\right) \\
&+\frac{U''''(q)a}{3!(m\omega)^2}G^{0,3}_0 G^{a-1,n-1}_0 - \frac{U''''(q)a}{6(m\omega)^2}\left(G^{a-1,n+2}_0 - \frac{(a-1)(a-2)}{4}G^{a-3,n-2}_0\right).
\end{aligned} \tag{55}$$

At zeroth order in the adiabatic approximation, the left-hand side is zero. For $a = 0$, we find that $G^{1,n}_{2,0} = 0$, as at $O(\hbar^{1/2})$. In particular, $G^{1,2}_{2,0} = 0$. The $a = 2$-equation gives no new information, but confirms that $G^{1,3}_{1,0} = 0$, as we found in Sec. III B 1. The $a = 1$-equation is

$$0 = \omega G^{2,2}_{2,0} - \omega\left(1 + \frac{U''(q)}{m\omega^2}\right)G^{0,2}_{2,0} - \frac{U'''(q)}{2(m\omega)^{3/2}}G^{0,3}_{1,0} - \frac{U''''(q)}{6(m\omega)^2}G^{0,4}_{0,0}\,. \tag{56}$$

The coefficients $G^{0,3}_{1,0}$ and $G^{0,4}_{0,0}$ are given by equations (47) and (20), respectively, so we can express $G^{2,2}_{2,0}$ in terms of $G^{0,2}_{2,0}$:

$$G^{2,2}_{2,0} = \left(1 - \frac{U''(q)}{m\omega^2}\right) G^{0,2}_{2,0} - \frac{(U'''(q))^2}{24m^3\omega^5}\left(1 - \frac{U''(q)}{m\omega^2}\right)^{-2} + \frac{U''''(q)}{8m^2\omega^3}\left(1 - \frac{U''(q)}{m\omega^2}\right)^{-1} . \quad (57)$$

In order to find $G^{0,2}_{2,0}$, we would have to go to first order in $\lambda$.

## IV. EQUATION OF MOTION FOR THE OSCILLATOR UP TO $O(\hbar^{3/2})$ AND THE FOURTH ADIABATIC ORDER

It is evident from (40) compared to the previous equations that higher time derivatives appear at higher orders of the adiabatic expansion. This pattern continues at higher adiabatic orders, even going beyond the second derivative order of the classical equations. Genuine higher-derivative equations are then obtained when solutions for moments are inserted in (12). Not surprisingly, it becomes more and more complicated to find explicit solutions to higher orders, valid for generic $a$ and $n$. Still, individual moments, such as $G^{0,2}$ as needed for the first corrections in (11), can be computed more easily because specific numbers take the place of coefficients such as $A'_n$ and $B'_n$ subject to complicated recurrence relations.

### A. Higher-derivative equation of motion

From the preceding section it is clear how such calculations are organized, and it suffices here to quote the results needed for the leading corrections in the equations of motion of the anharmonic oscillator, given as before by

$$\begin{aligned} \dot{q} &= m^{-1}p \quad (58) \\ \dot{p} &= -m\omega^2 q - U'(q) - \sum_{n=2}^{\infty} \frac{1}{n!}\left(\frac{1}{m\omega\hbar}\right)^{n/2} U^{(n+1)}(q) G^{0,n} . \end{aligned}$$

Taking the time derivative of the $\dot{q}$ equation, we may write, correct up to $O(\hbar^{3/2})$ in quantum corrections,

$$\ddot{q} = -\omega^2 q - U'(q)/m - \frac{\hbar}{2m^2\omega} U'''(q)\left(\sum_\lambda G^{0,2}_{0,\lambda} + \sqrt{\hbar}\sum_\lambda G^{0,2}_{1,\lambda}\right) , \quad (59)$$

showing which moments and orders we need. (Moments of orders higher than $n = 2$ would be required at the next order, $O(\hbar^2)$.) Here we have already used the fact that $G^{0,3}_{0,i} = 0$ for any value of $i$, according to (22).

