Off-center coherent-state representation and an application to semiclassics

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By using the overcompleteness of coherent states we find an alternative form of the unit operator for which the ket and the bra appearing under the integration sign do not refer to the same phase-space point. This defines a new quantum representation in terms of Bargmann functions, whose basic features are presented. A continuous family of secondary reproducing kernels for the Bargmann functions is obtained, showing that this quantity is not necessarily unique for representations based on overcomplete sets. We illustrate the applicability of the presented results by deriving a semiclassical expression for the Feynman propagator that generalizes the well-known van Vleck formula and seems to point a way to cope with long-standing problems in semiclassical propagation of localized states.

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I. INTRODUCTION

In addressing a quantum mechanical problem a crucial point is the choice of a convenient representation, which is made operational by its closure relation. These relations may be expressed in a number of ways, e.g., in terms of position eigenstates \{ |x\rangle \}, as an integration in configuration space. It is a common belief that once a basis in the Hilbert space is chosen the representation of the unit operator is unique. However, this is not necessarily true if one deals with overcomplete basis, such as the set of eigenstates \{ |z\rangle \} of the annihilation operator, the so-called canonical coherent states \[.\] Despite the fact that the label \( z \) can take any complex value, a theorem by Cahill \[\] asserts that the kets related to an arbitrary convergent sequence \{ \( z_i \) \} of points in the \( z \)-complex plane (\( \mathbb{C} \)) suffice to generate the space of states. Therefore, we have a large amount of redundancy in the full set and a general state ket \( |\psi\rangle \) may, in principle, be written in different ways in terms of the vectors \{ \( z \) \}. An immediate corollary is that any path in the complex plane enables a complete quantum representation. Examples are the results given in reference \[\], where only the vectors on a circle (\( z = Re^{i\theta} \)) are used to express an arbitrary state; and the line representation \[\], for which only coherent states of vanishing momentum are considered. Nevertheless, in these cases the identity operator is not explicitly expressed. The redundant nature of coherent states can also be made evident by an example which is not encompassed by the theorem of Cahill, namely, the Wigner lattice \( z = \sqrt{\pi}(l + im) \) with \( l \) and \( m \) integers, that constitutes a basis of the Hilbert space. Thus, in principle, the unit operator does not have a unique representation in terms of coherent states.

In this work we shall explore the overcompleteness from a different perspective, namely, by focusing on the fact that the overlap between any two states \( |z'\rangle \) and \( |z''\rangle \) is non-vanishing and finite. In a more technical terminology this means that the reproducing kernel of the coherent-state representation is not a Dirac delta distribution. As we shall see, it is possible to use the full \( z \)-complex plane in a non-standard way, where the operator under the integration sign in the resolution of unity is not the projector \( |z\rangle\langle z| \).

In the next section we give an account of some basic properties of coherent states. In section III we derive an alternative form of the unit operator [see equation (19)], which, in turn, gives rise to a broader way to deal with the analytic representation associated to the coherent states. Basic properties such as general state and operator representations, reproducing kernels and constraints are presented and discussed.

This sort of result may be of use for, at least, two reasons. First, although the final result of a calculation does not depend on which particular representation we use, a convenient choice may lead to a drastic simplification in calculations. Second, and most importantly, approximate results do depend on the particular form of the identity operator used in the intermediate steps. Perhaps the clearest example is the semiclassical evaluation of quantum propagators via the stationary exponent method. In section IV we use the new unit operator to generalize the van Vleck semiclassical expression for the Feynman propagator \( \langle x''|\hat{K}(t)|x'\rangle \). In fact, we obtain a family of semiclassical propagators parameterized by a real number \( \lambda \), of which the van Vleck formula is a particular case (\( \lambda = 1 \)). While the original result involves real classical paths that begin at \( x' \) and end at \( x'' \), we show that complex trajectories may appear in the semiclassical evaluation of a position-position propagator and not only in problems involving Gaussian initial states, as has been reported so far \[\] \[\]. Yet, within the realm of semiclassical approximations, since \( \lambda \) is a continuous parameter, it may be used in variational and optimization processes, although we do not address these issues in the present work. In the appendix we present alternative forms of the unit operator whose application, however, must be made under restricted conditions due to their weak convergence properties.
II. THE CANONICAL COHERENT STATES

