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Canonical variables for the Poisson algebra of quantum moments are introduced here, expressing semiclassical quantum mechanics as a canonical dynamical system that extends the classical phase space. New realizations for up to fourth order in moments for a single classical degree of freedom and to second order for a pair of classical degrees of freedom are derived and applied to several model systems. It is shown that these new canonical variables facilitate the derivation of quantum-statistical quantities and effective potentials. Moreover, by formulating quantum dynamics in classical language, these methods result in new heuristic pictures, for instance of tunneling, that can guide further investigations.

I. INTRODUCTION

Semiclassical physics can often be described by classical equations of motion amended by correction terms and possible new degrees of freedom. For instance, Ehrenfest's theorem shows that the expectation values of position and momentum in an evolving quantum state obey equations of motion which are identical with the classical equations to zeroth order in $\hbar$ but, in general, have a modified quantum force given by $-\langle \nabla V(\hat{x}) \rangle$ not equal to the classical force $-\nabla V(\langle \hat{x} \rangle)$ evaluated at $\langle \hat{x} \rangle$. The difference depends on $\langle \hat{x} \rangle$, but also on the variance $(\Delta x)^2$ and higher moments, which constitute new, non-classical degrees of freedom.

A moment expansion can be used to derive quantum corrections systematically. In this way, one can formulate quantum dynamics as classical-type dynamics on an extended phase space, given by expectation values and moments equipped with a Poisson bracket that follows from the commutator of operators [1, 2]. Moments, however, do not directly form canonical variables on this Poisson manifold, which complicates some of the usual procedures of canonical mechanics. Darboux' theorem guarantees the existence of local canonical coordinates, but it is not always easy to find them. Using a proce-

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dure we developed in [3], as well as other new methods, we present here detailed derivations of canonical variables for moments of up to fourth order for a single degree of freedom, as well as to second order for a pair of degrees of freedom. The resulting expressions can be used to make interesting observations about the behavior of states, and they are crucial for the derivation of effective potentials. We present several applications, including tunneling. This application is discussed in more detail in [4] where we demonstrate the usefulness of our present methods in atomic physics, related to an ongoing debate of evaluations of recent experiments [5–17].

II. CANONICAL EFFECTIVE METHODS

We use a quantum system of N degrees of freedom with basic operators $\hat{q}_j$ and $\hat{\pi}_k$, $1 \leq j, k \leq N$ that are canonically conjugate,

$$[\hat{q}_j, \hat{\pi}_k] = i\hbar \delta_{jk}. \tag{1}$$

In a semiclassical truncation [1, 2], the state space is described by a finite-dimensional phase space with coordinates given by the basic expectation values $q_j = \langle \hat{q}_j \rangle$ and $\pi_k = \langle \hat{\pi}_k \rangle$ and, for positive integers k_i and l_i such that $\sum_{i=1}^{N}(k_i + l_i) \geq 2$, the moments

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$$\Delta\left(q_1^{k_1} \cdots q_N^{k_N} \pi_1^{l_1} \cdots \pi_N^{l_N}\right) = \langle (\hat{q}_1 - q_1)^{k_1} \cdots (\hat{q}_N - q_N)^{k_N} (\hat{\pi}_1 - \pi_1)^{l_1} \cdots (\hat{\pi}_N - \pi_N)^{l_N} \rangle_{\text{Weyl}}, \tag{2}$$

where the product of operators is Weyl (totally symmetrically) ordered. (For low orders, these central moments agree with the cumulants of a probability distribution.) The phase-space structure is defined by the Poisson bracket

$$\{\langle \hat{A} \rangle, \langle \hat{B} \rangle\} = \frac{1}{i\hbar} \langle [\hat{A}, \hat{B}] \rangle, \tag{3}$$

extended to all moments by using linearity and the Leibniz rule. The phase space has boundaries according to Heisenberg's uncertainty relation

$$\Delta(q_j^2)\Delta(\pi_k^2) - \Delta(q_j \pi_k)^2 \geq \frac{\hbar^2}{4}\delta_{jk} \tag{4}$$

and higher-order analogs.

Any given state (which may be pure or mixed) is therefore represented by a point in phase space defined by the

corresponding basic expectation values and moments. A state is considered semiclassical if its moments obey the hierarchy

$$\Delta \left(q_1^{k_1} \cdots q_N^{k_N} \pi_1^{l_1} \cdots \pi_N^{l_N} \right) = O \left(\hbar^{\frac{1}{2} \sum_n (l_n + k_n)} \right) \quad (5)$$

which is satisfied, for instance, by a Gaussian, but includes also a more general class of states. A semiclassical truncation of order s of the quantum system is defined as the submanifold spanned by the basic expectation values and moments such that $\sum_n (l_n + k_n) \leq s$, which implies variables up to order $\frac{1}{2} s$ in $\hbar$ according to the semiclassical hierarchy. The Poisson bracket that results from (3) can consistently be restricted to any semiclassical truncation by ignoring in $\{\Delta_1, \Delta_2\}$ all terms of order higher than s in moments. In this restriction, the product of a moment of order s_1 and a moment of order s_2 is considered of semiclassical order $s_1 + s_2$, while the product of a moment of order s_1 with $\hbar^{s_2}$ is of order $s_1 + 2s_2$ [18]. For given s, the Poisson tensor on the semiclassical truncation of order s is, in general, not invertible. Therefore, semiclassical truncations and the resulting effective potentials cannot be formulated within symplectic geometry.

We note that the semiclassical truncations used here impose stronger conditions than usually used in studies of the semiclassical limit, using for instance WKB-type or Maslov methods [19] or the Wigner function [20]. In particular, while both methods assume that a certain dimensionless combination of parameters proportional to $\hbar$ is small or even approaches zero, our semiclassicality condition also restricts the class of states. Our definition here ensures that quantum corrections, for instance in the total energy, are well-defined at least in the sense of a formal power series in $\hbar$. From other methods, such as Wigner functions [20], it is known that the semiclassical limit, applied to unrestricted states, generically gives rise to terms that are non-analytic in $\hbar$; see for instance [21]. Our condition avoids this behavior, while still maintaining access to interesting problems, as our examples will demonstrate.

The Hamilton operator $\hat{H}$ determines a Hamilton function $\langle \hat{H} \rangle$ on state space, which can be restricted to any semiclassical truncation of order s to define an effective Hamilton function of semiclassical order s. We assume that each contribution to the Hamilton operator is Weyl-ordered in basic operators. Any Hamilton operator that does not obey this condition can be brought to Weyl-ordered form by using the canonical commutation relations, which results in terms that explicitly depend on $\hbar$. In order to compute an effective Hamiltonian of order s for a given Hamilton operator $H(\hat{q}_j, \hat{\pi}_k)$, we use

$$
\begin{aligned}
H_{\text{eff},s} &= \langle H(q_j + (\hat{q}_j - q_j), \pi_k + (\hat{\pi}_k - \pi_k)) \rangle \\
&= H(q_j, \pi_k) + \sum_{\sum_n (j_n + k_n) = 2}^{s} \frac{\partial^n H(q, \pi)}{\partial q_1^{j_1} \cdots \partial q_N^{j_N} \partial \pi_1^{k_1} \cdots \partial \pi_N^{k_N}} \frac{\Delta \left(q_1^{j_1} \cdots q_N^{j_N} \pi_1^{k_1} \cdots \pi_N^{k_N} \right)}{j_1! \cdots j_N! k_1! \cdots k_N!}.
\end{aligned}
\quad (6)
$$

This expansion is reduced to a finite sum if $\hat{H}$ is polynomial in basic operators, in which case the expansion serves the purpose of expressing the expectation value of products of basic operators in terms of central moments. For a non-polynomial Hamilton operator, the expansion is a formal power series in $\hbar$. The definition of our Poisson bracket ensures that Hamilton's equations

$$\dot{f}(\langle \cdot \rangle, \Delta) = \{f(\langle \cdot \rangle, \Delta), H_{\text{eff,s}}\} \quad (7)$$

on any semiclassical truncation are consistent with Heisenberg's equations of motion evaluated in a state.

Equations of motion such as (7) require initial values for particular solutions. In our case, this means that we should select suitable expectation values and moments of an initial state. However, moments of a state are not arbitrary because a state, interpreted as a map from the algebra of quantum operators to complex-valued expectation values, must fulfill a positivity condition: $\langle \hat{A}^\dagger \hat{A} \rangle \geq 0$ for all operators $\hat{A}$. Positivity implies an infinite set of inequalities for the moments, the best-known example being Heisenberg's uncertainty relation. The remaining inequalities are correspondingly called 'generalized uncertainty relations' [22, 23]. They provide necessary conditions for a set of moments to belong to a positive state. While it remains unknown whether these conditions are also sufficient, it is clear that any initial set of moments must obey all the generalized uncertainty relations. In practice, it is often more convenient to select initial moments by calculating them for a given initial wave function or density matrix (defining a positive state). The evolved moments, using (7), are then guaranteed to belong to a positive state to within the order of approximation used.

A. Examples

For a single pair of classical degrees of freedom, $N = 1$, the phase space of the semiclassical truncation of order two is five-dimensional (and therefore cannot be symplec-

tic). In addition to the basic expectation values q and π, there are two fluctuation variables, $\Delta(q^2)$ and $\Delta(\pi^2)$, and the covariance $\Delta(q\pi)$. The non-zero Poisson brackets of these variables are given by

$$\{q, \pi\} = 1 \tag{8}$$
$$\{\Delta(q^2), \Delta(q\pi)\} = 2\Delta(q^2) \tag{9}$$
$$\{\Delta(q\pi), \Delta(\pi^2)\} = 2\Delta(\pi^2) \tag{10}$$
$$\{\Delta(q^2), \Delta(\pi^2)\} = 4\Delta(q\pi) \tag{11}$$

which are linear and equivalent to the Lie algebra $\mathrm{sp}(2, \mathbb{R})$.

More generally, the second-order semiclassical truncation for N pairs of classical degrees of freedom is equivalent to $\mathrm{sp}(2N, \mathbb{R})$ [3]. Third-order semiclassical truncations also have linear Poisson brackets which are no longer semisimple: Within a higher-order semiclassical truncation, the Poisson bracket of two third-order moments is a sum of fourth-order moments and products of

second-order moments, all of which are of order four and set to zero in a third-order truncation. Moreover, the Poisson bracket of a second-order moment and a third-order moment is proportional to a third-order moment, for instance

$$\{\Delta(q^2), \Delta(q^2\pi)\} = 2\Delta(q^3)$$
$$\{\Delta(q^2), \Delta(q\pi^2)\} = 4\Delta(q^2\pi)$$
$$\{\Delta(q^2), \Delta(\pi^3)\} = 6\Delta(q\pi^2)$$

for $N = 1$. The third-order moments in a semiclassical truncation of order three therefore form an Abelian ideal, and the corresponding Lie algebra is not semisimple. (For $N = 1$, the Lie algebra is the semidirect product $\mathrm{sp}(2, \mathbb{R}) \ltimes \mathbb{R}^4$ where $\mathrm{sp}(2, \mathbb{R})$ acts according to its spin-3/2 representation [3].)

For orders higher than three, the Poisson brackets are non-linear and therefore do not define Lie algebras. A general expression is given by [1, 24]

$$\{\Delta(q^b p^a), \Delta(q^d p^c)\} = a\, d\, \Delta(q^b p^{a-1})\Delta(q^{d-1} p^c) - bc\Delta(q^{b-1}p^a)\Delta(q^d p^{c-1})$$
$$+ \sum_{\mathrm{odd}\ n=1}^{M} \left(\frac{i\hbar}{2}\right)^{n-1} K^n_{abcd}\, \Delta(q^{b+d-n} p^{a+c-n}) \tag{12}$$

where $M = \min(a+c, b+d, a+b, c+d)$ and

$$K^n_{abcd} = \sum_{m=0}^{n} (-1)^m m!(n-m)! \binom{a}{m}\binom{b}{n-m}\binom{c}{n-m}\binom{d}{m}. \tag{13}$$

The inclusion of only odd n in the sum ensures that all coefficients are real. Terms containing $\Delta(q)$ or $\Delta(p)$ are considered zero: They correspond to expectation values of the form $\langle \hat{a} - a \rangle = 0$ which are identically zero.

B. Purity

The collection of all moments determines a state, provided it obeys conditions that follow from (generalized) uncertainty relations. Since moments are defined using expectation values, which can be computed from a pure or mixed state, they may describe a pure or mixed state. In general, it is not easy to determine the purity of a state described by moments without first reconstructing a density matrix from them. As we will see, however, canonical variables for moments can provide indications as to possible impurity parameters. In preparation of this application, we discuss here ingredients for possible reconstructions of states from a given set of moments.

If the state is pure, it is sufficient to consider only the moments $\Delta(q^n)$ and $\Delta(q^{n-1}\pi)$ to reconstruct a wave

function [1]. For instance, we can use Hermite polynomials $H_n(q)$ and their coefficients $h_{n,l}$ defined such that $H_n(q) = \sum_l h_{n,l} q^l$. The expectation values $a_n = \langle \hat{q}^n \rangle$ can then be used to compute

$$c_n = \sum_l h_{n,l} a_l = \int \mathrm{d}q |\psi(q)|^2 H_n(q), \tag{14}$$

from which we obtain the probability density

$$|\psi(q)|^2 = e^{-q^2} \sum_n \frac{c_n}{2^n \pi n!} H_n(q) \tag{15}$$

using the orthonormality relation of Hermite polynomials.