In order to evaluate (58) completely, we need to compute $G^{0,2}$ to orders $O(\hbar^0)$ and $O(\hbar^{1/2})$ in the semiclassical expansion. The previous section contains results up to the second adiabatic order, at which the right-hand side of (59) would be of second order in time derivatives. In particular, we have

$$G^{0,2}_{0,0} = \frac{1}{2}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-1/2} \tag{60}$$

from (20), while

$$G^{0,2}_{1,1} = G^{0,2}_{1,0} = G^{0,2}_{0,1} = 0\,. \tag{61}$$

At second adiabatic order, we have

$$G^{0,2}_{0,2} = \frac{U'''(q)\ddot{q} + U''''(q)\dot{q}^2}{16m\omega^4}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-5/2} - \frac{5(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-7/2} \tag{62}$$

while

$$G^{0,2}_{1,2} = 0\,. \tag{63}$$

Higher adiabatic orders cannot be obtained from the previous general formulas for $G^{a,n}$, but the relevant contributions to the specific moment $G^{0.2}$ can be computed with the previous methods. Up to fourth adiabatic order, we have $G^{0,2}_{0,3} = 0$ (which holds for all moments of even $a$ and $n$) by using (28) at higher adiabatic order and observing that $G^{a,n}_{0,2} = 0$ for odd $a$ and even $n$. Moreover, $G^{0,2}_{1,3} = 0$ and $G^{0,2}_{1,4} = 0$ vanish. The final moment we need, $G^{0,2}_{0,4}$ is more difficult to derive, and we just sketch the procedure we followed. The fourth-order equations can be manipulated to show a relation of the form

$$G^{2,2}_{0,4} = XG^{0,2}_{0,4} + \frac{\Theta}{w} \tag{64}$$

where $X = 1 + U''(q)/m\omega^2$ and

$$
\begin{aligned}
\Theta \;=\; & X^{-5/2}\left(\frac{1}{32m\omega^5}\right)\left[U'''(q)\ddddot{q} + 4U''''(q)\dddot{q}\,\dot{q} + 3U''''(q)\ddot{q}^2 + 6U'''''(q)\dot{q}^2\ddot{q} + U''''''(q)\dot{q}^4\right] \\
& -X^{-7/2}\left\{\left(\frac{5}{32m^2\omega^7}\right)\left[U''''(q)\dot{q}^2 + U'''(q)\ddot{q}\right]^2\right. \\
& \qquad \left. + \left(\frac{15}{64m^2\omega^7}\right)\left[U'''(q)\dot{q}\right]\left[U'''(q)\dddot{q} + U'''''(q)\dot{q}^3 + 3U''''(q)\dot{q}\ddot{q}\right]\right\} \\
& +X^{-9/2}\left(\frac{245}{256m^3\omega^9}\right)\left[U'''(q)\dot{q}\right]^2\left[U'''(q)\ddot{q} + U''''(q)\dot{q}^2\right] \\
& -X^{11/2}\left(\frac{315}{512m^4\omega^11}\right)\left[U'''(q)\dot{q}\right]^4
\end{aligned}
\tag{65}
$$

Then using the consistency equation (34) from [2], we get

$$
2X\dot{G}^{0,2}_{0,4} + \left(\frac{U'''(q)\dot{q}}{mw^2}\right)G^{0,2}_{0,4} + \frac{1}{\omega}\dot{\Theta} = 0\,. \tag{66}
$$

Choosing $G^{0,2}_{0,4} = AX^{-7/2} + BX^{-9/2} + CX^{-11/2} + DX^{-13/2}$ as an ansatz, we solve for these functions $A$, $B$, $C$ and $D$. However, we have five equations (corresponding to the five different powers of $X$ in (66)) with four unknowns. This generates another consistency equation which turns out to be satisfied by the coefficients in

$$
\begin{aligned}
G^{0,2}_{0,4} \;=\; & -\frac{U'''(q)\ddddot{q} + 4U''''(q)\dddot{q}\,\dot{q} + 3U''''(q)\ddot{q}^2 + 6U'''''(q)\dot{q}^2\ddot{q} + U''''''(q)\dot{q}^4}{64m\omega^6}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-7/2} \\
& + \left(\frac{21(U''''(q)\dot{q}^2 + U'''(q)\ddot{q})^2}{256m^2\omega^8}\right. \\
& \qquad \left. + \frac{7(U'''(q)\dot{q})(U'''(q)\dddot{q} + 3U''''\ddot{q}\dot{q} + U'''''(q)\dot{q}^3)}{64m^2\omega^8}\right)\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-9/2} \\
& - \frac{231(U'''(q)\dot{q})^2(U'''(q)\ddot{q} + U''''(q)\dot{q}^2)}{512m^3\omega^{10}}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-11/2} \\
& + \frac{1155(U'''(q)\dot{q})^4}{4096m^4\omega^{12}}\left(1 + \frac{U''(q)}{m\omega^2}\right)^{-13/2}\,.
\end{aligned}
\tag{67}
$$

