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## ADVERTISEMENT



## Semiclassical propagator for SU(*n*) coherent states

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We present a detailed derivation of the semiclassical propagator in the SU(*n*) coherent state representation. In order to provide support for immediate physical applications, we restrict this work to the fully symmetric irreducible representations, which are suitable for the treatment of bosonic dynamics in *n* modes, considering systems with conservation of total particle number. The derivation described here can be easily extended to other classes of coherent states, thus representing an alternative approach to previously published methods. © 2011 American Institute of Physics. [doi:10.1063/1.3583996]

## I. INTRODUCTION

The coherent states are a fundamental tool in quantum mechanics. They were initially envisioned by Schrödinger<sup>1</sup> as minimum uncertainty Gaussian states whose dynamics has maximum similarity to the classical oscillator. The interest in these states, which are related to the Weyl-Heisenberg algebra, was again aroused by the work of Glauber,<sup>2–4</sup> Klauder,<sup>5–7</sup> and Sudarshan,<sup>8</sup> with the emergence of the first applications directed to quantum optics and semiclassical approximations.

The generalization of the coherent states to arbitrary Lie groups was initially studied by Klauder, but a complete and detailed definition of the generalized coherent states was only later developed by Perelomov<sup>9</sup> and Gilmore.<sup>10</sup> In this way, important properties of the harmonic-oscillator coherent states were extended to other algebras of physical interest, resulting in an ideal setting for the study of the quantum-classical correspondence.<sup>11</sup>

Although the semiclassical methods also have their origin in the early days of quantum mechanics, the first calculations concerning semiclassical propagators in the representation of harmonicoscillator coherent states were only developed in the last decades of the past century,<sup>12–15</sup> as an attempt to transpose the practical difficulties of semiclassical propagators in the coordinate and momentum representations.

However, similar to the very definitions of coherent states, the generalization of semiclassical propagators for arbitrary groups occurred only in the decades following the semiclassical approximations with Gaussian states. In particular, aiming at the treatment of systems with spin, various correct derivations of the SU(2) semiclassical propagator<sup>16–18</sup> were obtained independently. Amidst these different methods, Kochetov<sup>19,20</sup> generalized his results to arbitrary Lie groups.

The study of semiclassical propagators is motivated mainly by the computational gain in relation to exact quantum calculations, considering practical applications in systems with many degrees of freedom or large quantum numbers, in which cases it is believed that the semiclassical approximation is efficient and accurate. From the less pragmatic point of view, the use of classical quantities for the calculation of quantum corrections allows us a greater understanding of the quantum-classical correspondence principle, since it establishes more precisely the boundaries and intersections between the two theories.

We propose in this paper an independent approach for the derivation of the semiclassical propagator in arbitrary coherent state representations. However, to make this text clearer and more

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accessible, here we exemplify our method only for the coherent states related to the fully symmetric representations of the SU(n) group.<sup>21</sup> These coherent states are appropriate for the treatment of bosonic systems with a finite number of modes and conservation of the total particle number. Therefore, the SU(n) coherent states are important for several physical applications, as for example, the research on Bose-Einstein condensates in multiwell traps.<sup>22–24</sup>

The major technical difficulty encountered in the derivation of semiclassical propagators is related to the explicit calculation of path integrals for quadratic approximations of the action functional. The topology and dimensionality of the classical phase space can make this task quite complex. Recently, Braun and  $\text{Garg}^{25,26}$  developed a simple and transparent solution to the semiclassical propagator for an arbitrary number of degrees of freedom, but considering only the direct product of many harmonic-oscillator or SU(2) coherent states. Using a slightly modified form of their previous findings and a suitable transformation of variables, we extend the path integral calculation to the SU(*n*) coherent states.

The remainder of this paper is divided as follows: in large part of Sec. II we reproduce the main results of Braun and Garg<sup>25</sup> concerning the semiclassical propagator for multidimensional harmonicoscillator coherent states. At the end of this section, we reformulate the identity that relates the path integral resulting from the semiclassical approximation to dynamical quantities calculated on the classical trajectory. This fundamental result is used in Sec. III, where we make a detailed derivation of the semiclassical propagator in the SU(n) coherent state representation. Finally, the Sec. IV is intended to our concluding remarks.

## II. SEMICLASSICAL PROPAGATOR FOR (n-1) HARMONIC MODES

### A. Harmonic-oscillator coherent states

The coherent state for (n - 1) harmonic modes is given by

$$|z\rangle = e^{-\frac{z^{*}z}{2}} \sum_{m_1, m_2, \dots, m_{n-1}=0}^{\infty} \left( \prod_{j=1}^{n-1} \frac{z_j^{m_j}}{\sqrt{m_j!}} \right) |m_1, m_2, \dots, m_{n-1}\rangle,$$
(1)

where  $\{|m_1, m_2, ..., m_{n-1}\rangle\}$  is the usual basis of the bosonic Fock space  $B^{n-1}$  for (n-1) modes, such that  $m_j$  is the occupation in the *j*th mode. The complex vector  $z = (z_1, z_2, ..., z_{n-1})^T$ , with (n-1) entries, parametrizes the entire set of coherent states. Also, according to the adopted notation, the juxtaposition of two vectors *a* and *b* represents the matrix product  $ab = a_1b_1 + a_2b_2 + ... + a_{n-1}b_{n-1}$ .