Using $b_n = \langle \hat{q}^n \hat{\pi} \rangle$, the phase $\alpha(q)$ of the wave function $\psi(q) = \exp(i\alpha(q))|\psi(q)|$ then follows from

$$\mathrm{Re}\, b_n = \mathrm{Re} \int \mathrm{d}q\, \psi^* q^n \frac{\hbar}{i} \frac{\mathrm{d}\psi}{\mathrm{d}q}$$
$$= \mathrm{Re} \int \mathrm{d}q\, e^{-i\alpha} |\psi| q^n \frac{\hbar}{i} \left(i\frac{\mathrm{d}\alpha}{\mathrm{d}q} e^{i\alpha} |\psi| + e^{i\alpha} \frac{\mathrm{d}|\psi|}{\mathrm{d}q} \right)$$
$$= \hbar \int \mathrm{d}q |\psi|^2 q^n \frac{\mathrm{d}\alpha}{\mathrm{d}q}. \tag{16}$$

If we define

$$d_n = \sum_l h_{n,l} \mathrm{Re} b_n = \hbar \int \mathrm{d}q |\psi|^2 \frac{\mathrm{d}\alpha}{\mathrm{d}q} H_n(q) , \qquad (17)$$

we reconstruct

$$\frac{\mathrm{d}\alpha}{\mathrm{d}q} = \frac{e^{-q^2}}{\hbar |\psi|^2} \sum_n \frac{d_n}{2^n \pi n!} H_n(q) . \qquad (18)$$

Integration gives $\alpha(q)$ up to an arbitrary constant phase.

In order to reconstruct a density matrix, we need all moments. First, position moments are given by

$$\Delta(q^a) = \mathrm{tr}((\hat{q} - \langle \hat{q} \rangle)^a \hat{\rho}) = \int (q - \langle \hat{q} \rangle)^a \rho(q, q) \mathrm{d}q \quad (19)$$

from which we can reconstruct the diagonal part $\rho(q, q)$ using orthogonal polynomials. Using momentum-dependent moments, we can compute the values of

$$\mathrm{tr}((\hat{q} - \langle \hat{q} \rangle)^a \hat{\pi}^b \hat{\rho}) = \left(\frac{\hbar}{i} \right)^b \int (q - \langle \hat{q} \rangle)^a \left. \frac{\partial^b \rho(y, q)}{\partial y^b} \right|_{y=q} \mathrm{d}q \qquad (20)$$

and use them in

$$\sum_b \frac{1}{b!} \left(\frac{id}{\hbar} \right)^b \mathrm{tr}((\hat{q} - \langle \hat{q} \rangle)^a \hat{\pi}^b \hat{\rho}) = \int (q - \langle \hat{q} \rangle)^a \sum_b \frac{d^b}{b!} \left. \frac{\partial^b \rho(y, q)}{\partial y^b} \right|_{y=q} \mathrm{d}q$$

$$= \int (q - \langle \hat{q} \rangle)^a \rho(q + d, q) \mathrm{d}q \qquad (21)$$

to reconstruct $\rho(q + d, q)$ for arbitrary q and d.

In a semiclassical truncation we have incomplete information about the moments and it may be impossible to tell with certainty whether truncated moments correspond to a pure or mixed state. However, if there are parameters that appear only in moments of the form $\Delta(q^a \pi^b)$ with $b > 1$, they may be considered candidates for impurity parameters. We will see several examples in our derivation of canonical variables for moments.

C. Casimir–Darboux coordinates

Since the brackets (12) are non-canonical, it is not possible to interpret the moments directly in terms of configuration variables and momenta. However, the Darboux theorem and its generalization to Poisson manifolds guarantee that one can always choose coordinates that are canonical, together with a set of Casimir coordinates that have vanishing Poisson brackets with all other variables. The required transformation from moments to Casimir–Darboux variables of this form is, in general, non-linear. In [3], we have developed a systematic method to derive such transformations, based on a proof of Darboux' theorem given in [25]. We have applied this method to semiclassical truncations in [3]. Here we review the simplest case of a single pair of classical degrees of freedom at the second order in $\sqrt{\hbar}$. In this case, Casimir–Darboux variables had already been found independently in [26, 27]. Derivations for the more complicated cases are relegated to the Appendices A and B with further details on the

relevant integrations. These new results will be applied in the following section.

The relevant Poisson brackets of second-order moments are given in (9)–(11). The procedure starts by choosing a function that plays the role of the first canonical coordinate. It is convenient to have a quantum fluctuation as one of the configuration variables, and therefore we choose $s = \sqrt{\Delta(q^2)}$. This function, viewed formally as a Hamiltonian, is the generator of a Hamiltonian flow on phase space defined by

$$\frac{\mathrm{d}f(\Delta(q^2), \Delta(q\pi), \Delta(\pi^2))}{\mathrm{d}\epsilon} = \{ f(\Delta(q^2), \Delta(q\pi), \Delta(\pi^2)), s \} . \qquad (22)$$

If we already knew canonical coordinates, it would be obvious that the Poisson bracket on the right-hand side of this equation changes only the variable p_s canonically conjugate to s, and therefore the derivative should be equal to the (negative) partial derivative of f by p_s. Since we do not know p_s yet, we revert this argument and implicitly define p_s such that the derivatives in (22) equal the negative partial derivative by p_s for any function f. In particular, for the three second-order moments we obtain

$$\frac{\partial \Delta(q^2)}{\partial p_s} = -\{\Delta(q^2), \sqrt{\Delta(q^2)}\} = 0 \qquad (23)$$

$$\frac{\partial \Delta(q\pi)}{\partial p_s} = -\{\Delta(q\pi), \sqrt{\Delta(q^2)}\} = \sqrt{\Delta(q^2)} = s \qquad (24)$$

$$\frac{\partial \Delta(\pi^2)}{\partial p_s} = -\{\Delta(\pi^2), \sqrt{\Delta(q^2)}\} = 2\frac{\Delta(q\pi)}{\sqrt{\Delta(q^2)}} = 2\frac{\Delta(q\pi)}{s} \qquad (25)$$

By construction, these are partial differential equations in which s is held constant. We can easily solve (24) by

$$\Delta(q\pi) = sp_s + f_1(s) \qquad (26)$$

with a free function f_1 depending only on s. Inserting this solution in (25), we have

$$\Delta(\pi^2) = p_s^2 + 2\frac{f_1(s)}{s}p_s + f_2(s) \qquad (27)$$

with another free function f_2 depending only on s.

Computing $\{\Delta(q\pi), \Delta(\pi^2)\}$ using the canonical nature of the variables s and p_s, and requiring that it equal $2\Delta(\pi^2)$ implies two equations:

$$\frac{\mathrm{d}f_1}{\mathrm{d}s} = \frac{f_1}{s} \quad , \quad \frac{\mathrm{d}f_2}{\mathrm{d}s} = 2\frac{f_1}{s^2}\frac{\mathrm{d}f_1}{\mathrm{d}s} - 2\frac{f_2}{s} . \qquad (28)$$

They are solved by

$$f_1(s) = U_2 s \quad , \quad f_2(s) = \frac{U_1}{s^2} + U_2^2 \qquad (29)$$

with constants U_1 and U_2. We can eliminate U_2 by a canonical transformation replacing p_s with $p_s + U_2$. The constant U_1 is the Casimir coordinate which has vanishing Poisson brackets with all other functions. The resulting moments in terms of Casimir–Darboux variables are

$$\Delta(q^2) = s^2 \quad , \quad \Delta(q\pi) = sp_s \quad , \quad \Delta(\pi^2) = p_s^2 + \frac{U_1}{s^2} \qquad (30)$$

as in [26, 27].

In general, it may be difficult to recognize a variable such as U_1 as a Casimir coordinate. In such a case, the flow generated by s or $s^2 = \Delta(q^2)$ is again useful:

$$\frac{\mathrm{d}\Delta(q\pi)}{\mathrm{d}\epsilon} = -2\Delta(q^2) \quad , \quad \frac{\mathrm{d}\Delta(\pi^2)}{\mathrm{d}\epsilon} = -4\Delta(q\pi) . \qquad (31)$$

The solutions are similar to what we already used, $\Delta(q\pi)[\epsilon] = -2\Delta(q^2)\epsilon + d$ for the first equation and $\Delta(\pi^2)[\epsilon] = 4\Delta(q^2)\epsilon^2 - 4d\epsilon + e$ for the second equation, with constants d and e. But now we use these equations to eliminate ϵ instead of solving for p_s. Inserting $\epsilon = \frac{1}{2}(d - \Delta(q\pi)[\epsilon])/s^2$ in $\Delta(\pi^2)[\epsilon]$ implies

$$\Delta(\pi^2)[\epsilon] = \frac{\Delta(q\pi)[\epsilon]^2}{\Delta(q^2)} - 3\frac{d^2}{\Delta(q^2)} + e . \qquad (32)$$

The combination $U_1 = \Delta(q^2)\Delta(\pi^2)[\epsilon] - \Delta(q\pi)[\epsilon]^2 = -3d^2 + es^2$ is therefore independent of ϵ. Since $\mathrm{d}U_1/\mathrm{d}\epsilon = \{U_1, \Delta(q^2)\} = 0$, U_1 is a coordinate Poisson orthogonal to s. It is also Poisson orthogonal to p_s by construction, and therefore represents the Casimir variable of this system.

III. APPLICATIONS

As shown in the preceding section, the inclusion of moments in semiclassical truncations leads to several new degrees of freedom. In this section, we highlight some of the physical effects implied by them. At the same time, we show that the form in which canonical variables appear in various realizations of the moment algebras suggests truncations to smaller canonical subsystems which are easier to analyze by analytic means and often show physical effects more intuitively.

A. Partition and two-point function of a free massive scalar field

Our first example is an application of the second-order mapping (30), rederived here from [26, 27], to a free field theory. We start with the Hamiltonian,

$$H = \int \mathrm{d}x \left(\frac{1}{2}\pi^2 + \frac{1}{2}(\partial_x\phi)^2 + \frac{1}{2}m^2\phi^2 \right) \qquad (33)$$

of a 1-dimensional real scalar field with mass m. We transform to momentum space by writing

$$\phi_k = \frac{1}{\sqrt{2\pi}}\int \mathrm{d}x\, \phi(x)e^{-ikx} \quad , \quad \pi_k = \frac{1}{\sqrt{2\pi}}\int \mathrm{d}x\, \pi(x)e^{-ikx} \qquad (34)$$

with a real wave number k. Reality of $\phi(x)$ and $\pi(x)$ implies that $\phi_k^* = \phi_{-k}$ and $\pi_k^* = \pi_{-k}$.

If we assume that the spatial manifold with coordinate x is compact and of length 2π, thus describing a scalar field on a unit circle, k takes integer values and we have finite Poisson brackets

$$\{\phi_k, \pi_{k'}\} = \delta_{kk'} \qquad (35)$$

replacing the field-theory Poisson brackets $\{\phi(x), \pi(y)\} = \delta(x - y)$ in the position representation. Each mode with fixed k is then described by an independent canonical pair (ϕ_k, π_k), which can easily be quantized to a pair $(\hat{\phi}_k, \hat{\pi}_k)$ of operators.

The classical reality condition implies the adjointness relations

$$\hat{\phi}_k^\dagger = \hat{\phi}_{-k} \quad , \quad \hat{\pi}_k^\dagger = \hat{\pi}_{-k} . \qquad (36)$$

The Hamilton operator can therefore be expressed as

$$\hat{H} = \frac{1}{2}\sum_{k=-\infty}^{\infty}\left(\hat{\pi}_k\hat{\pi}_k^\dagger + \omega_k^2\hat{\phi}_k\hat{\phi}_k^\dagger\right) \qquad (37)$$

with $\omega_k = \sqrt{m^2 + k^2}$. A further transformation,

$$\hat{\phi}_k = \frac{1}{2}\left(\hat{\phi}_k^\mathrm{R} - i\hat{\phi}_k^\mathrm{L}\right) \quad , \quad \hat{\pi}_k = \frac{1}{2}\left(\hat{\pi}_k^\mathrm{R} + i\hat{\pi}_k^\mathrm{L}\right) , \qquad (38)$$

explicitly decouples left and right-moving modes, $\hat{\phi}_k^{\mathrm{L}}$ and $\hat{\phi}_k^{\mathrm{R}}$, respectively. The Hamilton operator then reads

$$\hat{H} = \frac{1}{2} \sum_{k=-\infty}^{\infty} \left(\left(\hat{\pi}_k^{\mathrm{R}}\right)^2 + \left(\hat{\pi}_k^{\mathrm{L}}\right)^2 + \frac{1}{4}\omega_k^2 \left(\hat{\phi}_k^{\mathrm{R}}\right)^2 + \frac{1}{4}\omega_k^2 \left(\hat{\phi}_k^{\mathrm{L}}\right)^2 \right)$$

(39)

1. Partition function

Since all the modes decouple and have harmonic Hamiltonians, the mapping for a single degree of freedom at the second order provides an exact effective description in any state in which cross-correlations between different modes vanish. In the absence of interaction terms in the Hamiltonian, the latter condition is satisfied in the ground state. More generally, we can also consider ensemble averages in finite-temperature states. Since cross-correlations do not contribute the the energy of our non-interacting system, they will not be affected by turning on a finite temperature. Moreover, correlations in harmonic systems have oscillatory solutions around zero and therefore vanish in an ensemble average.