We may now rewrite the equation of motion (58) as:

$$
\begin{aligned}
\ddot{q} \;=\; & -\omega^2 q - U'(q)/m \qquad (68) \\
& -\frac{\hbar}{2m^2\omega}U'''(q)\left[f(q,\dot{q}) + f_1(q,\dot{q})\ddot{q} + f_2(q)\ddot{q}^2 + f_3(q,\dot{q})\dddot{q} + f_4(q)\ddddot{q}\right]
\end{aligned}
$$

where

$$
\begin{aligned}
f(q,\dot q) \;=\; & \frac{1}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-1/2}+\frac{U''''(q)\dot q^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2}-\frac{5(U'''(q))^2\dot q^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}\\
&-\frac{U''''''(q)\dot q^4}{64m\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}+\frac{21(U''''(q))^2\dot q^4}{256m^2\omega^8}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-9/2}\\
&+\frac{7U'''''(q)U'''(q)\dot q^4}{64m^2\omega^8}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-9/2}-\frac{231U''''(q)(U'''(q))^2\dot q^4}{512m^3\omega^{10}}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-11/2}\\
&+\frac{1155(U'''(q))^4\dot q^4}{4096m^4\omega^{12}}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-13/2}\;,
\end{aligned}
\tag{69}
$$

$$
\begin{aligned}
f_1(q,\dot q) \;=\; & \frac{U'''(q)}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2}-\frac{3U'''''(q)\dot q^2}{32m\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}\\
&+\frac{63U''''(q)U'''(q)\dot q^2}{128m^2\omega^8}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-9/2}-\frac{231(U'''(q))^3\dot q^2}{512m^3\omega^{10}}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-11/2},
\end{aligned}
\tag{70}
$$

$$
f_2(q) \;=\; -\frac{3U''''(q)}{64m\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}+\frac{21(U'''(q))^2}{256m^2\omega^8}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-9/2}\;, \tag{71}
$$

$$
f_3(q,\dot q) \;=\; -\frac{U''''(q)\dot q}{16m\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}+\frac{7(U'''(q))^2\dot q}{64m^2\omega^8}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-9/2}\;, \tag{72}
$$

$$
f_4(q) \;=\; -\frac{U'''(q)}{64m\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2} \tag{73}
$$

Once these coefficients are inserted in (58) we have the equation of motion for $q$ correct up to the fourth adiabatic order, for quantum corrections up to $\hbar^{3/2}$. From (67), it is now clear that higher time derivatives result, up to fourth order with the present approximation. The equations for moments shown in this section demonstrate that it is the adiabatic order, rather than the semiclassical expansion or the order of moments, that determines the order of derivatives. Although back-reaction of moments on expectation values is responsible for higher time derivatives, the new degrees of freedom that higher-derivative equations would imply if used at face value, are not identical to the moments as true quantum degrees of freedom.

### B. Uncertainty Relation and Zero-Point Energy

Having derived solutions for second-order moments, we need to make sure that they obey the uncertainty relation so that they can correspond to a state. This requires us to compute not only the moment $G^{0,2}$, as used in corrected equations of motion, but also $G^{1,2}$ and $G^{2,2}$. Since expressions with these moments get more lengthy, we restrict the orders to $(0,0)+(0,1)+(1,0)+(1,1)+(0,2)$. (Especially $G^{1,2}$ is more difficult to obtain to higher orders.) We then have

$$\begin{aligned}
G^{0,2} &= \frac{1}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-1/2} + \frac{U'''(q)\ddot{q}+U''''(q)\dot{q}^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2} \\
&- \frac{5(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2} && (74)\\
G^{2,2} &= \frac{1}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{1/2} - \frac{U'''(q)\ddot{q}+U''''(q)\dot{q}^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-3/2} \\
&+ \frac{7(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2} && (75)\\
G^{1,2} &= -\frac{U'''(q)\dot{q}}{8m\omega^3}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-3/2}. && (76)
\end{aligned}$$

To check the uncertainty relation $G^{0,2}G^{2,2}-(G^{1,2})^2 \geq 1/4$, it is useful to write $G^{0,2} = \frac{1}{2}X^{-1/2}+Y$ while $G^{2,2} = \left(\frac{1}{2}X^{-1/2} - Y + \frac{(U'''(q)\dot{q})^2}{32m^2\omega^6}X^{-7/2}\right)X$, where $X = 1+\frac{U''(q)}{m\omega^2}$ and

$$Y = \frac{U'''(q)\ddot{q}+U''''(q)\dot{q}^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2} - \frac{5(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2}.$$