The canonical coherent states are the eigenstates of the annihilation operator, \( \hat{a} |z\rangle = z |z\rangle \). All the unusual properties of this basis come from the non-hermiticity of \( \hat{a} \), e.g., the spectral theorem does not apply, neither the eigenvalues are real numbers nor are the eigenvectors mutually orthogonal. In terms of harmonic oscillator eigenstates a normalized coherent state reads

\[
|z\rangle = e^{-\frac{1}{2}|z|^2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} |n\rangle ,
\]

with the complex label \( z \) given by

\[
z = \frac{q}{\sqrt{2b}} + i \frac{bp}{\sqrt{2\hbar}},
\]

\( q \) and \( p \) being the expected values of position and momentum for the state \(|z\rangle\), and \( \sqrt{2b} = \Delta q \) its position uncertainty. The standard way to express the closure relation is in terms of a phase-space integration:

\[
\hat{I} = \int \frac{d^2z}{\pi} |z\rangle \langle z| \equiv \int \frac{dp dq}{2\pi \hbar} |z\rangle \langle z| .
\]

Since all states \(|z\rangle\) are of minimum uncertainty their position representation are given by wave functions that lead to Gaussian probability densities,

\[
\langle x|z\rangle = \frac{1}{\pi^{1/4}\hbar^{1/2}} e^{-\frac{1}{2}(\frac{x-q}{\hbar})^2 + \frac{1}{2}z(z^*)} = \frac{1}{\pi^{1/4}\hbar^{1/2}} e^{-\frac{1}{2} \frac{(x-p)^2}{\hbar^2} + \frac{1}{2}p(p^*)},
\]

with a completely analogous relation holding for the momentum representation \( \langle p,z|\rangle \).

Finally, we briefly refer to the analytic representation associated to the canonical coherent states, the so-called Bargmann representation. In this formalism, a state ket \(|\psi\rangle\) is represented in phase space by its projection onto a non-normalized coherent state \(|z\rangle = e^{\frac{i}{2}|z|^2} |z\rangle\), in terms of which the standard resolution of unit is expressed as

\[
\hat{I} = \int \frac{d^2z}{\pi} e^{-|z|^2} |z\rangle \langle z| .
\]

The state of the system is completely determined by the entire function \( \psi(z^*) = (z|\psi\rangle \), i.e.,

\[
\psi(z^*) = \int \frac{d^2z'}{\pi} e^{-|z'|^2} (z|z'|\langle z'|\psi) = \int \frac{d^2z'}{\pi} e^{-|z'|^2} (z|z')\psi(z'^*) .
\]

The reproducing kernel \( K(z^*,z') = (z|z') = e^{z^* z'} \) plays the role of the delta function in the position and momentum representations. Note, however that the above relation represents an actual constraint to be satisfied by the function \( \psi(z^*) \), which has no parallel in the other mentioned representations. We will describe further developments on the Bargmann representation with the help of the results presented in the next section.

III. OFF-CENTER COHERENT-STATE REPRESENTATIONS

The previous discussion motivates the inspection of the following kind of integral operator

\[
\hat{A} = \int \frac{d^2z}{\pi} \mu(z,z^*) |f(z,z^*)\rangle \langle z| ,
\]

where the integration runs in the whole phase space \((d^2z/\pi = dp dq /2\pi \hbar)\), \( \mu \) is a weighting function, and \( f \) maps points on the complex plane \( C \) to a subset \( D \) of \( C \). It is a key point to realize that \(|f(z,z^*)\rangle\) is itself a coherent state with the same uncertainty in position as \(|z\rangle\), i.e., given an annihilation operator \( \hat{a} \), if \( \hat{a}|z\rangle = z |z\rangle \) then \( \hat{a}|f(z,z^*)\rangle = f(z,z^*)|f(z,z^*)\rangle \), where \( f \) can always be put in the form \( f = Q(q,p) / \sqrt{2b} + ib P(q,p) / \sqrt{2\hbar} \). Note that, for \( f = z \) and \( \mu = 1 \) we get the standard coherent-state closure relation \([43] \).