Mode fluctuations parameterized by the canonical variable s_k with momentum p_k and Casimir U_k, by contrast, are bounded from below by the uncertainty relation and do not average to zero. For every fixed mode and at finite temperature T, we can compute the partition function

$$\mathcal{Z}(\beta, \omega_k, \lambda) = \int_0^\infty \int_{-\infty}^\infty \int_{U_{\mathrm{min}}}^\infty \mathrm{d}s_k \, \mathrm{d}p_k \, \mathrm{d}U_k \exp\left(-\beta\left(\frac{1}{2}p_k^2 + \lambda\frac{U_k}{2s_k^2} + \frac{1}{8}\omega_k^2 s_k^2 \right) \right),$$

(40)

where $\beta = 1/k_{\mathrm{B}}T$ and $U_{\mathrm{min}} = \hbar^2/4$ and we have restricted s_k to positive values. We have inserted the auxiliary parameter λ in anticipation of an application below in which a λ-derivative of $\mathcal{Z}$ will give us the ensemble average of the quantum uncertainty U_k. For all other purposes, we use the physical value $\lambda = 1$. If we perform the U_k-integral before the s_k-integral, the partition function

$$\mathcal{Z}(\beta, \omega_k, \lambda) = 4\pi \frac{2 + \beta\omega_k\sqrt{U_{\mathrm{min}}\lambda}}{\lambda\omega_k^3\beta^3} \exp\left(-\frac{1}{2}\beta\omega_k\sqrt{U_{\mathrm{min}}\lambda} \right)$$

(41)

can be obtained in closed form.

A derivative by ω_k (at $\lambda = 1$) results in the ensemble averages

$$\langle (s_k^{\mathrm{R}})^2 \rangle_{\mathrm{E}} = \langle (s_k^{\mathrm{L}})^2 \rangle_{\mathrm{E}} = \frac{12}{\omega_k^2\beta} + \frac{U_{\mathrm{min}}\beta}{1 + \frac{1}{2}\sqrt{U_{\mathrm{min}}}\omega_k\beta}. \quad (42)$$

of dispersions in a thermal state. Moreover, the average energy per mode is

$$\langle E_k \rangle_{\mathrm{E}} = -\frac{\partial \log \mathcal{Z}}{\partial \beta} = \frac{12 + \beta\omega_k \left(6\sqrt{U_{\mathrm{min}}} + U_{\mathrm{min}}\omega_k\beta\right)}{2\beta \left(2 + \beta\sqrt{U_{\mathrm{min}}}\omega_k\right)}.$$

(43)

In the limit $T \to 0$, the value

$$\langle E_k \rangle_E = \sqrt{U_{\mathrm{min}}}\frac{\omega_k}{2}$$

(44)

agrees with the ground-state energy if we use $U_{\mathrm{min}} = \hbar^2/4$, noting that a single mode used here appears with frequency $\omega_k/2$ in (39). (The combination of ϕ_k^{R} and ϕ_k^{L} has the standard harmonic-oscillator energy $\frac{1}{2}\hbar\omega_k$ on average.) Finally, the ensemble average of the quantum uncertainty in a thermal state can be determined as

$$\begin{aligned} \langle U_k \rangle_{\mathrm{E}} &= \frac{8}{\beta^2\omega_k} \frac{1}{\mathcal{Z}} \frac{\partial^2 \mathcal{Z}}{\partial\omega_k\partial\lambda}\bigg|_{\lambda=1} \\ &= U_{\mathrm{min}} + \frac{24}{\beta^2\omega_k^2} + \frac{4U_{\mathrm{min}}}{2 + \sqrt{U_{\mathrm{min}}}\beta\omega_k}, \end{aligned} \quad (45)$$

which approaches U_{min} as $T \to 0$. For $T \neq 0$, $\langle U_k \rangle_{\mathrm{E}} > U_{\mathrm{min}}$ in a mixed, finite-temperature state. The difference $U - U_{\mathrm{min}}$ is therefore an impurity parameter in this situation, which is in agreement with our discussion in Sec. II B and the fact that the Casimir U only appears in the second-order moment $\Delta(\pi^2)$.

We see that canonical variables for semiclassical truncations can give easy access to thermodynamical quantities by rewriting a quantum statistical system in the form of a classical system. The canonical nature of variables parameterizing quantum moments makes it possible to determine the correct phase-space volume for the partition function.

2. Two-point function

We extend the definition of moments to our field theory by applying the quantum-mechanics definition to each mode ϕ_k. Introducing $\widehat{\delta\phi}_k = \hat{\phi}_k - \langle\hat{\phi}_k\rangle_{\mathrm{Q}}$, we then have $\Delta(\phi_k\phi_{k'}) = \langle\widehat{\delta\phi}_k\widehat{\delta\phi}_{k'}\rangle_{\mathrm{Q}}$, from which we can obtain correlations in the position representation by Fourier transformation. In these definitions, we have explicitly indicated that expectation values $\langle\cdot\rangle_{\mathrm{Q}}$ refer to a quantum state as opposed to the ensemble average used in (42).

The two-point function

$$\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \sum_{kk'}\langle\langle\widehat{\delta\phi}_k\widehat{\delta\phi}_{k'}\rangle_{\mathrm{Q}}\rangle_{\mathrm{E}}e^{ikx}e^{ik'y}$$

$$= \frac{1}{4}\sum_{kk'}\left\langle\left\langle\left(\widehat{\delta\phi}_k^{\mathrm{R}} - i\widehat{\delta\phi}_k^{\mathrm{L}}\right)\left(\widehat{\delta\phi}_{k'}^{\mathrm{R}} - i\widehat{\delta\phi}_{k'}^{\mathrm{L}}\right)\right\rangle_{\mathrm{Q}}\right\rangle_{\mathrm{E}}e^{ikx}e^{ik'y}$$

combines both types of averages. We can simplify the double summation using $\widehat{\delta\phi}_{-k}^{\mathrm{L}} = -\widehat{\delta\phi}_k^{\mathrm{L}}$, which follows from the adjointness relation for $\hat{\phi}_k$. Using zero cross-covariances between the modes as well as the fact that the fluctuations only depend on the wave number k but not on whether the mode is left or right-moving, the double summation is then reduced to

$$\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\sum_k\langle\langle\widehat{\delta\phi}_k^{\mathrm{R}}\widehat{\delta\phi}_k^{\mathrm{R}}\rangle_{\mathrm{Q}}\rangle_{\mathrm{E}}\cos\left(k(x-y)\right). \tag{46}$$

Inserting (42), we obtain

$$\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\sum_k\left(\frac{12}{\omega_k^2\beta} + \frac{U_{\mathrm{min}}\beta}{1 + \frac{1}{2}\sqrt{U_{\mathrm{min}}}\omega_k\beta}\right)\cos\left(k(x-y)\right). \tag{47}$$

In the limit of large $k \gg 1$, or of wave lengths much smaller than the circumference of our circle, we can replace $\sum_k$ by $(2\pi)^{-1}\int\mathrm{d}k$, such that

$$\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{1}{2}\int\frac{\mathrm{d}k}{2\pi}\left(\frac{12}{\omega_k^2\beta} + \frac{U_{\mathrm{min}}\beta}{1 + \frac{1}{2}\sqrt{U_{\mathrm{min}}}\omega_k\beta}\right)\cos\left(k(x-y)\right). \tag{48}$$

It is instructive to consider the low-temperature limit $\beta \to \infty$. The result,

$$\lim_{\beta\to\infty}\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \hbar\int\frac{\mathrm{d}k}{4\pi\omega_k}\cos\left(k(x-y)\right)$$

$$= \frac{\hbar}{2\pi}K_0(m|x-y|) \tag{49}$$

with a Bessel function K_0, agrees exactly with the equal-time two-point function obtained using path integral methods.

We can also consider the case where the temperature is nonzero but still small enough for the semi-classical approximation to be valid. Taylor expanding the integrand about $\beta = \infty$, the first-order temperature correction to the two-point function is $8/(\omega_k^2\beta)$:

$$\langle\Delta\left(\phi(x)\phi(y)\right)\rangle_{\mathrm{E}} = \frac{\hbar}{2\pi}K_0(m|x-y|) + \frac{9kT}{4m}\exp\left(-m|x-y|\right) + O(T^2). \tag{50}$$

The asymptotic behavior $K_0(z) \sim \sqrt{\frac{1}{2}\pi/z}\,e^{-z}$ for large z shows that the term linear in the temperature decreases more slowly with the distance than the temperature-independent term. For large-distance correlations, this correction from a non-zero temperature may therefore be relevant.

B. Closure conditions

Our third and fourth order mappings from App. A suggest new closure conditions (in the sense of [28]) that can be used to describe moments by a small number of parameters. In particular, we may assume that the second-order fluctuation parameter s contributes to higher-order moments such that $\Delta(q^n) = s^n$, at least for even n. For the third-order moments $\Delta(q^3)$ in the fourth-order truncation, Eq. (A49), the cubic dependence on s_i is multiplied by a free parameter, given by the Casimir variable C, unlike in even-order moments $\Delta(q^2)$ and $\Delta(q^4)$, Eq. (A50). Since odd-order moments are often subdominant, for instance in the family of Gaussian states, we can set $C = 0$ and assume that this behavior extends to higher orders. These considerations suggest the closure conditions

$$\Delta(q^n) = \begin{cases} s^n & \text{for even } n \\ 0 & \text{for odd } n \end{cases} \tag{51}$$

for all moments, replacing a truncation to finite order. In an effective Hamiltonian, we then obtain the *all-orders effective potential*

$$
\begin{aligned}
V_{\text{all-orders}}(q,s) &= V(q) + \frac{U}{2ms^2} + \sum_n \frac{1}{(2n)!} \frac{d^{2n}V(q)}{dq^{2n}} s^{2n} \\
&= \frac{U}{2ms^2} + \frac{1}{2}\left(V(q+s) + V(q-s)\right) \quad (52)
\end{aligned}
$$

for a classical potential $V(q)$. The Casimir variable U may be set equal to the minimum value $\hbar^2/4$ allowed by the uncertainty relation.

It is interesting to note that a similar potential has appeared before, based on an analysis of the Wigner function in [21]; see in particular Eq. (4.19b) there. However, in this derivation, the argument q of the classical potential is shifted by terms which in general are not real and depend on more than just a single parameter. For some choices of these parameter, our all-orders effective potential can be reproduced with a very different derivation. This relationship lends additional support to our constructions. To the best of our knowledge, the effective potential derived in [21] has not been applied in concrete examples such as those we now turn to.

1. Non-differentiable potentials

Semiclassical physics is usually based on an expansion which requires a smooth potential. Our all-orders effective potential, by contrast, explicitly sums up a perturbative series and expresses quantum effects via finite shifts of the classical potential. It can therefore be applied to potentials that are not smooth or not even differentiable.

As an example, consider the potential $V(q) = |q|$. In particular, we can check the ground state energy. In the static case of zero momentum (and using atomic units in which $\hbar = 1$ and $m = 1$), we have

$$
V_{\text{all-orders}}(q,s) = \frac{1}{8s^2} + \frac{1}{2}\left(|q+s| + |q-s|\right). \quad (53)
$$

This function has a minimum at $q = 0$ and $s = 2^{-2/3}$, and the minimum value is $E_{\text{ground}} = 0.94$. We can calculate the exact value of the ground state energy using a truncated oscillator basis. The result is $E_{\text{ground}}^{\text{exact}} = 0.81$.

It is possible to obtain this non-differentiable potential as a limit of a differentiable one. To this end, consider the Hamiltonian

$$
H = \sqrt{1+\pi^2} + \frac{1}{2}q^2 \quad (54)
$$

which can be interpreted as describing a relativistic particle with position-dependent mass $\sqrt{H^2 - \pi^2} = \sqrt{1 + \frac{1}{2}q^2}$. After a simple canonical transformation $(q,\pi) \mapsto (-\pi, q)$ the Hamiltonian

$$
H = \frac{\pi^2}{2} + \sqrt{1+q^2} \quad (55)
$$

appears in standard form for a non-relativistic system. Now the all-orders effective potential with $U = 1/4$ (setting $\hbar = 1$ for the purpose of numerical comparisons) is given by

$$
V_{\text{all-orders}}(q,s) = \frac{1}{8s^2} + \frac{1}{2}\left(\sqrt{1+(q+s)^2} + \sqrt{1+(q-s)^2}\right) \quad (56)
$$

and minimized in q when $q = 0$. Minimizing

$$
V_{\text{all-orders}}(0,s) = \frac{1}{8s^2} + \sqrt{1+s^2} \quad (57)
$$

with respect to s, we find the minimum value

$$
E_{\text{ground}} = 1.47. \quad (58)
$$

The exact ground state energy is

$$
E_{\text{ground}}^{\text{exact}} = 1.44. \quad (59)
$$

The agreement here is better than in the preceding example, which can be interpreted as a limit of a potential in which $\sqrt{1+q^2}$ is replaced by $\lim_{d\to 0}\sqrt{d+q^2}$.

2. Canonical tunneling time in polynomial potentials

The regimes of validity of the all-orders potential can be tested in the case of tunneling escape. For this purpose, we consider a fourth-order polynomial potential in order to describe tunneling escape from a metastable state:

$$
V_{\text{poly}}(q) = \frac{27}{4}V_{\text{top}}\gamma q^2(q-1)\left(q - \frac{1}{\gamma}\right), \quad (60)
$$

where V_{top} is a parameter that controls the height of the barrier and γ controls the location of the global minimum of this potential. When γ is small, this potential has the following approximate critical points with the corresponding potential values: The top of the barrier is characterized by

$$
q_{\text{top}} \approx \frac{2}{3} \quad , \quad V_{\text{poly}}(q_{\text{top}}) = V_{\text{top}} \quad (61)
$$

and the global minimum is characterized by

$$
q_{\text{min}} \approx \frac{3}{4\gamma} \quad , \quad V_{\text{poly}}(q_{\text{min}}) \approx -\frac{729\,V_{\text{top}}}{1024\gamma^3}. \quad (62)
$$

In addition to the global minimum, there is a local minimum at $q = 0$ with $V_{\text{poly}}(0) = 0$.