The coherent states (1) constitute an overcomplete set in Hilbert space, which enables us to write the following diagonal resolution of the identity in  $B^{n-1}$ ,

$$\int_{\mathbf{C}^{n-1}} d\mu(z^*, z) |z\rangle \langle z| = 1, \qquad d\mu(z^*, z) = \prod_{j=1}^{n-1} \frac{d^2 z_j}{\pi},$$
(2)

where  $d^2 z_j = dq_j dp_j = \frac{dz_j dz_j^*}{2i}$ , with  $q_j = \operatorname{Re}(z_j)$  and  $p_j = \operatorname{Im}(z_j)$ .

## B. Coherent state propagator

The quantum propagator in the coherent state representation is defined as the matrix element of the time evolution operator between the initial coherent state  $|z_i\rangle$  and the final coherent state  $|z_f\rangle$ , assuming a propagation period  $\tau$ ,

$$K(z_f^*, z_i; \tau) = \langle z_f | e^{-iH\tau} | z_i \rangle.$$
(3)

In the above definition, for simplicity, we assumed  $\hbar = 1$  and the temporal independence of the Hamiltonian *H*. However, the main results presented in this work, including the semiclassical approximation of the propagator, are also valid for Hamiltonians with explicit time dependence.<sup>27</sup>

Expanding the propagator (3) to second order around the classical trajectory, which is defined later, we obtain the following form for its semiclassical approximation:

$$K_{sc}(z_f^*, z_i; \tau) = e^{iS_c - \frac{1}{2}(|z_i|^2 + |z_f^*|^2)} K_{red}(z_f^*, z_i; \tau),$$
(4)

where  $S_c$  is the action functional S calculated on the classical trajectory, and  $K_{red}$  is the reduced propagator, which introduces quantum corrections. The classical trajectories, by definition, are the extremes of the action functional,

$$iS(z_f^*, z_i; \tau) = \int_0^t \left\{ \frac{1}{2} (\dot{\bar{z}}z - \bar{z}\dot{z}) - i\mathcal{H}(\bar{z}, z) \right\} dt + \frac{1}{2} [z_f^* z(\tau) + \bar{z}(0)z_i].$$
(5)

In the previous equation, to emphasize the independence of the variables z and  $z^*$ , we made the change of notation  $z^* \to \overline{z}$ . Also in (5), we defined the function  $\mathcal{H}(\overline{z}, z) = \frac{\langle \overline{z}^* | H | z \rangle}{\langle \overline{z}^* | z \rangle}$ , which represents the effective classical Hamiltonian. The extremization of the action functional implies the following classical equations of motion:<sup>28</sup>

$$\dot{z} = -i\frac{\partial\mathcal{H}}{\partial\bar{z}}, \qquad \dot{\bar{z}} = i\frac{\partial\mathcal{H}}{\partial\bar{z}}.$$
 (6)

According to (3), the correct classical trajectory must respect the boundary conditions  $z(0) = z_i$ and  $\overline{z}(\tau) = z_f^*$ . Generally, if we consider the variables  $\overline{z}$  as the complex conjugates of z, then the boundary conditions would make the system of differential equations (6) overdetermined, since the two vector equations would become redundant. Therefore, for arbitrary classical trajectories,  $\overline{z}(t)$ is not the complex conjugate of z(t), henceforth denoted by  $z^*(t)$ , except for a specific boundary condition in which accidentally  $\overline{z}(0) = z_i^*$ .

The reduced propagator corresponds to an infinite dimensional integral of the second variation of the action  $\delta^2 S_c$ ,

$$K_{red}(z_f^*, z_i; \tau) = \int D\mu(\overline{\eta}, \eta) \exp\left\{\frac{i}{2}\delta^2 S_c\right\}, \quad D\mu(\overline{\eta}, \eta) = \lim_{M \to \infty} \prod_{k=1}^{M-1} \left[\prod_{j=1}^{n-1} \frac{d^2 \eta_j^k}{\pi}\right].$$
(7)

The integration variables  $\eta^k = z^k - z_c^k$  and  $\overline{\eta}^k = \overline{z}^k - \overline{z}_c^k$  represent the departure from the classical trajectory, denoted by  $z_c^k$  and  $\overline{z}_c^k$ , at the time  $t_k = k\varepsilon$ , for k = 0, 1, 2, ..., M and  $\varepsilon = \frac{\tau}{M}$ . These variables are subject to the boundary conditions  $\eta^0 = \eta(0) = 0$  and  $\overline{\eta}^M = \overline{\eta}(\tau) = 0$ , also in agreement with the propagator (3).

By linearization of Eq. (6), we can also obtain the classical equations of motion for deviations from the classical trajectory. In this way we define the matrices  $R_{jk}$ , which are essential for later results,<sup>29</sup>

$$\begin{pmatrix} \delta \dot{z}(t) \\ \delta \dot{\overline{z}}(t) \end{pmatrix} = \begin{pmatrix} -i \frac{\partial^2 \mathcal{H}}{\partial \overline{z} \partial z} & -i \frac{\partial^2 \mathcal{H}}{\partial \overline{z}^2} \\ i \frac{\partial^2 \mathcal{H}}{\partial z^2} & i \frac{\partial^2 \mathcal{H}}{\partial z \partial \overline{z}} \end{pmatrix} \begin{pmatrix} \delta z(t) \\ \delta \overline{z}(t) \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} \delta z(t) \\ \delta \overline{z}(t) \end{pmatrix}.$$
(8)

The quantities in the previous equation are calculated on the classical trajectory. Notice that  $\delta z$  and  $\delta \overline{z}$ , which represent the dynamical variables of Eq. (8), deserve different notation from the integration variables  $\eta^k$  and  $\overline{\eta}^k$  due to their fundamentally unrelated purposes and definitions.