Due to the mentioned non-vanishing overlap between distinct coherent states, we may hope that it is possible to obtain representations of \( \hat{I} \) for which \( f \neq z \) and, consequently, \( \mu \neq 1 \). In what follows we show that this is indeed the
case by giving the explicit representation of a non-standard identity operator. Because of the non-equality between \( f \) and \( z \) we name this resolution of unity “off-center”. Notice that a definition analogous to equation (7) involving position or momentum eigenstates, for example, could not result in the identity operator.

We recall that for vector spaces of bounded dimension it is a necessary and sufficient condition for the equivalence \( A \equiv I \), that \( \langle i|A|j \rangle = A_{i,j} = \delta_{i,j} \), for all pairs \( i,j \), where \( |i \rangle \) and \( |j \rangle \) belong to a discrete basis \( \{|i\} \) of the Hilbert space. Let \( |\psi \rangle = \sum_i a_i |i \rangle \) be an arbitrary ket, so \( A|\psi \rangle = \sum_i a_i |A_i \rangle \). If \( A_{i,j} = \delta_{i,j} \), then \( \langle j|A|\psi \rangle = \sum_i a_i \langle j|A_i |i \rangle = a_j \). But \( A_{i,j} = \langle j|\psi \rangle \), so \( A|\psi \rangle \) and \( |\psi \rangle \) have the same components in all directions. Therefore \( A|\psi \rangle = |\psi \rangle \) for an arbitrary ket \( |\psi \rangle \), implying \( A \equiv I \). The converse is immediate. For infinite-dimensional spaces \( \langle i|A|j \rangle = \delta_{i,j} \) is certainly a necessary condition, but by no means a sufficient one. In the appendix this will become particularly clear with two explicit examples.

We focus our study on a very simple family of trial operators

\[
\hat{A} = \int \frac{d^2z}{\pi} \mu(z,z^*;\lambda) |\lambda z \rangle \langle z|,
\]

where \( f = \lambda z \), with \( D = C \), \( \lambda \) being a real number. Our task is to find out the weighting function \( \mu \) that turns this expression into the unit operator. Let \( \{|n\} \) be the harmonic oscillator basis associated to the annihilation operator \( \hat{a} \) that defines the set \( \{|z\} \). Note that if \( |\lambda z \rangle \) is a coherent state associated to the same annihilation operator, its expected values of position and momentum are uniquely determined by \( \lambda q = \mu q = \mu p \). Therefore, we have

\[
\langle n|\hat{A}|m \rangle \equiv A_{n,m} = \int \frac{d^2z}{\pi} \mu(z,z^*;\lambda) \langle n|\lambda z \rangle \langle z|m \rangle = \frac{-1}{\sqrt{n!m!}} \int \frac{d^2z}{\pi} \mu e^{-\frac{\lambda}{2}z^2} \lambda^n e^{-\frac{1}{2}|z|^2} \lambda^m z
\]

where we used the relation (11). Writing the above expression in polar coordinates \( z = re^{i\phi} \) we obtain

\[
A_{n,m} = \frac{1}{\sqrt{n!m!}} \int \frac{d\phi dr}{\pi} \mu \lambda^n e^{-\frac{\lambda}{2}(\lambda^2+1)r^2} e^{r(n-m)} = \frac{2\delta_{n,m}}{n!} \int_0^\infty dr \lambda^n e^{-\frac{\lambda}{2}(\lambda^2+1)r^2}.
\]

By writing \( x = \lambda r^2 \), we get

\[
A_{n,m} = \frac{\delta_{n,m}}{\lambda n} \int_0^\infty dx \mu x^n e^{-\frac{1}{2}(\lambda^2+1)x} = \frac{\lambda e^{\frac{1}{2}x} \Gamma(n+1/2)}{\sqrt{\pi} \lambda n!} \int_0^\infty dx \mu x^n e^{-\frac{1}{2}(\lambda^2+1)x},
\]

where the integral converges only if \( \lambda > 0 \). Now, we see that the measure must be given by

\[
\mu = \lambda e^{\frac{1}{2}(\lambda^2+1)} x e^{-x} = \lambda e^{\frac{1}{2}(\lambda^2+1-2\lambda)x},
\]