Classically, if the particle starts close to the local minimum at $q = 0$ with an energy less than V_{top}, the particle will remain confined. However if quantum degrees of freedom are taken into account, we know that the particle can tunnel through the barrier and into the lower basin. We can account for this modified dynamics using second-order variables if the barrier is sufficiently small. If the barrier is large, higher-order corrections need to be taken

into account in order to see tunneling. The all-orders effective potential, given by

$$V_{\text{all–orders}}(q, s) = \frac{U}{2ms^2} + \frac{1}{2}\left(V_{\text{poly}}(q + s) + V_{\text{poly}}(q - s)\right)$$
(63)

includes some of the terms that result from higher-order moments.

For escape from a metastable state, the particle is initially at the local minimum at $q = 0$, around which

$$V_{\text{poly}}(q) \approx \frac{27}{4}V_{\text{top}}q^2 .$$
(64)

For this quadratic approximation, the effective potential is

$$V_{\text{eff}}(q, s) \approx \frac{27}{4}V_{\text{top}}\left(q^2 + s^2\right) + \frac{U}{2s^2} .$$
(65)

This potential has a minimum at

$$q = 0 \quad , \quad s = \left(\frac{2U}{27V_{\text{top}}}\right)^{1/4}$$
(66)

which give the approximate ground state energy

$$V_0 \approx \frac{3}{8}\sqrt{\frac{3U}{V_{\text{top}}}}\left(V_{\text{top}} + 2\right) .$$
(67)

Given the initial conditions (66) we can track the particle dynamics numerically; see Fig. 1. If the parameter V_{top} becomes large the particles no longer tunnels if one only considers the second-order canonical mapping. Second-order dynamics can provide good approximations in certain regimes, but for "deep" tunneling, in which case the expectation value spends a long time within the barrier and the moments have time to change considerably, we need an extension to higher orders. The all-orders effective potential is then useful for understanding the escape from a local minimum in deep tunneling situations.

Using the all-orders potential, we estimate the tunneling time as a function of the tunnel exit position of the particle, which corresponds to the particle position around the critical point $q_{\text{top}} \approx 2/3$. Figures 2 and 3 show a numerical comparison of the canonical tunneling time and the exit momentum of the particle, using the all-orders potential and exact solutions, respectively.

In [4] we used the all-orders effective potential for atomic systems, based on the all-orders closure condition. In a further approximation, it was possible to eliminate some of the basic variables such that $s \approx q$ inside the barrier. For the polynomial potential we can test the same behavior by computing the evolution of the expectation value q and its fluctuation s. As shown Fig. 4, the approximate relationship between q and s during tunneling is maintained also here.

Finally, it is interesting to note that the tunneling time can be sensitive to the parameter γ which specifies the location of the global minimum of the classical potential (60). We estimate the tunneling time in terms of γ, starting with $\gamma = 0.1$, as shown in Fig. 5.
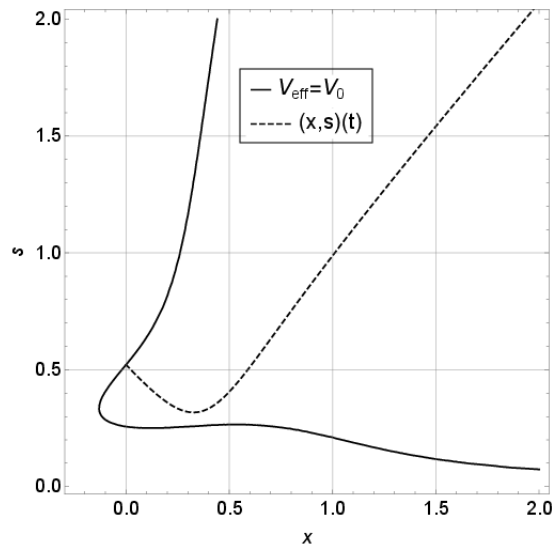

FIG. 1: Dynamics in the all-orders effective potential (63): The potential is represented by its ground-state equipotential curve $V_{\text{eff}} = V_0$ (solid line), together with a tunneling trajectory starting from the local minimum (dashed line). For this plot we chose the parameters $V_{\text{top}} = 1$, $\gamma = 0.1$, $U = 1/4$. The "extra dimension" given by the fluctuation parameter s provides the particle with an escape route around the classical barrier, without violating energy conservation. (All figures are shown in atomic units.)
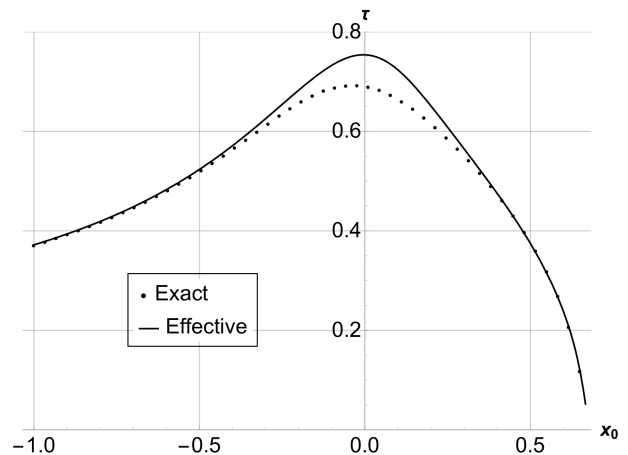

FIG. 2: Tunneling times as a function of the starting position, for an exact calculation and the all-orders potential, respectively. There is good agreement, with larger discrepancies close to the origin where we have deep tunneling.

C.   Effective potentials

Casimir–Darboux coordinates for moments, in combination with the effective Hamiltonian (6), allow us to identify the dynamics of a semiclassical truncation with a dynamical canonical system. The classical momentum
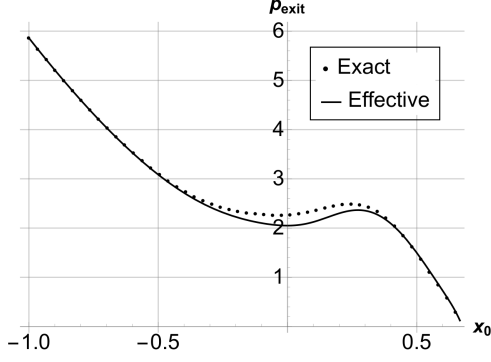
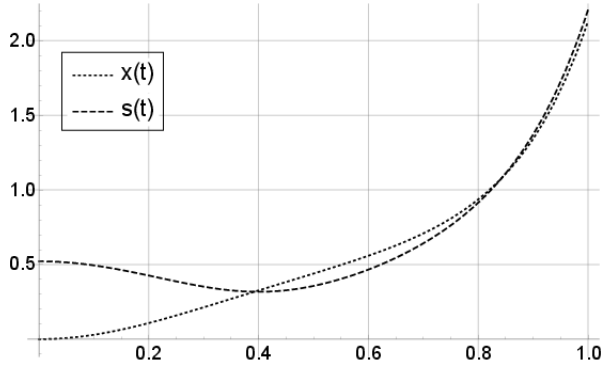FIG. 3: The exit momentum of the particle as a function of the initial position.

FIG. 4: Trajectories of t4he tunneling coordinate q and its fluctuation s for the all-orders effective potential (63).

π (derived from the momentum expectation value) is then accompanied by one or more new momenta that parameterize fluctuations, correlations, and higher moments.

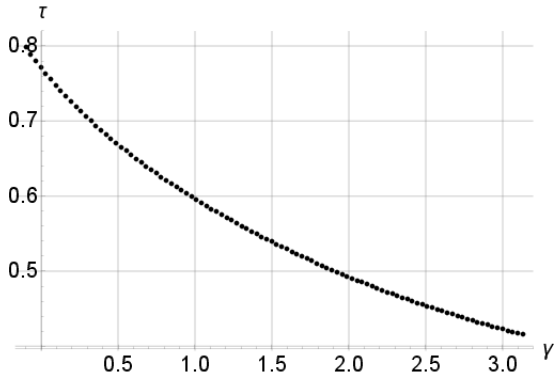For a single classical pair of degrees of freedom to second semiclassical order, the moments are quadratic in

FIG. 5: The tunneling time as a function of γ in the potential (60).

the new momentum p_s with constant coefficients. A dynamical system with standard kinetic term is therefore obtained [27]:

$$
\begin{aligned}
\langle \hat{H} \rangle &= \frac{\langle \hat{\pi}^2 \rangle}{2m} + V(\hat{q}) \qquad (68) \\
&= \frac{\pi^2 + \Delta(\pi^2)}{2m} + V(q) + \frac{1}{2}V''(q)\Delta(q^2) + \cdots \\
&= \frac{\pi^2}{2m} + \frac{p_s^2}{2m} + \frac{U}{2ms^2} + V(q) + \frac{1}{2}V''(q)s^2 + \cdots
\end{aligned}
$$

with effective potential

$$
V_{\text{eff}}(q,s) = \frac{U}{2ms^2} + V(q) + \frac{1}{2}V''(q)s^2 . \qquad (69)
$$

Our third-order moments provide an extension to the next order, now with three non-classical momenta. The first version, (A24), is quadratic in momenta but with coefficients depending on the configuration variables s_i. The second version, (A34), results in a simplified system with constant coefficients in the extended kinetic term.

However, for two pairs of degrees of freedom, it is not possible to have momentum fluctuations which are quadratic in Darboux momenta with constant coefficients [3]. The resulting effective theories are therefore more involved in such cases. Nevertheless, it is possible to extract an effective potential. Using the Taylor expansion (6) of the effective Hamiltonian $\langle \hat{H} \rangle$ and setting all canonical momenta equal to zero, we obtain an expression depending only on the canonical coordinates. We do not require that the momenta vanish for all solutions of interest, which would then be adiabatic, but rather extract a term from the effective Hamiltonian that serves as an effective potential. For this purpose, canonical variables are required in order to know which functions of the moments should be considered momenta.

For two classical degrees of freedom to second semiclassical order, this procedure leads to a more complicated effective potential. We derive this potential for a classical Hamiltonian of the form

$$
H = \frac{1}{2}\pi_1^2 + \frac{1}{2}\pi_2^2 + V(q_1, q_2) \qquad (70)
$$

as it appears in quantum-mechanics models of field theories used in particle physics. (The masses of the two degrees of freedom then appear in quadratic contributions $\frac{1}{2}m_1^2 q_1^2$ and $\frac{1}{2}m_2^2 q_2^2$ to the potential.) The second-order moment expansion of the expectation value $\langle \hat{H} \rangle$ then leads to non-classical contributions $\frac{1}{2}\Delta(\pi_1^2)$ and $\frac{1}{2}\Delta(\pi_2^2)$ from the kinetic terms, as well as

$$
\frac{1}{2}V_{11}(q_1, q_2)\Delta(q_1^2) + V_{12}(q_1, q_2)\Delta(q_1 q_2) + \frac{1}{2}V_{22}(q_1, q_2)\Delta(q_2^2),
$$

where we have used the notation $V_{ij} = \partial^2 V/\partial q_i \partial q_j$.

According to App. B, it is possible to choose canonical variables s_1, s_2 and β in Casimir–Darboux coordinates such that $\Delta(q_1^2) = s_1^2$, $\Delta(q_2^2) = s_2^2$ and $\Delta(q_1 q_2) =$

$s_1 s_2 \cos\beta$; see Eq. (B65). The moments $\Delta(\pi_1^2)$ and $\Delta(\pi_2^2)$ take more complicated forms in canonical variables, which are shown in Eqs. (B58)–(B61). These moments depend on a fourth canonical variable, α, in addition to s_1, s_2 and β. Moreover, there are two Casimir variables, U_1 and U_2. When all the momenta are set equal to zero, the effective potential derived from these moments is given by

$$
\begin{aligned}
V_{\text{eff}}^{(1)}(q_1, q_2, s_1, s_2, \alpha, \beta, U_1, U_2) \;=\; & V(q_1, q_2) \\
& + \frac{1}{4\sin^2(\beta)}\left(\frac{U_1 - \sqrt{U_2}\sin(\alpha+\beta)}{s_1^2} + \frac{U_1 - \sqrt{U_2}\sin(\alpha-\beta)}{s_2^2} \right) \\
& + \frac{1}{2}V_{11}(q_1,q_2)s_1^2 + V_{12}(q_1,q_2)s_1 s_2 \cos(\beta) + \frac{1}{2}V_{22}(q_1,q_2)s_2^2
\end{aligned}
\tag{71}
$$

The two Casimir coordinates U_1 and U_2 are constants of motion for any classical dynamics and can be considered (state-dependent) parameters of the effective potential, while the remainder in the effective Hamiltonian for non-zero momenta (not used here) is a non-standard kinetic term.

We define the low-energy effective potential $V_{\text{low}}(q_1, q_2)$ as the effective potential V_{eff} restricted to values of the moments (that is, s_1, s_2, α, β, U_1 and U_2) obtained in the ground state of the interacting system. We therefore determine the moments by minimizing the effective potential with respect to s_1, s_2, α, β and the two Casimir coordinates while keeping the classical-type variables q_1 and q_2 free.