With these definitions, the required expression is of the form

$$\begin{aligned}
& G^{0,2}G^{2,2}-(G^{1,2})^2 \\
&= X\left[\left(\tfrac{1}{4}X^{-1}-Y^2\right) + \left(\tfrac{1}{2}X^{-1/2}+Y\right)\frac{(U'''(q)\dot{q})^2}{32m^2\omega^6}X^{-7/2} - \frac{(U'''(q)\dot{q})^2}{64m^2\omega^6}X^{-4}\right] \\
&= 1/4 - XY^2 + \frac{(U'''(q)\dot{q})^2}{32m^2\omega^6}X^{-5/2}Y\,. && (77)
\end{aligned}$$

In the limit $U(q)\to 0$, we have $X=1$ and $Y=0$, yielding a value of $1/4$ for the above expression and exact saturation of the uncertainty relation, in accordance with our assumption of the Gaussian ground state in the harmonic limit. With anharmonicity, it is not obvious to see the sign of $G^{0,2}G^{2,2}-(G^{1,2})^2-1/4$. It is, however, clear that we need $Y\geq 0$. The adiabaticity condition for the anharmonic ground state is therefore not guaranteed to be valid automatically, but with our equations the uncertainty relation can easily be monitored when numerical solutions are analyzed.

Finally, having determined the moments $G^{0,2}$ as well as $G^{2,2}$ to some orders, we can compute anharmonic corrections to the zero-point energy $Z = \frac{1}{2}\hbar\omega(G^{0,2}+G^{2,2}) =: \frac{1}{2}\hbar\omega Z'$.

With (74) and (75) we have, now valid up to the order $(1,3)$,

$$\begin{aligned}
Z' &= G^{0,2} + G^{2,2} \\
&= \frac{1}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-1/2} + \frac{U'''(q)\ddot{q} + U''''(q)\dot{q}^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2} \\
&\quad -\frac{5(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-7/2} \\
&\quad +\frac{1}{2}\left(1+\frac{U''(q)}{m\omega^2}\right)^{1/2} - \frac{U'''(q)\ddot{q} + U''''(q)\dot{q}^2}{16m\omega^4}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-3/2} \\
&\quad +\frac{7(U'''(q)\dot{q})^2}{64m^2\omega^6}\left(1+\frac{U''(q)}{m\omega^2}\right)^{-5/2} \\
&= \frac{1}{2}X^{-1/2}(1+X) + Y(1-X) + \frac{(U'''(q)\dot{q})^2}{32m^2\omega^6}X^{-5/2}\,. \qquad (78)
\end{aligned}$$

## V. CONCLUSIONS

We have shown explicitly how higher time derivatives arise in effective equations of canonical quantum systems. Physically, quantum back-reaction by moments of a state on expectation values implies correction terms, which in an adiabatic approximation (combined with a semiclassical one) can be solved for in terms of higher time derivatives. The quantum degrees of freedom are then removed from direct view, analogous to integrating out variables in a path integral. Although the quantum equations are local, given by differential equations of finite order, the effective system in which infinitely many degrees of freedom have been expressed by higher time derivatives becomes non-local.

### A. General properties

Our analysis has revealed several general properties of the expansions considered.

First, some coefficients of moments vanish at all orders in one of the expansions, irrespective of the harmonic state perturbed around. For instance, as already mentioned, $G^{a,n}_{0,i} = 0$ for odd $n$. This observation simplifies some computations of moments relevant for corrected equations of motion. The interesting moments that appear in quantum corrections, however, satisfy equations that become progressively more involved as the orders increase. The methods employed here can be extended to higher orders, but a general solution seems out of reach.

Secondly, while coefficients of explicit solutions for moments are usually complicated, the relationship between the adiabatic and derivative order is evident from the general form of equations (16). Going to higher adiabatic orders requires the use of time derivatives of lower-order coefficients, starting with zeroth adiabatic order in which coefficients depend on $q$. In this way, higher and higher time derivatives enter solutions as seen explicitly in the preceding section.

Thirdly, as in our explicit examples (19), (25) and (30), odd adiabatic orders mainly change moments $G^{a,n}$ with odd $a$ (correlations), while even adiabatic orders lead to corrections in moments with even $a$.