After a lengthy derivation, the result of the Gaussian integral (7) can be written in terms of dynamical quantities calculated on the classical trajectory,<sup>30</sup>

$$K_{red}(z_f^*, z_i; \tau) = e^{\frac{1}{2} \int_{0}^{\tau} \operatorname{Tr}[R_{22}(t)] dt} \sqrt{\det\left[\frac{\partial \overline{z}(0)}{\partial \overline{z}(\tau)}\right]}.$$
(9)

The matrix  $\frac{\partial \overline{z}(0)}{\partial \overline{z}(\tau)}$  represents the response of the "free" trajectory extreme  $\overline{z}(0)$  to a change in the boundary condition  $\overline{z}(\tau) = z_f^*$ . Employing the functional (5), we can show the identity  $\frac{\partial \overline{z}(0)}{\partial \overline{z}(\tau)} = i \frac{\partial^2 S_c}{\partial z_i \partial z_f^*}$ , relating the second factor of (9) to a second derivative of the action.

## C. Continuous limit of $\delta^2 S_c$

In the original text of Braun and Garg,<sup>25</sup> only the time discretized form of  $\delta^2 S_c$  was employed in order to obtain the result (9). In this approach, the Gaussian integrals in (7) are calculated sequentially, before the application of the continuous-time limit ( $\varepsilon \rightarrow 0, M \rightarrow \infty$ , and  $\varepsilon M = \tau$ ). However, we can write the continuous form of  $\delta^2 S_c$  directly from (5),

$$i\delta^2 S_c = \int_0^t dt \left\{ (\dot{\eta}\eta - \overline{\eta}\dot{\eta}) - \eta R_{21}\eta - \eta R_{22}\overline{\eta} + \overline{\eta}R_{11}\eta + \overline{\eta}R_{12}\overline{\eta} \right\}.$$
 (10)

Substituting (10) in (7), we obtain a new expression for the reduced propagator,

$$K_{red}(z_f^*, z_i; \tau) = \int D\mu(\overline{\eta}, \eta) \exp\left\{\frac{1}{2} \int_0^{\tau} dt \left[ (\dot{\overline{\eta}}\eta - \overline{\eta}\dot{\eta}) - \eta R_{21}\eta - 2\eta R_{22}\overline{\eta} + \overline{\eta}R_{12}\overline{\eta} \right] \right\}, \quad (11)$$

where we used the identity  $R_{22}^T = -R_{11}$ . Comparing the representations (9) and (11) of  $K_{red}$ , we can write a formal identity between the path integral of  $\delta^2 S_c$  in its continuous form and the corresponding solution described by classical quantities,

$$\int D\mu(\overline{\eta},\eta) \, e^{\frac{1}{2} \int \limits_{0}^{\tau} dt \left[ (\dot{\overline{\eta}}\eta - \overline{\eta}\eta) - \eta R_{21}\eta - 2\eta R_{22}\overline{\eta} + \overline{\eta}R_{12}\overline{\eta} \right]} = e^{\frac{1}{2} \int \limits_{0}^{\tau} \mathrm{Tr}[R_{22}(t)]dt} \sqrt{\det\left[ \frac{\partial \overline{z}(0)}{\partial \overline{z}(\tau)} \right]}.$$
(12)

We must always remember that the previous expression is associated with the boundary conditions  $\eta(0) = 0$  and  $\overline{\eta}(\tau) = 0$ . Equation (12) is the main result of this section, since its generalization to SU(*n*) coherent states is almost straightforward, as shown below.

## III. PATH INTEGRAL FOR SU(n) COHERENT STATES

## A. SU(n) coherent states

The coherent states related to the *fully symmetric irreducible representations* of SU(n) are given by<sup>21</sup>

$$|N;w\rangle = \sum_{m_1+m_2+\ldots+m_n=N} \left(\frac{N!}{m_1!m_2!\ldots m_n!}\right)^{\frac{1}{2}} \left(\prod_{j=1}^{n-1} w_j^{m_j}\right) \frac{|m_1,m_2,\ldots,m_n\rangle}{(1+w^*w)^{\frac{N}{2}}}.$$
 (13)

Here again  $\{|m_1, m_2, ..., m_n\rangle\}$  is the usual basis of the bosonic Fock space  $\mathbb{B}_N^n$  for *n* modes and *N* particles, such that  $m_j$  is the occupation of the *j*th mode. Similar to the vector *z* defined in Eq. (1), the number of entries of the complex vector  $w = (w_1, w_2, ..., w_{n-1})^T$  is (n - 1). However, the number of bosonic modes is now *n*, but with occupations restricted by  $\sum_{j=1}^n m_j = N$ . Note that the total number of particles *N* is the only index needed to uniquely specify a fully symmetric irreducible representation of SU(*n*).