In this process, we have to respect the boundaries imposed by uncertainty relations. Since W is linear in U_1 and $\sqrt{U_2}$, minimization sends these two values to the boundary. (From (B44), we know that $U_2 > 0$ for $p_4 = 0$ to be possible.) The relevant boundary components, at zero momenta, can be obtained from Heisenberg's uncertainty relation applied to each canonical pair: As shown in App. B, there are functions Φ and Γ such that

$$
\frac{\hbar^2}{4} \le \Delta(q_1^2)\Delta(\pi_1^2) - \Delta(q_1\pi_1)^2 = \Phi(\beta, p_\beta, \alpha, p_\alpha) \tag{72}
$$

$$
\frac{\hbar^2}{4} \le \Delta(q_2^2)\Delta(\pi_2^2) - \Delta(q_2\pi_2)^2 = \Gamma(\beta, p_\beta, \alpha, p_\alpha); \tag{73}
$$

see Eqs. (B58)–(B61). For zero momenta p_α and p_β, the expressions simplify to

$$
\Phi(\beta, 0, \alpha, 0) \;=\; \frac{1}{2\sin(\beta)^2}\left(U_1 - \sqrt{U_2}\sin(\alpha+\beta) \right) \ge \frac{\hbar^2}{4} \tag{74}
$$

$$
\Gamma(\beta, 0, \alpha, 0) \;=\; \frac{1}{2\sin(\beta)^2}\left(U_1 - \sqrt{U_2}\sin(\alpha-\beta) \right) \ge \frac{\hbar^2}{4} \tag{75}
$$

For fixed U_1 and U_2, these two relations must be true for all α and β. Moreover, for any choice of U_1 and U_2 there must be solutions of α and β such that both relations are saturated: If the coupling between the two degrees of freedom is turned off adiabatically we expect saturation in the ground state. Since U_1 and U_2 are constants of motion for any Hamiltonian, their values do not change during this adiabatic decoupling. Therefore, any choice of U_1 and U_2 must allow some solutions of α and β such that the uncertainty relations are saturated.

At saturation, we can subtract (74) and (75) and obtain

$$
-\frac{1}{2}\sqrt{U_2}\frac{\cos(\alpha)}{\sin(\beta)} = 0, \tag{76}
$$

and thus $U_2 = 0$ or $\cos(\alpha) = 0$. In the latter case, the U_2-dependent term in the effective potential,

$$
V_{U_2} = -\frac{\sqrt{U_2}\cos(\beta)}{4\sin^2(\beta)}\left(\frac{1}{s_1^2} + \frac{1}{s_2^2} \right), \tag{77}
$$

is, for any classical potential, unbounded from below in $\sqrt{U_2}$ for any β such that $\cos(\beta) > 0$. This solution of (76) is therefore ruled out by the condition that a stable ground state must exist for a large class of classical potentials. We conclude that $U_2 = 0$.

Given this solution, the smallest value of U_1 for which (74) can be fulfilled is $U_1 = \hbar^2/2$. Therefore,

$$
\Phi|_{p_3=p_4=U_2=0, U_1=\hbar^2/2} = \frac{\hbar^2}{4\sin\beta^2} = \Gamma_{p_3=p_4=U_2=0, U_1=\hbar^2/2}. \tag{78}
$$

The effective potential then reads

$$
V_{\text{eff}}^{(2)}(q_1, q_2, s_1, s_2, \beta) = V(q_1, q_2) + \frac{\hbar^2}{8\sin(\beta)^2 s_1^2} + \frac{\hbar^2}{8\sin(\beta)^2 s_2^2} + \frac{1}{2}V_{11}s_1^2 + V_{12}s_1 s_2\cos(\beta) + \frac{1}{2}V_{22}s_2^2. \tag{79}
$$

Although we have not minimized the potential in the direction of α, the α-dependence has disappeared. There should, however, be a unique pure state that corresponds to the ground state where the effective potential has its minimum. Since minimization does not determine α, it must be the pure-state condition that fixes its value. This conclusion is in agreement with our earlier discussion of impurity parameters: In the mapping (B58)–(B65), α appears only in moments of the form $\Delta(\pi_i\pi_j)$ which are not required to reconstruct a pure state in the position representation.

Minimization by s_1, s_2 and β gives us three equations:

$$0 = \frac{\partial V_{\text{eff}}^{(2)}}{\partial s_1} = -\frac{\hbar^2}{4s_1^3 \sin^2 \beta} + V_{11}s_1 + V_{12}s_2 \cos \beta \tag{80}$$

$$0 = \frac{\partial V_{\text{eff}}^{(2)}}{\partial s_2} = -\frac{\hbar^2}{4s_2^3 \sin^2 \beta} + V_{22}s_2 + V_{12}s_1 \cos \beta \tag{81}$$

$$0 = \frac{\partial V_{\text{eff}}^{(2)}}{\partial \beta} = -\frac{\hbar^2(s_1^2 + s_2^2) \cos \beta}{4s_1^2 s_2^2 \sin^2 \beta} - V_{12}s_1 s_2 \sin \beta . \tag{82}$$

Subtracting s_2 times (81) from s_1 times (80), we obtain

$$\sin^2 \beta = \frac{\hbar^2}{4s_1^2 s_2^2} \frac{s_2^2 - s_1^2}{V_{11}s_1^2 - V_{22}s_2^2} . \tag{83}$$

Using the sum of s_2 times (81) and s_1 times (80), we derive

$$
\begin{aligned}
4V_{12}^2 s_1^2 s_2^2 \cos^2 \beta &= \left(\frac{\hbar^2(s_1^2 + s_2^2)}{4s_1^2 s_2^2 \sin^2 \beta} - (V_{11}s_1^2 + V_{22}s_2^2) \right)^2 = \left(\frac{s_1^2 + s_2^2}{s_1^2 - s_2^2}(V_{11}s_1^2 - V_{22}s_2^2) + (V_{11}s_1^2 + V_{22}s_2^2) \right)^2 \\
&= 4\frac{(V_{11}s_1^4 - V_{22}s_2^4)^2}{(s_1^2 - s_2^2)^2} .
\end{aligned}
\tag{84}
$$

Alternatively, we can derive $4V_{12}^2 s_1^2 s_2^2 \cos^2 \beta$ as follows: The sum of $s_1 \sin^2 \beta$ times (80) and $\cos \beta \sin \beta$ times (82) implies

$$0 = -\frac{\hbar^2(s_1^2 + s_2^2)}{4s_1^2 s_2^2 \sin^2 \beta} + \frac{\hbar^2}{4s_2^2} + V_{11}s_1^2 \sin^2 \beta = \frac{s_1^2 + s_2^2}{s_1^2 - s_2^2}(V_{11}s_1^2 - V_{22}s_2^2) + \frac{\hbar^2}{4} \frac{V_{11} - V_{22}}{V_{11}s_1^2 - V_{22}s_2^2} \tag{85}$$

using (83). This equation together with (83) also gives us

$$
\begin{aligned}
4V_{12}^2 s_1^2 s_2^2 \cos^2 \beta &= 4V_{12}^2 s_1^2 s_2^2 \left(1 - \frac{2\hbar^2}{s_1^2 s_2^2} \frac{s_2^2 - s_1^2}{V_{11}s_1^2 - V_{22}s_2^2} \right) = 4V_{12}^2 \left(s_1^2 s_2^2 + (s_1^2 + s_2^2) \frac{V_{11}s_1^2 - V_{22}s_2^2}{V_{11} - V_{22}} \right) \\
&= 4V_{12}^2 \frac{V_{11}s_1^4 - V_{22}s_2^4}{V_{22} - V_{11}} .
\end{aligned}
\tag{86}
$$

Equating (84) and (86), we have

$$V_{11}s_1^4 - V_{22}s_2^4 = \frac{V_{12}^2}{V_{22} - V_{11}}(s_1^2 - s_2^2)^2 \tag{87}$$

which can be interpreted as a quadratic equation for s_1^2/s_2^2 with solution

$$\frac{s_1^2}{s_2^2} = \frac{(V_{22} - V_{11})\sqrt{V_{11}V_{22} - V_{12}^2} - V_{12}^2}{V_{11}(V_{22} - V_{11}) - V_{12}^2} . \tag{88}$$

(There is a unique sign choice implied by $s_1^2/s_2^2 > 0$.)

This solution implies

$$\frac{s_1^2 + s_2^2}{s_1^2 - s_2^2} = \frac{(V_{22} - V_{11})\left(\sqrt{V_{11}V_{22} - V_{12}^2} + V_{11}\right) - 2V_{12}^2}{(V_{22} - V_{11})\left(\sqrt{V_{11}V_{22} - V_{12}^2} - V_{11}\right)} \tag{89}$$

$$V_{11}\frac{s_1^2}{s_2^2} - V_{22} = (V_{22} - V_{11})\sqrt{V_{11}V_{22} - V_{12}^2}\frac{V_{11} - \sqrt{V_{11}V_{22} - V_{12}^2}}{V_{11}(V_{22} - V_{11}) - V_{12}^2} \tag{90}$$

which can be used in (85) to obtain

$$s_2^4 = \frac{\hbar^2}{4}\frac{V_{11}V_{22} - V_{12}^2 - V_{11}^2}{V_{11}V_{22} - V_{12}^2}\frac{V_{11} + \sqrt{V_{11}V_{22} - V_{12}^2}}{(V_{22} - V_{11})\sqrt{V_{11}V_{22} - V_{12}^2} + V_{11}V_{22} - V_{11}^2 - 2V_{12}^2}. \tag{91}$$

We also have

$$s_1^4 = s_2^4(V_{11} \leftrightarrow V_{22}) \tag{92}$$

$$= \frac{\hbar^2}{4}\frac{V_{11}V_{22} - V_{12}^2 - V_{22}^2}{V_{11}V_{22} - V_{12}^2}\frac{V_{22} + \sqrt{V_{11}V_{22} - V_{12}^2}}{(V_{11} - V_{22})\sqrt{V_{11}V_{22} - V_{12}^2} + V_{11}V_{22} - V_{22}^2 - 2V_{12}^2}, \tag{93}$$

and the angle β can be obtained by (83).

If we insert these solutions in the effective potential, the results can be seen to equal the low-energy effective potential [29]

$$V_{\text{low}}(q_1, q_2) = V(q_1, q_2) + \frac{\hbar}{2}\sqrt{\frac{1}{2}\left(V_{11} + V_{22} + \sqrt{(V_{11} - V_{22})^2 + 4V_{12}^2}\right)}$$

$$+ \frac{\hbar}{2}\sqrt{\frac{1}{2}\left(V_{11} + V_{22} - \sqrt{(V_{11} - V_{22})^2 + 4V_{12}^2}\right)}. \tag{94}$$

although it initially appears in a rather different algebraic form. Our derivation automatically provides results for the ground-state variances and covariance at the minimum of the effective potential. For instance, while the actual expression for β is quite complicated and not given here, for small V_{12} we can use a Taylor expansion and obtain

$$\beta = \frac{\pi}{2} + \frac{V_{12}}{(V_{11}V_{22})^{1/4}\left(\sqrt{V_{11}} + \sqrt{V_{22}}\right)} + O(V_{12}^2). \tag{95}$$

In the limit of weak coupling, the moment $\Delta(q_1 q_2)$ therefore goes to zero.

As a simple example, consider the Hamiltonian

$$H = \frac{1}{2}\pi_1^2 + \frac{1}{2}\pi_2^2 + \frac{\omega^2}{2}q_1^2 + \frac{\omega^2}{2}q_2^2 + \gamma\omega^2 q_1 q_2. \tag{96}$$

Its quantization has the exact ground-state energy

$$E = \frac{1}{2}\hbar\omega\left(\sqrt{1 + \gamma} + \sqrt{1 - \gamma}\right) \tag{97}$$

agreeing with what we get from (94).

IV. DISCUSSION

Our extensions of canonical variables for moments from second order for a single degree of freedom demonstrate several new features of semiclassical states and their dynamics. In particular, we have identified various parameters related to the impurity of a state, a result which also plays a role in the determination of semiclassical potentials. Canonical moment variables are therefore useful tools to understand features of the quantum state space.

Our other applications illustrate the fact that canonical mappings of the form derived here can be relevant in a large set of different physical fields. For instance, they allow one to rewrite quantum statistics in classical terms and thereby provide convenient access to new types of variables (Section III A). Interestingly, there is a well-defined partition function for second-order moments even though these variables are subject to a non-invertible Poisson structure. For a derivation of the correct phase-space volume element it is therefore crucial to identify Casimir–Darboux variables. Casimir variables do not have momenta and therefore do not contribute the usual $2\pi\hbar$-volume to a partition function. Nevertheless, in our example we saw that we have to integrate over them in order to obtain the correct thermodynamical re-

sults for fluctuations. In tunneling situations, canonical moment variables demonstrate a new heuristic picture in which an external field literally opens up a tunnel through a higher-dimensional extension of the classical potential (Fig. 1). During tunneling, higher than second-order moments are crucial, which we have captured by the new all-orders effective potential (52) defined here for any classical potential.

The present paper has given mainly illustrative applications in simplified models. Our presentation here sets the basis for a detailed analysis [4] to tunneling ionization in atoms with a successful comparison with recent discussions [8–17] of experimental results [5–7]. In particular, the closure conditions discussed here provide the foundation for our analysis of tunneling in 3-dimensional atomic systems subject to a time-dependent external force.

Appendix A: Single pair of degrees of freedom at higher orders

In this appendix, we present derivations of canonical moment variables for a single degree of freedom at third and fourth order. Different approaches are compared, which allows us to highlight interesting features of moment systems.