### B. Higher time derivatives in quantum cosmology

Our results apply to all quantum systems, but are especially relevant for quantum gravity and cosmology. In these settings, canonical techniques are often crucial or at least applied widely, and it has remained unclear if and how higher time derivatives should result. The present article shows this unambiguously and provides a systematic procedure for their computation. As an example for the importance of higher time derivatives, we may look at loop quantum cosmology [8, 10]. In this setting, one would generically expect effective equations with higher time derivatives, as a result of higher-curvature corrections. (We are dealing here with quantizations of finite-dimensional systems, and must therefore leave unaddressed the intriguing possibility that strong quantum corrections may lead to signature change from space-time to a 4-dimensional quantum version of Euclidean space [11–13]. The question of how the "evolution" of states and quantum back-reaction can be formulated to compute quantum effects in timeless Euclidean space requires further detailed study. But quantum effective equations should still be non-local and require higher derivatives, including spatial ones.)

However, higher derivative terms or the more general moment-dependent corrections as in (11) have not yet been computed in all cases; adiabatic regimes may even be non-existing. (After all, non-perturbative quantum gravity may lack a ground state with slowly evolving moments.) Instead, for a first impression of implications of quantum effects one often ignored quantum back-reaction altogether, considering only quantum-geometry corrections in homogeneous models which are easier to implement by simple modifications of classical equations. A prominent one is the so-called holonomy modification, by which the Hubble term $\mathcal{H}^2 = (\dot{a}/a)^2$ in the Friedmann equation is replaced by a periodic function such as $\sin(\ell\mathcal{H})^2/\ell^2$ with a length parameter $\ell$ (which could be the Planck length); see e.g. [14, 15]. This modification is motivated by a property in the full theory of loop quantum gravity [16, 17], according to which only holonomies but not the gravitational connection can be represented as operators. A heuristic interpretation often encountered, states that higher-order terms in an expansion of $\sin(\ell\mathcal{H})^2/\ell^2 = \mathcal{H}^2(1 - \frac{1}{3}\ell^2\mathcal{H}^2 + O((\ell\mathcal{H})^4))$ are related to higher-curvature terms. However, this interpretation overlooks the fact that higher-curvature terms also provide higher time derivatives, which are not included in most studies (and have not yet been computed). But if the higher-derivative part of curvature corrections is ignored, one cannot consider isolated higher powers of spatial curvature components as a reliable expansion. Generically, there is no reason to assume that a term of $\mathcal{H}^2$ is more important than, say, $\dot{\mathcal{H}}$, both of which contribute to the space-time curvature scalar. Expansions become inconsistent when only one type of terms is kept and, perhaps even more damningly, general covariance is put in jeopardy.

With holonomy corrections, the whole series expansion of $\sin^2(\ell\mathcal{H})/\ell^2$ by $\ell\mathcal{H}$ is used, but not a single higher time derivative. Such an approximation cannot be consistent unless one can show that there are no higher time derivatives whatsoever. There is indeed a harmonic system in loop quantum cosmology free of quantum back-reaction [6], given by a spatially flat isotropic model with a free, massless scalar. In this model, holonomy corrections correctly describe quantum evolution. If one departs from this model just slightly, when matter remains kinetic dominated and anisotropies and inhomogeneity are small, quantum back-reaction does arise [18, 19] but may be assumed weak; holonomy corrections can still be reliable. In all other cases, however, correct physical conclusions can be drawn only when all quantum corrections have been estimated and the relevant ones computed. For instance, when there is a phase of slow-roll inflation, the potential dominates and one must expect effective equations based on the assumption of kinetic domination to break down. The presence of higher-derivative terms means that holonomy corrections on their own are not reliable, but it also suggests interesting relationships with early-universe models based on higher-curvature or non-local derivative terms, especially regarding the singularity issue [20–22]. There is still much work to be done to apply the complete effective methods to quantum cosmology. At the very least, the present article serves to clarify the role of higher-derivative corrections.