The SU(*n*) coherent states are suitable for the treatment of bosonic systems with a finite number of modes and conservation of the total particle number. Therefore, henceforth we consider a system with a fixed number of bosons, so that the evolution of its state is restricted to only one SU(*n*) irreducible representation. Thus, we also simplify the notation by making  $|N; w\rangle \rightarrow |w\rangle$ . Just as in the harmonic-oscillator case, the coherent states in (13) are normalized, but they are not orthogonal. The overlap between two SU(n) coherent states is given by

$$\langle w'|w\rangle = \frac{(1+w'^*w)^N}{(1+w'^*w')^{\frac{N}{2}}(1+w^*w)^{\frac{N}{2}}}.$$
(14)

Using the SU(n) coherent states, we can write a diagonal resolution for the identity in  $B_N^n$ ,

$$\int_{e} \int_{e} d\mu(w^*, w) |w\rangle \langle w| = 1, \qquad d\mu(w^*, w) = \frac{\sigma(n) \dim(\mathbf{B}_N^n)}{(1 + w^* w)^n} \prod_{j=1}^{n-1} d^2 w_j.$$
(15)

Here again we use the notation  $d^2w_j = dx_j dy_j = \frac{dw_j dw_j^*}{2i}$ , where  $x_j = \operatorname{Re}(w_j)$  and  $y_j = \operatorname{Im}(w_j)$ . Notice that we can deform the integration domain by making  $w_j$  and  $w_j^*$  independent variables, which amounts to the complexification of  $x_j$  and  $y_j$ . We use this procedure in the following subsections to replace the complex plane by a surface of integration in C<sup>2</sup> for each value of j. Also note that the normalization constant in (15) can be divided into the factors  $\sigma(n) = \frac{(n-1)!}{\pi^{n-1}}$ , which is independent of the total particle number, and  $\dim(B_N^n) = \frac{(N+n-1)!}{N!(n-1)!}$ , the dimension of accessible Hilbert space.

The choice of parametrization defined in (13) for the SU(n) coherent states is quite appropriate, since the integration domain in (15) is the same of Eq. (2). Moreover, except for the normalization factor, the coherent states are entire functions of the variables w.

## B. SU(n) coherent state propagator

w

Similar to Eq. (3), we define the propagator in the SU(*n*) coherent state representation as the transition probability between the initial coherent state  $|w_i\rangle$  and the final coherent state  $|w_f\rangle$  after a time interval  $\tau$ ,

$$K(w_f^*, w_i; \tau) = \langle w_f | e^{-iH\tau} | w_i \rangle.$$
<sup>(16)</sup>

For simplicity, we have assumed again a time-independent Hamiltonian H. To write down a path integral representation for  $K(w_f^*, w_i; \tau)$ , we factorize the evolution operator into M identical propagation subintervals of length  $\varepsilon = \frac{\tau}{M}$ . Then, we introduce an identity of the form (15) between each pair of factors in the discretized evolution operator,

$$K(w_f^*, w_i; \tau) = \int \left[\prod_{k=1}^{M-1} d\mu(\overline{w}^k, w^k)\right] \prod_{j=1}^{M} \langle \overline{w}^{j*} | e^{-iH\varepsilon} | w^{j-1} \rangle.$$
(17)

In the previous equation we define the integration variables  $w^k = w(t_k)$  and  $\overline{w}^k = \overline{w}(t_k)$ , with  $t_k = k\varepsilon$  for k = 1, 2, ..., (M - 1). We also extend this notation to the propagator boundary conditions by setting  $w^0 = w(0) = w_i$  and  $\overline{w}^M = \overline{w}(\tau) = w_f^*$ . Note that we employ the notation  $w^*(t) \to \overline{w}(t)$  since the beginning of this section, already evidencing the future duplication of the classical phase space. However,  $w^k$  and  $\overline{w}^k$  need to be considered as independent integration variables only after the semiclassical approximation, when the integration domain is deformed to a surface in the doubled phase space which contains the *k*th point of the discretized classical trajectory. Nonetheless, to maintain the consistency of notation in this procedure, notice that the identities  $\overline{w}^0 = w^{0*} = w_i^*$  and  $w^M = \overline{w}^{M*} = w_f$  must always be preserved ( $\overline{w}^0$  and  $\overline{w}^M$  cannot be made independent of  $w^0$  and  $w^M$ ), since these quantities do not stand for integration variables, which can be designated to follow the classical trajectory in the doubled phase space.

052104-6 T. D. Viscondi and M. A. de Aguiar

Considering that at the some point of the calculations we will take the limit  $M \to \infty$ , we can expand each factor in the integrand of (17) to first order in  $\varepsilon$ ,

$$\langle \overline{w}^{j*} | e^{-iH\varepsilon} | w^{j-1} \rangle \approx \langle \overline{w}^{j*} | 1 - iH\varepsilon | w^{j-1} \rangle \approx \langle \overline{w}^{j*} | w^{j-1} \rangle e^{-i\varepsilon \mathcal{H}_{j,j-1}},$$

$$(18)$$

where  $\mathcal{H}_{j,j-1} = \frac{\langle \overline{w}^{j^*} | H | w^{j-1} \rangle}{\langle \overline{w}^{j^*} | w^{j-1} \rangle}$ , for j = 1, 2, ..., M. Then, substituting the expression (18) in (17), we can readily obtain

$$K(w_f^*, w_i; \tau) = \int \left[\prod_{k=1}^{M-1} d\mu(\overline{w}^k, w^k)\right] \exp\left[\sum_{j=1}^M \operatorname{Ln}\langle \overline{w}^{j*} | w^{j-1} \rangle - i\varepsilon \sum_{j=1}^M \mathcal{H}_{j,j-1}\right].$$
(19)

Employing Eq. (14), the argument of the exponential in (19) takes the following form:

$$i\widetilde{S}_{d} = \sum_{j=1}^{M} \left\{ \frac{N}{2} \operatorname{Ln} \left[ \frac{(1 + \overline{w}^{j} w^{j-1})^{2}}{(1 + \overline{w}^{j} w^{j})(1 + \overline{w}^{j-1} w^{j-1})} \right] - i\varepsilon \mathcal{H}_{j,j-1} \right\}$$

$$= iS_{d} - \frac{N}{2} \operatorname{Ln} \left[ (1 + |w_{j}^{*}|^{2})(1 + |w_{i}|^{2}) \right].$$
(20)

In order to achieve the correct continuous limit of  $\widetilde{S}_d$ , it is imperative to note that generally  $w(\tau) \neq w^M = w_f$  and  $\overline{w}(0) \neq \overline{w}^0 = w_i^*$ , thus ensuring the continuity of the trajectories in the independent variables w(t) and  $\overline{w}(t)$ . Although  $\widetilde{S}_d$  explicitly depends on  $w^M$  and  $\overline{w}^0$ , as we see in the first line of (20), it is possible to analytically isolate all dependence on these quantities in a single term, as shown in the last line of (20). The term  $S_d$  represents the discretized form of the action functional,<sup>31</sup> whose extremization correctly gives the classical equations of motion in the continuous-time limit.