1. Single pair of degrees of freedom at third order

Here we present an extension of the Casimir–Darboux coordinates from Sec. II C to third order. There are now seven moments, and the rank of the Poisson tensor shows that there is a single Casimir variable. We must therefore derive two additional pairs of canonical degrees of

freedom. Since Darboux coordinates are defined only up to canonical transformations, the form in which they appear in the moments is not unique and subject to choices. For now, we make a choice motivated by the canonical form we just derived at second order: We assume that $\Delta(q^2)$ depends only on one of the new canonical pairs,

$$\Delta(q^2) = s_1^2 \tag{A1}$$

from which it quickly follows, by a calculation similar to our second-order example, that

$$\Delta(q\pi) = s_1\, p_1 \tag{A2}$$

is a consistent (but not unique) choice of introducing the first momentum.

The remaining canonical pairs must be such that they have zero Poisson brackets with s_1 and p_1, or with $\Delta(q^2)$ and $\Delta(q\pi)$ according to our first choices. The same procedure that we used to derive U_1 as a coordinate Poisson orthogonal to both s and p_s at second order can also be used here, but now we have five additional moments which should be expressed in terms of functions Poisson orthogonal to s and p_s. By systematically computing the flows of all the remaining moments generated by s_1 and p_1 and eliminating flow parameters, it follows that the following functions of moments are Poisson orthogonal to s_1 and p_1:

$$f_1 = \Delta(q^2)\Delta(\pi^2) - \Delta(q\pi)^2 \tag{A3}$$

$$f_2 = \Delta(q^2)\frac{\Delta(q^2\pi)}{\Delta(q^3)} - \Delta(q\pi) \tag{A4}$$

$$f_3 = \frac{\Delta(q^2)^2}{\Delta(q^3)^2}\left(\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)\right) \tag{A5}$$

$$f_4 = 2\Delta(q\pi) + \Delta(q^2)\frac{\Delta(q^3)\Delta(\pi^3) - \Delta(q\pi^2)\Delta(q^2\pi)}{\Delta(q^2\pi)^2 - \Delta(q\pi^2)\Delta(q^3)} \tag{A6}$$

One additional variable can be derived independently from the Casimir function of the Lie algebra that corresponds to third-order moments,

$$f_5 := U_1^4 = \left(\Delta(q^2\pi)\Delta(q\pi^2) - \Delta(q^3)\Delta(\pi^3)\right)^2 - 4\left(\Delta(q\pi^2)^2 - \Delta(q^2\pi)\Delta(\pi^3)\right)\left(\Delta(q^2\pi)^2 - \Delta(q^3)\Delta(q\pi^2)\right). \tag{A7}$$

(The fourth power of U_1 is chosen such that U_1 is of third order just like the moment order considered here.) While f_5 Poisson commutes with all other f_i, (f_1, f_2, f_3, f_4) have non-linear brackets

$$\{f_1, f_2\} = 2f_1 + 2f_2^2 + 4f_3 \tag{A8}$$

$$\{f_1, f_3\} = 12f_2 f_3 + 2f_3 f_4 \tag{A9}$$

$$\{f_1, f_4\} = -4f_1 - f_4^2 + 4f_3 - (2f_2 + f_4)^2 \tag{A10}$$

$$\{f_2, f_3\} = -4f_3 \tag{A11}$$

$$\{f_2, f_4\} = -4f_2 - 2f_4 \tag{A12}$$

$$\{f_3, f_4\} = -8f_3 \tag{A13}$$

with one another.

We are now ready to choose our second configuration variable. We define

$$s_2 = f_3\,, \tag{A14}$$

such that

$$\frac{\partial f_1}{\partial p_2} = -12 s_2 f_2 - 2 s_2 f_4 \quad , \quad \frac{\partial f_2}{\partial p_2} = 4 s_2 \quad , \quad \frac{\partial f_4}{\partial p_2} = -8 s_2 \tag{A15}$$

can be used to determine the second momentum variable. Integrating the last two equations and inserting the results in the first one gives

$$f_1 = -16 s_2^2 p_2^2 - s_2 \left(12 g_2 + 2 g_4\right) p_2 + g_1 \tag{A16}$$
$$f_2 = 4 s_2 p_2 + g_2 \tag{A17}$$
$$f_4 = -8 s_2 p_2 + g_4 \tag{A18}$$

with three functions g_1, g_2 and g_4 independent of p_2. (They can therefore depend on s_2 and the remaining canonical pair, s_3 and p_3, as well as the Casimir variable U_1.) Since we are interested in deriving p_2, we can choose the free functions such that it is easy to invert (A16), (A17) or (A18) for p_2. A wrong choice at this point could result in a degenerate system that does not allow us to derive all canonical pairs. Since we know how many canonical pairs we obtain, a little bit of trial and error quickly shows when a choice is suitable. If we choose $g_4 = -6 g_2$, we obtain

$$p_2 = \frac{6 f_2 + f_4}{16 s_2} \tag{A19}$$

from a combination of (A17) and (A18), as well as

$$g_1 = f_1 + \frac{(6 f_2 + f_4)^2}{16} \quad , \quad g_2 = -\frac{1}{2} f_2 - \frac{1}{4} f_4 . \tag{A20}$$

By construction, g_1 and g_2 do not depend on p_2, but we have not made sure yet that they do not depend on s_2 either. Since s_2 is defined as s_3, the Poisson brackets (A8)–(A13) can be used to show that g_1 and g_2 do, in fact, depend on s_2. The same Poisson brackets determine the canonical flow generated by p_2 in (A19) on g_1 and g_2. By eliminating the flow parameter as in some of the previous steps, we find that the combinations

$$p_3 = \frac{g_2}{\sqrt{s_2}} \tag{A21}$$

$$s_3 = \frac{2 g_1 - 7 s_2 + 10 p_3^2 s_2}{6 \sqrt{s_2}(4 p_3^2 - 1)} \tag{A22}$$

are independent of s_2 and are therefore Poisson orthogonal to all previously constructed canonical pairs. They determine our final pair (s_3, p_3).

In order to express moments in terms of canonical pairs and the Casimir variable, we insert the functions

$$f_1 = 3\sqrt{s_2}\left(-1 + 4 p_3^2\right) s_3 + \frac{1}{2}\left(7 s_2 - 10 s_2 p_3^2\right) - 16 s_2^2 p_2^2$$
$$f_2 = \sqrt{s_2} p_3 + 4 s_2 p_2$$
$$f_3 = s_2$$
$$f_4 = -4\sqrt{s_2} p_3 - 8 s_2 p_2$$
$$f_5 = U_1^4$$

in (A3) and (A7) and invert the resulting relations for

$$\Delta(q^2) = s_1^2 \quad , \quad \Delta(q\pi) = s_1 p_1 \tag{A23}$$

$$\Delta(\pi^2) = p_1^2 + \frac{f_1}{s_1^2} = p_1^2 + \frac{3\sqrt{s_2}\left(4 p_3^2 - 1\right) s_3 + \frac{1}{2} s_2 \left(7 - 10 p_3^2\right) - 16 s_2^2 p_2^2}{s_1^2} \tag{A24}$$

$$\Delta(\pi^3) = \frac{U_1}{s_1^3 \sqrt{2 s_2^{3/2} \sqrt{1 - 4 p_3^2}}} \Phi(s_i, p_i) \tag{A25}$$

$$\Delta(q\pi^2) = \frac{U_1}{s_1 \sqrt{2 s_2^{3/2} \sqrt{1 - 4 p_3^2}}} \left(p_1 s_1 + (p_3 - 1)\sqrt{s_2} + 4 s_2 p_2\right) \tag{A26}$$

$$\times \left(p_1 s_1 + (1 + p_3)\sqrt{s_2} + 4 s_2 p_2\right) \tag{A27}$$

$$\Delta(q^2\pi) = \frac{U_1}{\sqrt{2 s_2^{3/2} \sqrt{1 - 4 p_3^2}}} \left(p_1 s_1^2 + s_1 \left(p_3 \sqrt{s_2} + 4 s_2 p_2\right)\right) \tag{A28}$$

$$\Delta(q^3) = \frac{U_1 s_1^3}{\sqrt{2 s_2^{3/2} \sqrt{1 - 4 p_3^2}}} , \tag{A29}$$

where

$$\Phi(s_i, p_i) = p_1^3 s_1^3 + 3 p_1^2 p_3 s_1^2 \sqrt{s_2} + 3 p_1 s_1 s_2 \left(-1 + p_3^2 + 4 p_1 s_1 p_2\right) + 64 p_3^3 s_2^3 \tag{A30}$$
$$+ p_3 s_2^{3/2} \left(-7 + p_3^2 + 24 p_1 p_2 s_1\right) + 48 p_3 p_2^2 s_2^{5/2} + 12 p_2 s_2^2 \left(-1 + p_3^2 + 4 p_1 s_1 p_2\right) .$$

More compactly, some of the momentum-dependent moments can be written as

$$\Delta(\pi^3) = \frac{U_1\left(P^3 - 3P - 4p_3 s_2^{3/2}\right)}{s_1^3 \sqrt{2s_2^{3/2}\sqrt{1 - 4p_3^2}}} \qquad (A31)$$

$$\Delta(q\pi^2) = \frac{U_1\left(P^2 - s_2\right)}{s_1\sqrt{2s_2^{3/2}\sqrt{1 - 4p_3^2}}} \qquad (A32)$$

$$\Delta(q^2\pi) = \frac{U_1 s_1 P}{\sqrt{2s_2^{3/2}\sqrt{1 - 4p_3^2}}} \qquad (A33)$$

if we introduce $P = p_1 s_1 + p_3\sqrt{s_2} + 4s_2 p_2$. Note that s_3 does not appear in any $\Delta(q^a\pi^b)$ with $b \leq 1$, and may therefore be a candidate for the impurity of a state.

2. Third order by ansatz

As we have seen, several choices have to be made in the process of deriving Casimir–Darboux coordinates. Some choices may lead to degenerate systems in which a smaller number of canonical pairs results, and which should therefore be discarded. However, even within the class of non-degenerate systems, there cannot be a unique set of Casimir–Darboux coordinates because one can always apply canonical transformations of Darboux variables. Depending on the application, some choices may lead to more useful realizations of canonical variables than others. Staying with the third-order system for a single pair of canonical degrees of freedom, we now apply an alternative method which works by ansatz and therefore is somewhat less systematic than the previous procedure. However, it makes it easier to implement certain properties such as a simplified version of $\Delta(\pi^2)$ in (A24) with s_i-independent coefficients. As we will see, such a version greatly simplifies the effective dynamics, but it does not always exist, in particular if we have more than one pair of classical degrees of freedom.

We make the ansatz

$$\Delta(\pi^2) = \sum_{i=1}^{3} p_i^2 + F(s_1, s_2, s_3) \quad , \quad \Delta(q\pi) = \sum_{i=1}^{3} s_i p_i \qquad (A34)$$

$$\Delta(q^2) = \sum_{i=1}^{3} s_i^2 \quad , \quad \Delta(q^3) = \sum_{i=1}^{3} s_i^3 \qquad (A35)$$

introducing three canonical pairs, as required. The function $F(s_1, s_2, s_3)$, which is assumed to be independent of the momenta, is subject to consistency conditions that follow from the required Poisson brackets of moments. Once we have a consistent F, we can generate all the remaining moments by taking successive Poisson brackets with $\Delta(\pi^2)$:

$$\Delta(q^{m-1}\pi^{n+1}) = -\frac{1}{2m}\left\{\Delta(\pi^2), \Delta(q^m\pi^n)\right\} , \qquad (A36)$$

starting with $m = 3$, $n = 0$ in which case we have defined $\Delta(q^3)$ in (A35) and can derive

$$\Delta(q^2\pi) = \sum_i p_i s_i^2$$

$$\Delta(q\pi^2) = \sum_i p_i^2 s_i - \frac{1}{4}\sum_i s_i^2 \frac{\partial F}{\partial s_i} \qquad (A37)$$

$$\Delta(\pi^3) = \sum_i p_i^3 - \frac{1}{4}\sum_i p_i\left(4s_i\frac{\partial F}{\partial s_i} + \sum_j s_j^2 \frac{\partial^2 F}{\partial s_i \partial s_j}\right) .$$

Since we have explicitly used all three canonical pairs expected for a third-order truncation, F depends on one further parameter, U, which will be the Casimir coordinate. Since F and therefore U appear only in moments which have at least two momentum factors, U is a candidate for an impurity parameter in this mapping.

Equation (A36) also applies to second-order moments, $m + n = 2$. Since we have defined all three second-order moments in (A34), we obtain consistency conditions on F. We first compute

$$\left\{\Delta(\pi^2), \Delta(q^2)\right\} = -4\sum_i s_i p_i \qquad (A38)$$

and from this

$$\left\{\Delta\pi^2, \left\{\Delta(\pi^2), \Delta(q^2)\right\}\right\} = 8\sum_i p_i^2 - 4\sum_i s_i \frac{\partial F}{\partial s_i}. \qquad (A39)$$

The condition

$$\left\{\Delta\pi^2, \left\{\Delta(\pi^2), \Delta(q^2)\right\}\right\} = 8\Delta(\pi^2) \qquad (A40)$$

then implies

$$\sum_i s_i \frac{\partial F}{\partial s_i} = -2F \qquad (A41)$$

and therefore F is homogeneous of degree -2 if all s_i are rescaled by the same constant.

Applying further Poisson brackets with $\Delta(\pi^2)$ does not give new conditions. For instance,

$$0 = \left\{\Delta(\pi^2), \left\{\Delta(\pi^2), \left\{\Delta(\pi^2), \Delta(q^2)\right\}\right\}\right\} \qquad (A42)$$

is equivalent to

$$0 = 8\left(3\sum_i p_i\frac{\partial F}{\partial s_i} + \sum_{i,j} p_i s_j \frac{\partial^2 F}{\partial s_i \partial s_j}\right) . \qquad (A43)$$

Since the s_i and p_i can be varied independently, the condition implies that all three $\partial F/\partial s_i$ are homogeneous of degree -3 if all s_i are rescaled by the same constant, which follows from F being of degree -2.