### C. The Role of Adiabaticity

The use of the adiabatic approximation as the key ingredient to arrive at higher time derivatives implies that not all quantum regimes may be amenable to a higher-derivative description. The validity of the adiabatic approximation is an assumption, which can be tested self-consistently but need not always be valid. We had to use equations of different orders to determine all coefficients, and depending on the given quantum dynamics, not all these equations may be mutually consistent, for instance if anharmonic constructions are attempted for fully squeezed, correlated harmonic coherent states, contradicting the condition $G^{a,n}_{0,0} = 0$ derived here for odd $a$ and even $n$. Moreover, the final solutions may be mathematically consistent, but could violate the uncertainty relation. If they do, there would be no state corresponding to the moment solutions. (See [23] for examples in quantum cosmology where these problems occur.) Solutions for moments describe a dynamical state, and not all states may allow moments to evolve adiabatically. Here, we have expanded around the ground state, which one can reasonably expect to evolve slowly. In other, more excited states, the condition may not be met. Unfortunately, since adiabaticity is a state-dependent property, it is not possible to give general estimates referring just to the constants at hand and the potential. A single model may allow states which evolve adiabatically and others that do not. In the canonical formalism, it is therefore the initial values chosen for the moments that determine whether the approximation can be used, but in general there is no simple a-priori condition that one could directly evaluate.

If the adiabatic approximation does not apply, there are still effective equations, and they can be expanded in a semiclassical approximation. However, it is then no longer possible to solve for the moments in terms of expectation values, and no higher-derivative effective equations exist. One would rather work with a higher-dimensional effective system, a dynamical system in which the expectation values together with all moments relevant to a given order in $\hbar$ are kept as in (11) and (12). The non-locality of the quantum system is then realized by the infinite number of moments if all orders are included. To any finite order in the moments, such a system can still be solved approximately, most often by numerical means, and evaluated for physical information; see e.g. [9, 24] for examples including a rather large number of moments. Effective equations in terms of moments, explicitly exhibiting the true quantum degrees of freedom, are therefore more general than higher-derivative effective equations, but higher-derivative equations, if they exist, can show some features more directly.

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[1] F. Cametti, G. Jona-Lasinio, C. Presilla, and F. Toninelli, in *Proceedings of the International School of Physics "Enrico Fermi", Course CXLIII* (IOS Press, Amsterdam, 2000), pp. 431–448, quant-ph/9910065.

[2] M. Bojowald and A. Skirzewski, Rev. Math. Phys. **18**, 713 (2006).

[3] J. Z. Simon, Phys. Rev. D **41**, 3720 (1990).

[4] M. Bojowald and A. Skirzewski, Int. J. Geom. Meth. Mod. Phys. **4**, 25 (2007).

[5] H. Halvorson, quant-ph/0110102.

[6] M. Bojowald, Phys. Rev. D **75**, 081301(R) (2007).

[7] K. Hepp, Commun. Math. Phys. **35**, 265 (1974).

[8] M. Bojowald, *Quantum Cosmology: A Fundamental Theory of the Universe* (Springer, New York, 2011).

[9] M. Bojowald *et al.*, Phys. Rev. D **84**, 043514 (2011).

[10] M. Bojowald, Living Rev. Relativity **11**, 4 (2008), `http://www.livingreviews.org/lrr-2008-4`.

[11] T. Cailleteau, J. Mielczarek, A. Barrau, and J. Grain, Class. Quant. Grav. **29**, 095010 (2012).

[12] M. Bojowald and G. M. Paily, arXiv:1112.1899.

[13] J. Mielczarek, arXiv:1207.4657.

[14] G. Date and G. M. Hossain, Class. Quantum Grav. **21**, 4941 (2004).

[15] K. Vandersloot, Phys. Rev. D **71**, 103506 (2005).

[16] C. Rovelli, *Quantum Gravity* (Cambridge University Press, Cambridge, UK, 2004).

[17] T. Thiemann, *Introduction to Modern Canonical Quantum General Relativity* (Cambridge University Press, Cambridge, UK, 2007).

[18] M. Bojowald, Gen. Rel. Grav. **40**, 2659 (2008).

[19] M. Bojowald, Phys. Rev. Lett. **100**, 221301 (2008).

[20] T. Biswas, A. Mazumdar, and W. Siegel, JCAP **0603**, 009 (2006).

[21] T. Biswas, E. Gerwick, T. Koivisto, and A. Mazumdar, Phys. Rev. Lett. **108**, 031101 (2012).

[22] T. Biswas, A. S. Koshelev, A. Mazumdar, and S. Y. Vernov, JCAP to appear (2012).

[23] M. Bojowald, H. Hernández, and A. Skirzewski, Phys. Rev. D **76**, 063511 (2007).

[24] M. Bojowald, D. Mulryne, W. Nelson, and R. Tavakol, Phys. Rev. D **82**, 124055 (2010).