leading to \( A_{n,m} = \delta_{n,m} \Gamma(n+1)/n! = \delta_{n,m} \). Thus, we conclude that a good candidate to represent the resolution of unity is

\[
\int \frac{d^2z}{\pi} \lambda e^{\frac{1}{2}(\lambda^2-1)|z|^2} |\lambda z \rangle \langle z|,
\]

with \( \lambda > 0 \), for it leads to the correct results whenever convergence is guaranteed. Note that for \( \lambda = 1 \) we obtain equation (3). Now we have to show that the above operator provides a consistent way to calculate the inner product for all vectors in the Hilbert space, that is, we have to demonstrate that

\[
\int \frac{d^2z}{\pi} \lambda e^{\frac{1}{2}(\lambda^2-1)|z|^2} \langle \psi|\lambda z \rangle \langle z|\psi \rangle,
\]

converges to \( \langle \psi|\psi \rangle \) for all vectors \( |\psi \rangle \). Note that once we show that \( \langle \psi|\psi \rangle < \infty \) we have \( \langle \psi|\phi \rangle < \infty \) since \( \langle \psi|\phi \rangle < \langle \psi|\psi \rangle \). In order to give a rigorous proof we will follow arguments similar to the ones given in (4) to validate the standard coherent-state closure relation. Consider the following quantity

\[
\int_0^R \int_0^{2\pi} \frac{d\phi dr}{\pi} \lambda e^{\frac{1}{2}(\lambda^2-1)r^2} \langle \psi|\lambda e^{i\phi} \rangle \langle e^{i\phi}|\psi \rangle.
\]

By using harmonic oscillator closure relations, and the fact that the above integration covers a finite region of phase space, justifying the interchange in the ordering of integrals and sums, one can write it as

\[
\sum_n \int_0^R \int_0^{2\pi} \frac{d\phi dr}{\pi} \lambda e^{\frac{1}{2}(\lambda^2-1)r^2} \frac{\lambda^{n+1} r^{n+m+1}}{\sqrt{n!m!}} e^{-\frac{1}{2}[1+\lambda^2]|z|^2} e^{i\phi(n-m)} \langle \psi|n \rangle \langle m|\psi \rangle
\]

\[
= \sum_n 2 \int_0^R \lambda^{n+1} e^{-\lambda r^2} r^{n+1} n! |\langle n|\psi \rangle|^2 = \sum_n |\langle n|\psi \rangle|^2 \gamma_n,
\]
where $\gamma_n$ can be rewritten as

$$\gamma_n = \frac{2}{n!} \int_0^R dr \, \lambda^{n+1} r^{2n+1} e^{-\lambda r^2} = \frac{1}{n!} \int_0^{\lambda R^2} dx \, x^n \, e^{-x},$$

(17)

with $\lambda > 0$. It is clear that for any positive $\lambda$ and real $R$ we have $0 < \gamma_n < 1$ and $\lim_{R \to \infty} \gamma_n = 1$. Then, we can write

$$\langle \psi|\psi \rangle = \sum_n |(n|\psi)^2 = \sum_n |\langle n|\psi \rangle|^2 \lim_{R \to \infty} \gamma_n = \lim_{R \to \infty} \sum_n |(n|\psi)^2 = \int \frac{d^2 z}{\pi} \, \lambda \, e^{\frac{1}{\lambda}(\lambda z)^2} \langle \psi|\lambda z \rangle \langle z|\psi \rangle,$$

(18)

where we used the fact that $\sum_n |(n|\psi)^2$ is absolutely convergent. This establishes the validity of

$$\hat{I} = \int \frac{d^2 w}{\pi} \, \lambda^{-1} \, e^{\frac{1}{\lambda \lambda^{-1} - 1} (\lambda z)^2} \langle \psi|\lambda z \rangle \langle z|\psi \rangle.$$