Another consistency condition can be derived by looking at the third order moments:

$$0 = \left\{\Delta(\pi^2), \left\{\Delta(\pi^2), \left\{\Delta(\pi^2), \left\{\Delta(\pi^2), \Delta(q^3)\right\}\right\}\right\}\right\} \qquad (A44)$$

is equivalent to

$$
\begin{aligned}
0 = \; & 6 \sum_i p_i^2 \frac{\partial F}{\partial s_i} + 4 \sum_{ij} p_i s_i p_j \frac{\partial^2 F}{\partial s_i \partial s_j} \\
& + \frac{1}{2} \sum_{ijk} s_i^2 p_j p_k \frac{\partial^3 F}{\partial s_i \partial s_j \partial s_k} \\
& - \frac{3}{2} \sum_i s_i \left(\frac{\partial F}{\partial s_i} \right)^2 - \frac{1}{4} \sum_{ij} s_i^2 \frac{\partial F}{\partial s_j} \frac{\partial^2 F}{\partial s_i \partial s_j}
\end{aligned} \quad \text{(A45)}
$$

This condition is generally independent from (A41). For example, the solution $F = \sum_i U/s_i^2$ of (A41) is not a solution of (A45).

One further condition has to be imposed, which is the invertibility of the mapping from moments to (s_i, p_{s_j}). (Otherwise one could choose the trivial solution $F = 0$.) For any given F, this condition can be checked by computing the Jacobian of the transformation, and it is fulfilled, for instance, by the solutions

$$
F(s_1, s_2, s_3) = \sum_{i<j} \frac{U}{(s_i - s_j)^2} \quad \text{(A46)}
$$

of (A41) and (A45), where U is the Casimir variable. Therefore, there is a faithful mapping from moments to canonical coordinates at the third order, such that moments are quadratic in the new momenta with s-independent coefficients. The ansatz used here provides a simplified procedure to compute Casimir–Darboux coordinates, but only if moments quadratic in momenta exist. The choice (A46) is not unique, but it is interesting because for $U > 0$ it implies repulsive potentials between the s_i in an effective potential.

At this point, we have obtained two different canonical systems for the third-order semiclassical truncation of a single classical degree of freedom, with Casimir variables U_1 and U, respectively. However, a direct comparison of these two versions of the Casimir variable is difficult because the two Poisson algebras we have canonically realized, in fact, differ from each other in a subtle way: For the mapping derived with the ansatz we have Poisson brackets of third order moments of the form $\left\{ \Delta_i^3, \Delta_j^3 \right\} = \mathcal{O}(\hbar^2)$. The right-hand side is considered zero in a third-order semiclassical truncation, which corresponds to an $\hbar$-order of $3/2$. For the mapping derived systematically, however, we were able to exactly impose $\left\{ \Delta_i^3, \Delta_j^3 \right\} = 0$. Therefore, the two Casimir variables are likely to differ from each other by terms of the order $\hbar^2$.

Nevertheless, it is instructive to compute the Poisson bracket of the moments derived with the ansatz with the Casimir U_1 that was derived systematically. Assuming that s and p are of the order $\mathcal{O}(\sqrt{\hbar})$ in a semiclassical state, computer algebra shows that the Taylor expansion of the Poisson brackets $\{\Delta_{\text{ansatz}}, U_1(\Delta_{\text{ansatz}})\} = \mathcal{O}(\hbar^{5/2})$ in $\sqrt{\hbar}$ is zero within the third-order truncation. Therefore, the Casimir variable derived systematically is a Casimir variable also for the realization derived using an ansatz, up to a truncation error.

3. Fourth order

The solution at the third order can be extended in a rather direct manner to the fourth order. Inspection of the rank of the Poisson tensor at this order shows that we expect five canonical pairs of quantum degrees of freedom and two Casimir variables. We then try the ansatz

$$
\Delta(\pi^2) = \sum_{i=1}^{5} p_i^2 + \sum_{i>j} \frac{U}{(s_i - s_j)^2} \quad \text{(A47)}
$$

$$
\Delta(q^2) = \sum_i s_i^2 \quad \text{(A48)}
$$

$$
\Delta(q^3) = C \sum_i s_i^3 . \quad \text{(A49)}
$$

In addition to an extension of the third-order ansatz to five pairs of canonical degrees of freedom, we have inserted a new parameter C which will play the role of the second Casimir variable.

The moment $\Delta(q^4)$ can be generated from the Poisson bracket $\left\{ \Delta(\pi q^2), \Delta(q^3) \right\} = 3\Delta(q^2)^2 - 3\Delta(q^4)$:

$$
\Delta(q^4) = C^2 \sum_i s_i^4 + \sum_{i,j} s_i^2 s_j^2 \quad \text{(A50)}
$$

We also need to check that the Poisson bracket is consistent at this order. For instance, while an expansion of the right-hand side of

$$
0 = \left\{ \Delta(\pi^2), \left\{ \Delta(\pi^2), \left\{ \Delta(\pi^2), \left\{ \Delta(\pi^2), \left\{ \Delta(\pi^2), \Delta(q^4) \right\} \right\} \right\} \right\} \right\} , \quad \text{(A51)}
$$

would be too complex to be shown here, computer algebra confirms that (A51) is indeed satisfied for our ansatz. This result supports the physical principle that (when $U > 0$) the quantum coordinates feel a repulsive potential between one another that goes as one over the square of the distance between them.

Appendix B: Second-order truncation for two pairs of classical degrees of freedom

For two pairs of classical degrees of freedom, we have a ten-dimensional submanifold of second-order moments. The Poisson tensor has rank eight, so that we have to construct four canonical pairs and two Casimir variables.

1. First step

The system contains two subalgebras that correspond to a single degree of freedom, given by $\langle \Delta(q_1^2), \Delta(q_1 \pi_1), \Delta(\pi_1^2) \rangle$ and $\langle \Delta(q_2^2), \Delta(q_2 \pi_2), \Delta(\pi_2^2) \rangle$. We can therefore make use of some of our previous derivations if we choose the first two configuration variables as $s_1 = \sqrt{\Delta(q_1^2)}$ and $s_2 = \sqrt{\Delta(q_2^2)}$. We obtain solutions

similar to (26) and (27) with (29), but now the free functions $f_{q_1\pi_1}$, $f_{\pi_1^2}$, $f_{q_2\pi_2}$ and $f_{\pi_2^2}$ in

$$\Delta(q_1\pi_1) = s_1 p_1 + f_{q_1\pi_1} \tag{B1}$$

$$\Delta(\pi_1^2) = p_1^2 + 2\frac{p_1}{s_1}f_{q_1\pi_1} + f_{q_1\pi_1}^2 + \frac{f_{\pi_1^2}}{s_1^2} \tag{B2}$$

and

$$\Delta(q_2\pi_2) = s_2 p_2 + f_{q_2\pi_2} \tag{B3}$$

$$\Delta(\pi_2^2) = p_2^2 + 2\frac{p_2}{s_2}f_{q_2\pi_2} + f_{q_2\pi_2}^2 + \frac{f_{\pi_2^2}}{s_2^2} \tag{B4}$$

may still depend on the remaining two canonical pairs, as well as the two Casimirs.

Since $f_{q_1\pi_1}$, $f_{\pi_1^2}$, $f_{q_2\pi_2}$ and $f_{\pi_2^2}$ do not depend on s_1, p_1, s_2 and p_2 by construction, they parameterize coordinate Poisson orthogonal to the first two canonical pairs. However, it is convenient to choose $f_{q_1\pi_1} = 0 = f_{q_2\pi_2}$ because the condition of being Poisson orthogonal to s_1, p_1, s_2 and p_2 is then equivalent to having vanishing Poisson brackets with the basic moments $\Delta(q_1^2) = s_1^2$, $\Delta(q_1\pi_1) = s_1 p_1$, $\Delta(q_2^2) = s_2^2$ and $\Delta(q_2\pi_2) = s_2 p_2$. This leaves two functions,

$$f_{\pi_1^2} = s_1^2\Delta(\pi_1^2) - s_1^2 p_1^2 = \Delta(q_1^2)\Delta(\pi_1^2) - \Delta(q_1\pi_1)^2 =: f_1 \tag{B5}$$

and

$$f_{\pi_2^2} = s_2^2\Delta(\pi_2^2) - s_2^2 p_2^2 = \Delta(q_2^2)\Delta(\pi_2^2) - \Delta(q_2\pi_2)^2 =: f_2, \tag{B6}$$

out of the original free functions in (B1) and (B3), which we can easily write in terms of moments.

In addition to f_1 and f_2, we need four further functions that Poisson commute with the first two canonical pairs, or with $\Delta(q_1^2)$, $\Delta(q_1\pi_1)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. As before, we find such variables by considering the flows generated by $\Delta(q_1^2)$, $\Delta(q_1\pi_1)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. For instance, for

$\Delta(q_1\pi_1)$, the flows $d/d\epsilon = \{\cdot, \Delta(q_1\pi_1)\}$ on the remaining moments are

$$\frac{d\Delta(q_1 q_2)}{d\epsilon} = \Delta(q_1 q_2) \quad , \quad \frac{d\Delta(q_1\pi_2)}{d\epsilon} = \Delta(q_1\pi_2)$$
$$\frac{d\Delta(q_2\pi_1)}{d\epsilon} = -\Delta(q_2\pi_1) \quad , \quad \frac{d\Delta(\pi_1\pi_2)}{d\epsilon} = -\Delta(\pi_1\pi_2)$$
$$\frac{d\Delta(q_1^2)}{d\epsilon} = 2\Delta(q_1^2) \quad . \tag{B7}$$

These linear differential equations can easily be solved by

$$\Delta(q_1 q_2) = c_1 e^{\epsilon} \quad , \quad \Delta(q_1\pi_2) = c_2 e^{\epsilon}$$
$$\Delta(q_2\pi_1) = c_3 e^{-\epsilon} \quad , \quad \Delta(\pi_1\pi_2) = c_4 e^{-\epsilon}$$
$$\Delta(q_1^2) = c_5 e^{2\epsilon} \quad . \tag{B8}$$

By eliminating ϵ, we find that $\Delta(q_1 q_2)\Delta(q_2\pi_1)$, $\Delta(q_1 q_2)\Delta(\pi_1\pi_2)$, $\Delta(q_1\pi_2)\Delta(q_2\pi_1)$, $\Delta(q_1\pi_2)\Delta(\pi_1\pi_2)$ and $\Delta(q_1^2)\Delta(\pi_1\pi_2)\Delta(q_2\pi_1)$ Poisson commute with $\Delta(q_1\pi_1)$. However, these combinations are not necessarily invariant under the flows generated by $\Delta(q_1^2)$, $\Delta(q_2^2)$ and $\Delta(q_2\pi_2)$. After computing variables invariant with respect to any one of these four flows, we find that the combinations

$$f_3 = \Delta(q_1\pi_2)\Delta(q_2\pi_1) - \Delta(q_1 q_2)\Delta(\pi_1\pi_2) \tag{B9}$$

$$f_4 = \Delta(q_1^2)\frac{\Delta(q_2\pi_1)}{\Delta(q_1 q_2)} - \Delta(q_1\pi_1) \tag{B10}$$

$$f_5 = \Delta(q_2^2)\frac{\Delta(q_1\pi_2)}{\Delta(q_1 q_2)} - \Delta(q_2\pi_2) \tag{B11}$$

$$f_6 = \frac{\Delta(q_1^2)\Delta(q_2^2)}{\Delta(q_1 q_2)^2}, \tag{B12}$$

in addition to f_1 and f_2, are Poisson orthogonal to s_1, p_1, s_2 and p_2. Moreover, their mutual Poisson brackets are closed,

$$\{f_1, f_2\} = 0 = \{f_1, f_3\} = \{f_2, f_3\} \tag{B13}$$

$$\{f_1, f_4\} = 2(f_1 + f_4^2) \quad , \quad \{f_1, f_5\} = 2f_3 f_6 \quad , \quad \{f_1, f_6\} = 4f_4 f_6 \tag{B14}$$

$$\{f_2, f_4\} = 2f_3 f_6 \quad , \quad \{f_2, f_5\} = 2(f_2 + f_5^2) \quad , \quad \{f_2, f_6\} = 4f_5 f_6 \tag{B15}$$

$$\{f_3, f_4\} = f_1 + f_3 f_6 + f_4^2 \quad , \quad \{f_3, f_5\} = f_2 + f_3 f_6 + f_5^2 \quad , \quad \{f_3, f_6\} = 2(f_4 + f_5)f_6 \tag{B16}$$

$$\{f_4, f_5\} = (f_5 - f_4)f_6 \quad , \quad \{f_4, f_6\} = -2f_6(1 - f_6) = \{f_5, f_6\} \tag{B17}$$

and therefore form a Poisson manifold on which we can iterate our procedure, expressing the f_1 in terms of further Casimir–Darboux variables.