Also in this limit, we can assume that consecutive values of  $w(t_k)$  and  $\overline{w}(t_k)$  are very close, forming a continuous trajectory. Therefore, according to (14), we can write the following identity, which is valid up to first order in  $|w(t_k) - w(t_k)|$  and  $|\overline{w}(t_k) - \overline{w}(t_k)|$ :

$$\operatorname{Ln}\langle \overline{w}^{*}(t_{k})|w(t_{k-1})\rangle \approx \frac{N}{2} \frac{[\overline{w}(t_{k}) - \overline{w}(t_{k-1})]w(t_{k-1}) - \overline{w}(t_{k})[w(t_{k}) - w(t_{k-1})]}{1 + \overline{w}(t_{k})w(t_{k-1})}.$$
 (21)

Adding and subtracting the appropriate terms dependent on  $w(\tau)$  and  $\overline{w}(0)$ , we can easily take the continuous limit of the action functional  $S_d$  with aid of expression (21),

$$iS(w_f^*, w_i; \tau) = \int_0^{\tau} dt \left\{ \frac{N}{2} \frac{\dot{\overline{w}}w - \overline{w}\dot{w}}{1 + \overline{w}w} - i\mathcal{H}(\overline{w}, w) \right\} + \frac{N}{2} \operatorname{Ln}\left\{ [1 + w_f^* w(\tau)] [1 + \overline{w}(0)w_i] \right\}.$$
(22)

In the previous equation we also defined the effective Hamiltonian  $\mathcal{H}(\overline{w}, w) = \frac{\langle \overline{w}^* | H | w \rangle}{\langle \overline{w}^* | w \rangle}$ , which represents the continuous limit of  $\mathcal{H}_{j,j-1}$ . The extremization of *S*, for fixed boundary conditions and propagation period, provides the classical equations of motion. So, by making  $\delta S = 0$ , we obtain<sup>32</sup>

$$\dot{w} = -\frac{i}{N}(1 + \overline{w}w)(1 + w \otimes \overline{w})\frac{\partial \mathcal{H}}{\partial \overline{w}} = -i\Xi\frac{\partial \mathcal{H}}{\partial \overline{w}},$$
  
$$\dot{\overline{w}} = \frac{i}{N}(1 + \overline{w}w)(1 + \overline{w} \otimes w)\frac{\partial \mathcal{H}}{\partial w} = i\overline{\Xi}\frac{\partial \mathcal{H}}{\partial w}.$$
(23)

Here we should remember again that the classical trajectory is contained in a doubled phase space, since w(t) and  $\overline{w}(t)$  must be treated as independent variables, preventing the overdetermination of the equations of motion caused by the boundary conditions  $w(0) = w_i$  and  $\overline{w}(\tau) = w_f^*$ . Notice that, in the case where  $\mathcal{H}/N$  is independent of N, the classical equations of motion, as well as their resulting solutions, are also independent of the total number of particles.

#### 052104-7 Semiclassical propagator for SU(*n*) coherent states

Analogously to (8), we can write equations of motion for deviations from the classical trajectory. Thus, we redefine the matrices  $R_{jk}$  for our new dynamical variables,

$$\begin{pmatrix} \delta \dot{w} \\ \delta \dot{\overline{w}} \end{pmatrix} = \begin{pmatrix} -i \frac{\partial}{\partial w} \left[ \Xi \frac{\partial \mathcal{H}}{\partial \overline{w}} \right] & -i \frac{\partial}{\partial \overline{w}} \left[ \Xi \frac{\partial \mathcal{H}}{\partial \overline{w}} \right] \\ i \frac{\partial}{\partial w} \left[ \overline{\Xi} \frac{\partial \mathcal{H}}{\partial w} \right] & i \frac{\partial}{\partial \overline{w}} \left[ \overline{\Xi} \frac{\partial \mathcal{H}}{\partial w} \right] \end{pmatrix} \begin{pmatrix} \delta w \\ \delta \overline{w} \end{pmatrix} = \begin{pmatrix} R_{11} & R_{12} \\ R_{21} & R_{22} \end{pmatrix} \begin{pmatrix} \delta w \\ \delta \overline{w} \end{pmatrix}.$$
(24)

Notice that the identity  $R_{22}^T = -R_{11}$  is no longer valid.