(19)

as genuine representations of the unit operator in the whole Hilbert space for $0 < \lambda \leq 1$. This limitation in the range of $\lambda$ is due to the fact that definition (17) is consistent for $\lambda \leq 1$ only. For $\lambda > 1$, the complex number $\lambda z$ associated to the ket in (17) will be outside the integration region (whose boundary is $|z| = R$) for $|z| > R/\lambda$. In order to guarantee that both, the labels of the bra and the ket in integration (17) are inside the integration region for all $r \leq R$ we have to set $0 < \lambda \leq 1$. Furthermore, despite $|\lambda z \rangle \langle z| \neq |z\lambda z \rangle \langle \lambda z|$, the second equality follows immediately from the Hermiticity of the unit operator. Now, it is quite simple to extend our result to $\lambda > 1$. By taking $w = \lambda z$ we get

$$\int \frac{d^2 w}{\pi} \, \lambda^{-1} \, e^{\frac{1}{\lambda \lambda^{-1} - 1} (\lambda z)^2} \langle w|\lambda z \rangle \langle \lambda z|\psi \rangle.$$

(20)

Since $0 < \lambda \leq 1$, we have that $\pi^{-1} \int d^2 w \, \sigma \, e^{\frac{1}{\lambda \lambda^{-1} - 1} (\lambda z)^2} \langle w|\sigma w \rangle$ is valid for $1 < \sigma \leq \infty$ with $\sigma = \lambda^{-1}$. This is exactly relation (19), which is, therefore, valid for any $\lambda > 0$.

Finally, the inner product of two arbitrary vectors and the matrix elements of an operator $\hat{B}$ can be safely written as

$$\langle \phi|\psi \rangle = \int \frac{d^2 z}{\pi} \, \lambda \, e^{\frac{1}{\lambda}(\lambda z)^2} \langle \phi|\lambda z \rangle \langle z|\psi \rangle, \quad \langle z|\hat{B}|z' \rangle = \int \frac{d^2 z}{\pi} \, \lambda \, e^{\frac{1}{\lambda}(\lambda z)^2} \langle z|\lambda z \rangle \langle \lambda z|\psi \rangle,$$

(21)

respectively.

### A. Bargmann Representation: secondary reproducing kernels

Let us analyze how the Bargmann functions are expressed via relation (19), which can also be written as

$$\hat{I} = \int \frac{d^2 z}{\pi} \, \lambda \, e^{-\lambda|z|^2} \langle \lambda z|\psi \rangle.$$

(22)

Then, we can write an arbitrary state as

$$\psi(z^*) = \int \frac{d^2 z'}{\pi} \, \lambda \, e^{-\lambda|z|^2} \langle z|\lambda z \rangle \langle z'|\psi \rangle = \int \frac{d^2 z'}{\pi} \, \lambda \, e^{-\lambda|z|^2} \mathcal{K}(z^*, z^*; \lambda) \psi(z'^*),$$

(23)

where the reproducing kernel of the representation is

$$\mathcal{K}(z^*, z^*; \lambda) = \langle z|\lambda z \rangle \langle \lambda z|z^* \rangle = e^{\lambda z^*z^*}.$$

(24)

By taking $|\psi \rangle = |\lambda z^* \rangle$ in equation (20) we show that $\mathcal{K}$ satisfies its own integral equation, i.e.,

$$\mathcal{K}(z^*, z^*; \lambda) = \int \frac{d^2 z'}{\pi} \, \lambda \, e^{-\lambda|z|^2} \mathcal{K}(z^*, z^*; \lambda) \mathcal{K}(z^*, z'^*; \lambda.$$}

(25)

Once we identified the reproducing kernel by inspection of the last part of equation (24), we now show that $\mathcal{K}$ is not uniquely defined even in the case $\lambda = 1$, in the sense that other phase-space functions also satisfy (23).
The fact that we are dealing with a continuous family of possible representations allows us to write the following differential relation for the kernel

\[ \frac{\partial^N K}{\partial \lambda^N} = (z^*z')^N K. \] (26)

Since the function \( \psi(z^*) \) does not depend on \( \lambda \), we can use relations (23) and (26) to write

\[ \frac{d\psi(z^*)}{d\lambda} = \frac{\psi(z^*)}{\lambda} + \int \frac{d^2 z'}{\pi} \lambda e^{-\lambda |z'|^2} K(z^*, z'; \lambda) z'(z^* - z'^*) \psi(z'^*) = 0, \] (27)

which leads to

\[ \psi(z^*) = -\int \frac{d^2 z'}{\pi} \lambda^2 e^{-\lambda |z|^2} K(z^*, z'; \lambda) z'(z^* - z'^*) \psi(z'^*). \] (28)