2. Second step

We now define $s_3 = f_6$, equal to the inverse of the correlation between the two positions. It generates a flow to be identified with the negative partial derivative with

respect tp p_3,

$$\frac{\partial f_1}{\partial p_3} = -\{f_1, f_6\} = -4s_3f_4 \tag{B18}$$

$$\frac{\partial f_2}{\partial p_3} = -4s_3f_5 \quad , \quad \frac{\partial f_3}{\partial p_3} = -2s_3(f_4 + f_5) \tag{B19}$$

$$\frac{\partial f_4}{\partial p_3} = 2s_3(1 - s_3) \quad , \quad \frac{\partial f_5}{\partial p_3} = 2s_3(1 - s_3). \tag{B20}$$

The last two equations are solved by

$$f_4 = 2s_3p_3(1 - s_3) + g_4 \quad \text{and} \quad f_5 = 2s_3p_3(1 - s_3) + g_5, \tag{B21}$$

after which the remaining equations can be solved by

$$f_1 = -4s_3^2(1 - s_3)p_3^2 - 4s_3p_3g_4 + g_1 \tag{B22}$$
$$f_2 = -4s_3^2(1 - s_3)p_3^2 - 4s_3p_3g_5 + g_2 \tag{B23}$$
$$f_3 = -4s_3^2(1 - s_3)p_3^2 - 2s_3p_3(g_4 + g_5) + g_3. \tag{B24}$$

The functions g_i are independent of p_3.

As before, a choice is required to proceed because we have five free functions g_i but only one more canonical pair and two Casimir variables. The choice $g_5 = -g_4$ simplifies f_3 and eliminates these functions from $f_4 + f_5$ according to (B21) and we obtain our third momentum

$$p_3 = \frac{f_4 + f_5}{4s_3(1 - s_3)}. \tag{B25}$$

We are left with four functions $g_1, \ldots, g_4$ which, by construction, are independent of p_3. But they may depend on s_3 and are therefore not Poisson orthogonal to the third canonical pair. In order to find combinations which Poisson commute with p_3, we consider the flow generated by $f_4 + f_5 = 4s_3(1 - s_3)p_3$. From

$$g_1 = f_1 + \frac{(f_4 + f_5)^2}{4(1 - f_6)} + \frac{1}{2}\frac{(f_4 + f_5)(f_4 - f_5)}{1 - f_6} \tag{B26}$$

$$g_2 = f_2 + \frac{(f_4 + f_5)^2}{4(1 - f_6)} - \frac{1}{2}\frac{(f_4 + f_5)(f_4 - f_5)}{1 - f_6} \tag{B27}$$

$$g_3 = f_3 + \frac{(f_4 + f_5)^2}{4(1 - f_6)} \tag{B28}$$

$$g_4 = \frac{1}{2}(f_4 - f_5), \tag{B29}$$

We obtain the brackets

$$\{g_1, f_4 + f_5\} = 2(g_1 + s_3g_3 + g_4^2) \tag{B30}$$
$$\{g_2, f_4 + f_5\} = 2(g_2 + s_3g_3 + g_4^2) \tag{B31}$$
$$\{g_3, f_4 + f_5\} = g_1 + g_2 + 2s_3g_3 + 2g_4^2 \tag{B32}$$
$$\{g_4, f_4 + f_5\} = -2s_3g_4. \tag{B33}$$

We see that $\{g_1 + g_2 - 2g_3, f_4 + f_5\} = 0$, and if we trace back all the dependencies on moments, we find that

$$g_1 + g_2 - 2g_3 = U_1 \tag{B34}$$

is, in fact, the quadratic Casimir. The remaining independent variables can conveniently be chosen as $g_1 + g_2$, $g_1 - g_2$ and g_4, with mutual Poisson brackets

$$\{g_1 + g_2, g_4\} = g_1 - g_2 \tag{B35}$$

$$\{g_1 - g_2, g_4\} = g_1 + g_2 - 2s_3g_3 + 2\frac{1 + s_3}{1 - s_3}g_4^2$$

$$\{g_1 + g_2, g_1 - g_2\} = 4\frac{g_4}{1 - s_3}(g_1 + g_2 + 2s_3g_3 + 2g_4^2).$$

3. Final step

We now consider the flow $\partial/\partial s_3 = \{\cdot, p_3\}$, using (B25):

$$\frac{\partial g_4}{\partial s_3} = \frac{g_4}{2(s_3 - 1)} \quad , \quad \frac{\partial(g_1 - g_2)}{\partial s_3} = \frac{g_1 - g_2}{2s_3(1 - s_3)} \quad ,$$

$$\frac{\partial(g_1 + g_2)}{\partial s_3} = \frac{g_1 + g_2 + 2s_3g_3 + 2g_4^2}{2s_3(1 - s_3)} = \frac{(g_1 + g_2)(1 + s_3) - s_3U_1 + 2g_4^2}{2s_3(1 - s_3)}. \tag{B36}$$

Solving these equations, we find that

$$h_1 = \frac{g_4}{\sqrt{s_3 - 1}} \tag{B37}$$

$$h_2 = (g_1 - g_2)\sqrt{\frac{s_3 - 1}{s_3}} \tag{B38}$$

$$h_3 = \frac{(1 - s_3)(g_1 + g_2) + s_3U_1 + 2(1 + s_3)(1 - s_3)^{-1}g_4^2}{\sqrt{s_3}}, \tag{B39}$$

in addition to U_1, are Poisson orthogonal to s_3 as well as p_3. They have closed brackets

$$\{h_1, h_2\} = h_3 \quad , \quad \{h_1, h_3\} = -h_2 \quad , \quad \{h_2, h_3\} = 8h_1U_1 - 32h_1^3. \tag{B40}$$

As our final canonical momentum, we choose $p_4 = h_1$. Its flow equations

$$\frac{\partial h_2}{\partial s_4} = -h_3 \quad , \quad \frac{\partial h_3}{\partial s_4} = h_2 \tag{B41}$$

have trigonometric solutions with a phase that can be set to zero by shifting s_4. Therefore,

$$h_2 = A(p_4)\cos(s_4) \quad , \quad h_3 = A(p_4)\sin(s_4) . \tag{B42}$$

The required Poisson brackets provide a condition on the function $A(p_4)$,

$$A(p_4)\frac{dA(p_4)}{dp_4} = -8p_4 U_1 + 32p_4^3 , \tag{B43}$$

solved by

$$A(p_4) = \sqrt{U_2 - 8p_4^2 U_1 + 16p_4^4} . \tag{B44}$$

The new free parameter U_2 is a constant and is our second Casimir variable.

4. Casimir–Darboux variables

Inverting all intermediate relations, we obtain the moments in terms of Casimir–Darboux variables,

$$\Delta(q_1^2) = s_1^2 \quad , \quad \Delta(q_1\pi_1) = s_1 p_1 \tag{B45}$$

$$\Delta(\pi_1^2) = p_1^2 + \frac{\Phi(s_3, p_3, s_4, p_4)}{s_1^2} \tag{B46}$$

with

$$\Phi(s_3, p_3, s_4, p_4) = -\frac{s_3 + 1}{s_3 - 1}p_4^2 - 4s_3\sqrt{s_3 - 1}p_3 p_4 + 4s_3^2(s_3 - 1)p_3^2 + \frac{1}{2}\frac{s_3}{s_3 - 1}U_1 \tag{B47}$$
$$-\frac{1}{2}\frac{\sqrt{s_3}}{s_3 - 1}\sqrt{U_2 - 8p_4^2 U_1 + 16p_4^4}\left(\sqrt{s_3 - 1}\cos(s_4) + \sin(s_4)\right) ,$$

for moments of the second classical pair of degrees of freedom,

$$\Delta(q_2^2) = s_2^2 \quad , \quad \Delta(q_2\pi_2) = s_2 p_2 \tag{B48}$$

$$\Delta(\pi_2^2) = p_2^2 + \frac{\Gamma(s_3, p_3, s_4, p_4)}{s_2^2} \tag{B49}$$

with

$$\Gamma(s_3, p_3, s_4, p_4) = -\frac{s_3 + 1}{s_3 - 1}p_4^2 + 4s_3\sqrt{s_3 - 1}p_3 p_4 + 4s_3^2(s_3 - 1)p_3^2 \tag{B50}$$
$$+\frac{1}{2}\frac{s_3}{s_3 - 1}U_1$$
$$-\frac{1}{2}\frac{\sqrt{s_3}}{s_3 - 1}\sqrt{U_2 - 8p_4^2 U_1 + 16p_4^4}\left(-\sqrt{s_3 - 1}\cos(s_4) + \sin(s_4)\right) ,$$

and

$$\Delta(\pi_1\pi_2) = \frac{p_1 p_2}{\sqrt{s_3}} + \sqrt{\frac{s_3 - 1}{s_3}}\left(\frac{p_2}{s_1} - \frac{p_1}{s_2}\right)p_4 \tag{B51}$$
$$-2\sqrt{s_3}(s_3 - 1)\left(\frac{p_1}{s_2} + \frac{p_2}{s_1}\right)p_3 + \frac{(3s_3 - 1)}{s_1 s_2\sqrt{s_3}(s_3 - 1)}p_4^2$$
$$-4\frac{(s_3 - 1)s_3^{3/2}}{s_1 s_2}p_3^2 - \frac{\sqrt{s_3}}{2s_1 s_2(s_3 - 1)}U_1$$
$$+\frac{s_3}{2s_1 s_2(s_3 - 1)}\sin(s_4)\sqrt{U_2 - 8p_4^2 U_1 + 16p_4^4}$$

$$\Delta(\pi_1 q_2) = \frac{p_1 s_2}{\sqrt{s_3}} + \sqrt{\frac{s_3 - 1}{s_3}}\frac{s_2}{s_1}p_4 - 2(s_3 - 1)\sqrt{s_3}\frac{s_2}{s_1}p_3 \tag{B52}$$

$$\Delta(\pi_2 q_1) = \frac{p_2 s_1}{\sqrt{s_3}} - \sqrt{\frac{s_3 - 1}{s_3}}\frac{s_1}{s_2}p_4 - 2(s_3 - 1)\sqrt{s_3}\frac{s_1}{s_2}p_3 \tag{B53}$$

$$\Delta(q_1 q_2) = \frac{s_1 s_2}{\sqrt{s_3}} \tag{B54}$$

for the cross-covariances.

5. Canonical transformation

We can change our Darboux coordinates by canonical transformations. An intersting example is suggested by the trigonometric form in which s_4 appears in the equations derived so far, which can be extended to s_3 by using the canonical pair

$$\beta = \arctan\sqrt{s_3 - 1} \quad , \quad p_\beta = 2s_3\sqrt{s_3 - 1}\,p_3 . \tag{B55}$$

Computing $s_3 = 1 + \tan^2\beta = 1/\cos^2\beta$, we see that the new variable β interprets the cross-correlation

$$\frac{\Delta(q_1 q_2)}{\sqrt{\Delta(q_1^2)\Delta(q_2^2)}} = \frac{1}{\sqrt{s_3}} = \cos\beta \tag{B56}$$

as an angle. Uncorrelated canonical pairs are therefore orthogonal to each other in the sense that $\cos\beta = 0$.

Because s_4 already appears in trigonometric functions in our realization, we rename it by defining

$$\alpha = s_4 \quad , \quad p_\alpha = p_4 . \tag{B57}$$

The canonical mapping then takes the form

$$\Delta(q_1^2) = s_1^2 \quad , \quad \Delta(q_1 \pi_1) = s_1 p_1 \quad , \quad \Delta(\pi_1^2) = p_1^2 + \frac{\Phi}{s_1^2} \tag{B58}$$

$$\Delta(q_2^2) = s_2^2 \quad , \quad \Delta(q_2 \pi_2) = s_2 p_2 \quad , \quad \Delta(\pi_2^2) = p_2^2 + \frac{\Gamma}{s_2^2} \tag{B59}$$

where

$$\Phi(\beta, p_\beta, \alpha, p_\alpha) = (p_\alpha - p_\beta)^2 \tag{B60}$$
$$+ \frac{1}{2\sin(\beta)^2}\left(U_1 - 4p_\alpha^2 - \sqrt{U_2 - U_1^2 + (U_1 - 4p_\alpha^2)^2}\sin(\alpha + \beta)\right)$$

$$\Gamma(\beta, p_\beta, \alpha, p_\alpha) = (p_\alpha + p_\beta)^2 \tag{B61}$$
$$+ \frac{1}{2\sin(\beta)^2}\left(U_1 - 4p_\alpha^2 - \sqrt{U_2 - U_1^2 + (U_1 - 4p_\alpha^2)^2}\sin(\alpha - \beta)\right) ,$$

as well as

$$\Delta(\pi_1 \pi_2) = p_2 p_2 \cos(\beta) - \frac{\cos(\beta)}{s_1 s_2}p_\beta^2 + \frac{\cos(\beta) + 2\cot(\beta)\csc(\beta)}{s_1 s_2}p_\alpha^2 \tag{B62}$$
$$- \sin(\beta)p_\beta\left(\frac{p_2}{s_1} + \frac{p_1}{s_1}\right) + p_\alpha\sin(\beta)\left(\frac{p_2}{s_1} - \frac{p_1}{s_2}\right)$$
$$- \frac{\cot(\beta)\csc(\beta)}{s_1 s_2}U_1 + \frac{\csc(\beta)^2\sin(\alpha)}{2s_1 s_2}\sqrt{16p_\alpha^2 - 8p_\alpha^2 U_1 + U_2}$$

$$\Delta(\pi_1 q_2) = p_1 s_2 \cos(\beta) + \sin(\beta)\frac{s_2}{s_1}(p_\alpha - p_\beta) \tag{B63}$$

$$\Delta(\pi_2 q_1) = p_2 s_1 \cos(\beta) + \sin(\beta)\frac{s_1}{s_2}(p_\beta + p_\alpha) \tag{B64}$$

$$\Delta(q_1 q_2) = s_1 s_2 \cos(\beta) . \tag{B65}$$

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