### C. Semiclassical approximation

Substituting the definition (20) in Eq. (19) and then taking the continuous limit, we obtain a new expression for the SU(n) propagator,

$$K(w_f^*, w_i; \tau) = \int D\mu(\overline{w}, w) \exp\left\{ i S(w_f^*, w_i; \tau) - \frac{N}{2} \operatorname{Ln}\left[ (1 + |w_f^*|^2)(1 + |w_i|^2) \right] \right\}.$$
 (25)

The quantity  $D\mu(\overline{w}, w)$  symbolizes the following infinite product of measures in the doubled phase space:

$$D\mu(\overline{w},w) = \lim_{M \to \infty} \prod_{k=1}^{M-1} \left[ \frac{\sigma(n)\operatorname{dim}(\mathbf{B}_N^n)}{(1+\overline{w}^k w^k)^n} \prod_{j=1}^{n-1} d^2 w_j^k \right].$$
 (26)

Now, we proceed to the semiclassical approximation. In the limit where the total number of particles becomes large and under realistic assumptions for the Hamiltonian H, one can show that the exponent of Eq. (25) increases linearly with N and a saddle-point approximation<sup>43</sup> to the integral is justified.<sup>33</sup> Indeed, the second term in the exponent of Eq. (25) is proportional to N and, according to Eq. (22), the action is also proportional to N, except for the term containing the Hamiltonian. However, in cases of physical interest, we expect that the effective energy per particle  $\mathcal{H}/N$  converges to a finite value, thus justifying the saddle-point procedure for  $N \gg 1$ . In a forthcoming article we present an explicit application of the SU(2) and SU(3) semiclassical propagators for a Bose-Einstein condensate trapped in a symmetric triple-well potential, where the above assumptions are exemplified.<sup>34</sup>

Expanding the action up to second order around the classical trajectory, which we denote by  $w_c(t)$  and  $\overline{w}_c(t)$ , we obtain

$$S \approx S_c + \frac{1}{2}\delta^2 S_c, \qquad \delta S_c = 0.$$
 (27)

Substituting the above approximation in the propagator (25), we obtain the semiclassical propagator in the SU(n) coherent state representation,

$$K_{sc}(w_f^*, w_i; \tau) = \exp\left\{iS_c - \frac{N}{2}\mathrm{Ln}\left[(1 + |w_f^*|^2)(1 + |w_i|^2)\right]\right\} \int D\mu(\overline{w}, w) \, e^{\frac{i}{2}\delta^2 S_c}.$$
 (28)

Therefore, it remains only to calculate the reduced propagator, defined by

$$K_{red}(w_f^*, w_i; \tau) = \int D\mu(\overline{\eta}, \eta) \, e^{\frac{i}{2}\delta^2 S_c},\tag{29}$$

where we have introduced new integration variables  $\eta(t) = w(t) - w_c(t)$  and  $\overline{\eta}(t) = \overline{w}(t) - \overline{w}_c(t)$ , which represent deviations from the classical trajectory. Note that these new variables are subject to the boundary conditions  $\eta(0) = \overline{\eta}(\tau) = 0$ . Expanding the action (22), we get the following quadratic terms in  $\eta$  and  $\overline{\eta}$  after some integrations by parts:

$$i\delta^2 S_c = \int_0^\tau dt \ \left\{ \eta \overline{\Theta} \dot{\overline{\eta}} - \overline{\eta} \Theta \dot{\eta} + \eta A \eta + 2\eta B \overline{\eta} + \overline{\eta} C \overline{\eta} \right\}.$$
(30)

052104-8 T. D. Viscondi and M. A. de Aguiar

The matrices  $\Theta$  and  $\overline{\Theta}$  are the inverses of  $\Xi$  and  $\overline{\Xi}$ , respectively. The explicit form of these matrices is given by

$$\Theta = N \frac{(1 + \overline{w}w)1 - w \otimes \overline{w}}{(1 + \overline{w}w)^2} = \overline{\Theta}^T.$$
(31)

The other quantities introduced in Eq. (30) are defined as follows:

$$\frac{A}{N} = \frac{2(\dot{w}w)\overline{w}\otimes\overline{w} - (1+\overline{w}w)(\overline{w}\otimes\dot{w}+\dot{w}\otimes\overline{w})}{(1+\overline{w}w)^3} - \frac{i}{N}\frac{\partial^2\mathcal{H}}{\partial w^2},$$

$$\frac{B}{N} = \frac{1}{2}\frac{(\dot{w}w-\overline{w}\dot{w})[2\overline{w}\otimes w - (1+\overline{w}w)1] + (1+\overline{w}w)(\overline{w}\otimes\dot{w}-\dot{w}\otimes w)}{(1+\overline{w}w)^3} - \frac{i}{N}\frac{\partial^2\mathcal{H}}{\partial w\partial\overline{w}}, \quad (32)$$

$$\frac{C}{N} = \frac{(1+\overline{w}w)(w\otimes\dot{w}+\dot{w}\otimes w) - 2(\overline{w}\dot{w})w\otimes w}{(1+\overline{w}w)^3} - \frac{i}{N}\frac{\partial^2\mathcal{H}}{\partial\overline{w}^2}.$$

Now we make a further change of integration variables, in order to compare the path integral (29) with the canonical result (12). To this end, we define the following matrices:

$$Q = \sqrt{N} \frac{w \otimes \overline{w} + \sqrt{1 + \overline{w}w} \left[ (\overline{w}w)1 - w \otimes \overline{w} \right]}{\overline{w}w(1 + \overline{w}w)} = \overline{Q}^{T},$$
(33)

such that  $Q^2 = \Theta$  and  $\overline{Q}^2 = \overline{\Theta}$ . Then, applying the linear transformations  $\nu = Q\eta$  and  $\overline{\nu} = \overline{Q}\overline{\eta}$  in (30), we get

$$i\delta^2 S_c = \int_0^\tau dt \ \left\{ (\nu \dot{\overline{\nu}} - \overline{\nu} \dot{\nu}) + \nu \widetilde{A}\nu + 2\nu \widetilde{B}\overline{\nu} + \overline{\nu}\widetilde{C}\overline{\nu} \right\}.$$
(34)