Differentiating (27) once again with respect to \( \lambda \) and using (28) we get

\[ \psi(z^*) = \int \frac{d^2 z'}{\pi} \lambda^3 e^{-\lambda |z|^2} K(z^*, z'; \lambda) [z'(z^* - z'^*)]^2 \psi(z'^*). \] (29)

By induction we get the following general relation

\[ \psi(z^*) = \int \frac{d^2 z'}{\pi} \lambda e^{-\lambda |z|^2} K^{(N)}(z^*, z'; \lambda) \psi(z'^*), \] (30)

with

\[ K^{(N)}(z^*, z'; \lambda) = \frac{\lambda^N}{N!} [z'(z'^* - z^*)]^N K(z^*, z'; \lambda), \] (31)

which defines a whole class of reproducing kernels, with \( K^{(0)} = K \). Note, however, that the secondary kernels do not satisfy their own integral equations. This is due to the fact that \( K^{(N)} \) can no longer be represented as an inner product for \( N \neq 0 \). The above relation can be directly derived from the observation that

\[ e^{-\lambda |z|^2} [z'(z'^* - z^*)]^N K(z^*, z'; \lambda) = [z'(z'^* - z^*)]^N K(z^* - z'^*, -z'; \lambda) = (-1)^N \frac{\partial^N K(z^* - z'^*, -z'; \lambda)}{\partial \lambda^N}, \] (32)

where the last equality comes from relation (26). Therefore, we can re-write equation (30) as

\[ \psi(z^*) = \frac{(-1)^N \lambda^{N+1}}{N!} \int \frac{d^2 z'}{\pi} \frac{\partial^N K(z^* - z'^*, -z'; \lambda)}{\partial \lambda^N} \psi(z'^*) = \frac{(-1)^N \lambda^{N+1}}{N!} \frac{\partial^N}{\partial \lambda^N} \int \frac{d^2 z'}{\pi} e^{-\lambda |z|^2} K(z^*, z'; \lambda) \psi(z'^*). \] (33)

By the primary relation (26) we see that the last integral is simply \( \psi(z^*)/\lambda \), which finishes the proof, since \( (-1)^N \lambda^{N+1} \frac{\partial^N}{\partial \lambda^N} = N! \). As a matter of fact, we note that the first equality in the above relation defines a family of reproducing kernels for the uniform measure:

\[ \tilde{K}^{(N)}(z^* - z'^*, -z'; \lambda) = \frac{(-1)^N \lambda^{N+1}}{N!} \frac{\partial^N K(z^* - z'^*, -z'; \lambda)}{\partial \lambda^N}, \] (34)

for any positive \( \lambda \) and \( N = 0, 1, 2, \ldots \). This makes clear that the infinity of ways to represent a reproducing integral equation for a general Bargmann state has its roots in the overcompleteness of coherent states, and not in a non-trivial measure.

IV. GENERALIZATION OF THE VAN-VLECK FORMULA

As an initial application of equation (19) we show that semiclassical results may be quite sensitive to the particular kind of identity operator one employs in the intermediate steps of asymptotic calculations. We start by recalling the van Vleck semiclassical formula for the Feynman propagator \( \langle x''|\hat{K}(t)|x'\rangle \),

\[ \langle x''|\hat{K}(t)|x'\rangle_{\nu V} = \frac{e^{S}}{b\sqrt{2\pi im_{aq}}}, \] (35)
where $S = S(x', x''; t)$ is the action integral of the classical trajectory that starts at $x'$ and ends at $x''$ in a time interval $t$, and $m_{qp}$ is an element of the stability matrix. This matrix specifies how a small rectangular spot in phase space with sides $\delta q_0$ and $\delta p_0$ develops in time, in the linear regime. Explicitly we have

$$\delta q_t = m_{qq} \delta q_0 + \frac{b^2}{\hbar} m_{qp} \delta p_0, \quad \delta p_t = \frac{b}{\hbar} m_{pq} \delta q_0 + m_{pp} \delta p_0.$$  \hfill (36)