Note that, in this new set of variables,  $\delta^2 S_c$  has the same form previously found in (10). The matrices above are related to variables of interest w and  $\overline{w}$  as follows:

$$\widetilde{A} = \overline{Q}^{-1} A Q^{-1},$$

$$\widetilde{B} = \overline{Q}^{-1} B \overline{Q}^{-1} - \frac{1}{2} \left( \dot{\overline{Q}} \overline{Q}^{-1} - \overline{Q}^{-1} \dot{\overline{Q}} \right),$$

$$\widetilde{C} = Q^{-1} C \overline{Q}^{-1}.$$
(35)

In the previous definitions we used the inverses of the matrices Q and  $\overline{Q}$ , which can be readily found,

$$Q^{-1} = \frac{1 + \overline{w}w}{\sqrt{N\overline{w}w}} \left\{ w \otimes \overline{w} + \frac{\left[(\overline{w}w)1 - w \otimes \overline{w}\right]}{\sqrt{1 + \overline{w}w}} \right\} = \left(\overline{Q}^{-1}\right)^{T}.$$
(36)

Under the same transformation applied to (34), the path measure (26) takes the following form:

$$D\mu(\overline{\nu},\nu) = \lim_{M \to \infty} \prod_{k=1}^{M-1} \left[ \frac{(N+n-1)!}{N!N^{n-1}} \prod_{j=1}^{n-1} \frac{d^2 \nu_j^k}{\pi} \right].$$
 (37)

Therefore,  $D\mu(\overline{\nu}, \nu)$  takes the same form found in (7) only when  $N \gg n$ . That is, the transformation given by (33) produces the desired result only for large number of particles (macroscopic limit). However, this is precisely the expected situation for the effectiveness of the semiclassical approximation, considering the computational gain and the quantitative agreement with respect to exact quantum results.

In order to go from Eqs. (26) to (37) we employed the explicit expression for det Q, which is trivially related to det  $\Theta$ . The determinant of  $\Theta$  can be easily calculated from the identity,

$$\det\left[(1+\overline{w}w)1-w\otimes\overline{w}\right] = (1+\overline{w}w)^{n-2}; \quad \text{for } n \ge 2.$$
(38)

Substituting (34) and (37) in (29), under the additional condition  $N \gg n$ , we can recast the reduced propagator in a similar way to Eq. (11),

$$K_{red}(w_f^*, w_i; \tau) = \int D\mu(\overline{\nu}, \nu) \, \exp\left\{\frac{1}{2} \int_0^{\tau} dt \, \left[(\nu \dot{\overline{\nu}} - \overline{\nu} \dot{\nu}) + \nu \widetilde{A}\nu + 2\nu \widetilde{B}\overline{\nu} + \overline{\nu} \widetilde{C}\overline{\nu}\right]\right\}. \tag{39}$$

The variables v(t) and  $\overline{v}(t)$  can be interpreted as deviations from the classical trajectory described in a new set of dynamical variables, such that  $v(t) = v(t) - v_c(t)$  and  $\overline{v}(t) = \overline{v}(t) - \overline{v}_c(t)$ . With this interpretation in mind, we can directly compare Eqs. (12) and (39), allowing us to solve the integral of the reduced propagator in an immediate way,

$$K_{red}(w_f^*, w_i; \tau) = \exp\left\{-\frac{1}{2}\int_0^{\tau} \operatorname{Tr}\left[\widetilde{B}(t)\right] dt\right\} \sqrt{\det\left[\frac{\partial \overline{v}(0)}{\partial \overline{v}(\tau)}\right]}.$$
(40)

However, the above result is not yet the desired solution, because we still need to return to the original variables w and  $\overline{w}$ . Comparing the transformation between the variables  $\eta$  ( $\overline{\eta}$ ) and  $\nu$  ( $\overline{\nu}$ ) with their respective definitions, it becomes evident the relation v(t) = Q(t)w(t) ( $\overline{v}(t) = \overline{Q}(t)\overline{w}(t)$ ). Therefore, we can write the following identity:

$$\det\left[\frac{\partial\overline{v}(0)}{\partial\overline{v}(\tau)}\right] = \det\left[\overline{Q}(0)\frac{\partial\overline{w}(0)}{\partial\overline{w}(\tau)}\overline{Q}^{-1}(\tau)\right] = \left[\frac{1+\overline{w}(\tau)w(\tau)}{1+\overline{w}(0)w(0)}\right]^{\frac{n}{2}}\det\left[\frac{\partial\overline{w}(0)}{\partial\overline{w}(\tau)}\right].$$
 (41)

In the last equation we used the expression for the determinant of  $\overline{Q}(t)$ , which can be easily calculated from (38). Furthermore, considering the quantities defined in (24), (31), (32) and (35) we can also obtain the relation,

$$\operatorname{Tr}\left[\widetilde{B}(t)\right] = \operatorname{Tr}\left[\overline{\Theta}^{-1}(t)B(t)\right] = \frac{1}{2}\operatorname{Tr}\left[R_{11}(t) - R_{22}(t)\right].$$
(42)

At last, substituting (41) and (42) into (40), we find the final expression for the semiclassical propagator of N bosons in n modes,

$$K_{sc}(w_f^*, w_i; \tau) = e^{i(S_c+I) - \frac{N}{2} \operatorname{Ln}\left[(1+|w_f^*|^2)(1+|w_i|^2)\right]} \sqrt{\left[\frac{1+\overline{w}(\tau)w(\tau)}{1+\overline{w}(0)w(0)}\right]^{\frac{n}{2}} \operatorname{det}\left[\frac{\partial \overline{w}(0)}{\partial \overline{w}(\tau)}\right]}.$$
 (43)