In analogy to the exact quantum mechanical relation

$$\langle x''|\hat{K}(t)|x'\rangle = \langle x''|\hat{K}(t)\hat{I}|x'\rangle = \int \frac{d^2 z}{\pi} \langle x''|\hat{K}(t)|z\rangle \langle z|x'\rangle,$$  \hfill (37)

it has been demonstrated that the following semiclassical relation holds

$$\langle x''|\hat{K}(t)|x'\rangle_{VV} = \int \frac{d^2 z}{\pi} \langle x''|\hat{K}(t)|z\rangle_{Heller} \langle z|x'\rangle,$$  \hfill (38)

where we used relation (34) and the Heller thawed approximation that is given by

$$\langle x''|\hat{K}(t)|z\rangle_{Heller} = \frac{\pi^{-1/4} b^{-1/2}}{\sqrt{m_{qq} + im_{qp}}} e^{-\frac{\pi}{b^2}(z'' - q_t)^2} e^{\pm \left[ S + p_t(x'' - q_t) + \frac{1}{2} \xi q_p \right]},$$  \hfill (39)

with $q_t$ and $p_t$ being the final points of the real trajectory that begins at $q$ with momentum $p$, and $\xi = (m_{pp} - im_{pq})/(m_{qq} + im_{qp})$.

Notice that equation (37) was obtained with the use of the standard closure relation (3). In complete analogy to this procedure, if $A$ is the identity operator, one can use relation (4) to write

$$\langle x''|\hat{K}(t)|x'\rangle = \int \frac{d^2 z}{\pi} \mu(z, z^*) \langle x''|\hat{K}(t)|f(z)\rangle \langle f(z)|x'\rangle,$$  \hfill (40)

and define an alternative family of semiclassical propagators from relation (19),

$$\langle x''|\hat{K}(t)|x'\rangle_{sc} = \int \frac{d^2 z}{\pi} \lambda e^{\frac{i}{2}(\lambda - 1)^2 |z|^2} \langle x''|\hat{K}(t)|z\rangle_{Heller} \langle \lambda z|x'\rangle,$$  \hfill (41)

where we used the second line of Eq. (40), which is valid due to the hermiticity of $\hat{I}$. The integral to be calculated can be written as

$$\langle x''|\hat{K}(t)|x'\rangle_{sc} = \frac{\lambda}{b \sqrt{\pi}} \int \frac{dq dp}{2\pi \hbar} \frac{e^{\Gamma(q, p, \lambda)}}{\sqrt{m_{qq} + im_{qp}}},$$  \hfill (42)

where

$$\Gamma(q, p, \lambda) = -\frac{\xi}{2b^2} (x'' - q_t)^2 + \frac{i}{\hbar} \left[ S + p_t(x'' - q_t) + \frac{1}{2} \xi q_p \right]$$

$$-\frac{1}{2} (\lambda^2 + 2\lambda - 1) \frac{q^2}{2b^2} + \frac{1}{2} (\lambda - 1)^2 b^2 p^2 + \frac{i\lambda^2}{2\hbar} q + \frac{\lambda x' - i\lambda x'}{\hbar} - \frac{p - x'^2}{2b^2}.$$  \hfill (43)

Now we evaluate the phase-space integral via the saddle point method. The stationary conditions $\Gamma_q = \partial \Gamma/\partial q = 0$ and $\Gamma_p = \partial \Gamma/\partial p = 0$, after some algebra, lead to

$$\left(1 - \lambda^2\right) \frac{q_0}{\sqrt{2}} + \lambda \frac{(x'' - q_0)}{b} + \frac{1}{m_{qq} + im_{qp}} \frac{(x'' - q_t)}{b} = 0,$$  \hfill (44)