In the previous equation, we introduced the correction term to the classical action in this quantization scheme,

$$I = \frac{1}{4} \int_{0}^{\tau} \operatorname{Tr}\left[\frac{\partial}{\partial \overline{w}} \left(\overline{\Xi} \frac{\partial \mathcal{H}}{\partial w}\right) + \frac{\partial}{\partial w} \left(\Xi \frac{\partial \mathcal{H}}{\partial \overline{w}}\right)\right] dt.$$
(44)

In comparison with the results for the harmonic-oscillator coherent states, we can also relate the factor under the square root symbol in (43) with a second derivative of the classical action,

$$\left[\frac{1+\overline{w}(\tau)w(\tau)}{1+\overline{w}(0)w(0)}\right]^{\frac{n}{2}}\det\left[\frac{\partial\overline{w}(0)}{\partial\overline{w}(\tau)}\right] = \left[1+w_f^*w(\tau)\right]^{\frac{n}{2}}\left[1+\overline{w}(0)w_i\right]^{\frac{n}{2}}\det\left[\frac{i}{N}\frac{\partial^2 S_c}{\partial w_i \partial w_f^*}\right].$$
 (45)

## **IV. CONCLUSION**

We presented in detail a derivation for the semiclassical propagator in the SU(n) coherent state representation based on previous findings for the multidimensional harmonic-oscillator coherent states. The main advantage of our method is that it can easily be extended to other groups of physical interest. The transformation given by (33), which allows a direct comparison between the SU(n) path integral and the results for the harmonic-oscillator coherent states, enables the immediate calculation of the semiclassical propagator in a phase space with more complex topology. This simple procedure can be readily generalized to a wide range of dynamical groups, thus avoiding an additional laborious derivation of the semiclassical propagator path integral for each new choice of coherent state representation, as usually done in previous publications.<sup>26,35</sup>

Equation (43) has direct application to the dynamical analysis of N bosonic particles in n modes. It is expected that the SU(n) semiclassical propagator provides accurate results, when compared to exact quantum calculations, for sufficiently large values of N. Nevertheless, we can safely suppose that the approximation prescribed by  $K_{sc}$  exceeds significantly the accuracy of mean-field methods, which are usually employed in the treatment of bosonic dynamics, even for a relatively small number of particles. We also expect the semiclassical propagation to be computationally more efficient, in relation to similar quantum calculations, for systems with many degrees of freedom (large values of n). In this case, the computational cost of calculation for the involved classical quantities grows slower with the number of modes than their quantum counterparts.

However, the explicit application of the formula (43) is not a simple task. First, we should note that semiclassical propagator is determined by *boundary-valued* solutions to the equations of motion (23). In general, the analytical or numerical search for these specific trajectories can be quite complicated, particularly in multidimensional and chaotic systems. Another recurrent difficulty in applying semiclassical coherent-state propagators is the appearance of classical trajectories that, although properly satisfying the boundary conditions, do not provide semiclassical propagators endowed with physical meaning.<sup>36–41</sup> The third major problem in the expression for  $K_{sc}$  comes from the factor det  $\left[\frac{\partial \overline{w}(0)}{\partial \overline{w}(\tau)}\right]$ , which happens to diverge at focal points in the variables  $\overline{w}$ .<sup>42</sup> For an example of implementation of the result (43) in a system of physical interest, we refer the reader to a recent work of the present authors,<sup>34</sup> in which we address all the issues mentioned above.

## ACKNOWLEDGMENTS

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#### 052104-11 Semiclassical propagator for SU(*n*) coherent states

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<sup>28</sup> According to the adopted notation, considering a scalar function f(a) and a vector a, we have that  $\frac{\partial f(a)}{\partial a}$  represents the vector whose elements are given by  $\left[\frac{\partial f(a)}{\partial a}\right]_j = \frac{\partial f(a)}{\partial a_j}$ , for j = 1, 2, ..., (n-1).

- <sup>29</sup> Following the adopted notation, considering a scalar function f(a, b) and two arbitrary vectors a and b, we have that  $\frac{\partial^2 f}{\partial a \partial b}$  represents the matrix whose elements are given by  $\left[\frac{\partial^2 f}{\partial a \partial b}\right]_{jk} = \frac{\partial^2 f}{\partial a_j \partial b_k}$ , for j, k = 1, 2, ..., (n-1).
- <sup>30</sup> For two vector quantities a and b, we denote by  $\frac{\partial a}{\partial b}$  the matrix whose elements follow from  $\left[\frac{\partial a}{\partial b}\right]_{jk} = \frac{\partial a_j}{\partial b_k}$ , for  $j, k = 1, 2, \dots, (n-1)$ .
- $^{31}$  The subindex *d* indicates the time discretization of dynamical quantities. Therefore, the omission of this index points out the continuous limit of the corresponding functionals.
- <sup>32</sup> Here, we introduce the notation for the dyadic product between vectors. Considering two arbitrary vectors a and b, the matrix elements of  $a \otimes b$  are given by  $(a \otimes b)_{jk} = a_j b_k$ .
- <sup>33</sup> The error incurred by this approximation is O(1/N) (see Ref. 43). The number of particles N plays the role of  $1/\hbar$  in the harmonic-oscillator coherent-state propagator (see Appendix B of Baranger *et al.* (see Ref. 27)).
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