and

$$\left(1 - \lambda^2\right) \frac{q_0}{\sqrt{2}} - \lambda \frac{(x'' - q_0)}{b} + \frac{1}{m_{qq} + im_{qp}} \frac{(x'' - q_t)}{b} = 0,$$  \hfill (45)
where we have to consider the action \( S = S(q_0, q(t), p_0, p(t); t) \) as an implicit function of \( q_0 \) and \( p_0 \) and use the relations \( \partial S/\partial q_0 = -p_0 \) and \( \partial S/\partial p_0 = p_t \). The subscript “0” denotes the stationary point in phase space and \( v_0 \equiv q_0/\sqrt{2b} - ibp_0/\sqrt{2}\hbar \). It must be realized that to obtain the above results, and in the rest of the calculations, we do not take into account variations of \( m_{qq} \), \( m_{qp} \), and \( \xi \) because they already involve second derivatives of the action integral, e. g., \( m_{qp} \propto (\partial^2 S/\partial q_0 \partial q_2)^{-1} \). Otherwise one would get terms with order higher than second (for a detailed discussion of the saddle point method applied to the evaluation of semiclassical propagators see ref. [11]). The previous conditions can be rewritten as

\[
(\lambda - 1)v_0 = \frac{\sqrt{2}}{b} (x' - q_0), \quad \text{and} \quad (\lambda - 1)v_0 = \frac{\sqrt{2}}{m_{qq} + im_{qp}} \frac{(x'' - q_t)}{b},
\]

which make clear that only for \( \lambda = 1 \) we have \( q_0 = x' \) and \( q_t = x'' \), the van Vleck boundary conditions. For other values of \( \lambda \) the classical path that comes from the stationary condition must have, both, complex position and momentum. Note that, in this case, \( v_0 \) does not coincide with \( z_0' = q_0'/\sqrt{2b} - ibp_0'/\sqrt{2}\hbar \). Complex trajectories naturally arise in the semiclassical evaluation of propagators involving coherent states, e. g., \( \langle x|\tilde{K}(t)|z \rangle \) \[3,8\], since a trajectory that begins with momentum \( p \) and position \( q \) and ends at \( x \) is clearly over-specified. We now see that they can also appear in the simpler case of a position-position propagator.

The next step is to expand the exponent around \( q_0 \) and \( p_0 \) up to second order. We write

\[
\Gamma = \Gamma_0 + \frac{b^2}{2} \Gamma_{qq} \dot{Q}^2 + \hbar \Gamma_{qp} \dot{Q} \dot{P} + \frac{\hbar^2}{2b^2} \Gamma_{pp} \dot{P}^2,
\]

where \( \dot{Q} = (q - q_0)/b \) and \( \dot{P} = (p - p_0)/\hbar \), and \( \Gamma_0 \) is the exponent evaluated at the stationary point. The semiclassical propagator becomes

\[
\langle x' | \tilde{K}(t) | x'' \rangle_{sc} = \frac{\lambda}{b\sqrt{\pi}} \frac{e^{\Gamma_0}}{\sqrt{m_{qq} + im_{qp}}} \int \frac{d\tilde{Q} d\tilde{P}}{2\pi} e^{\frac{i}{\hbar} \Gamma_{qq} \tilde{Q}^2 + \hbar \Gamma_{qp} \tilde{Q} \tilde{P} + \frac{\hbar^2}{2b^2} \Gamma_{pp} \tilde{P}^2},
\]

where the second derivatives of \( \Gamma \) read

\[
\Gamma_{qq} = \frac{1}{2b^2} (1 - 2\lambda - \lambda^2) - \frac{1}{b^2} \frac{m_{qq}}{m_{qq} + im_{qp}},
\]

\[
\Gamma_{qp} = \Gamma_{pq} = \frac{i}{2\hbar} (\lambda^2 - 1) \frac{m_{qp}}{\hbar (m_{qq} + im_{qp})},
\]

and

\[
\Gamma_{pp} = \frac{b^2}{2\pi^2} (\lambda - 1)^2 - \frac{i b^2}{\pi^2} \frac{m_{qp}}{m_{qq} + im_{qp}}.
\]

The integral (48) is convergent if the matrix associated to the quadratic form in the exponent has both eigenvalues \( (\sigma_{\pm}) \) with a negative real part. After some algebra we find \( (\sigma_{\pm}) = \lambda [-1 \pm (m_{qq} - im_{qp})/\sqrt{m_{qq}^2 + m_{qp}^2}] \), that satisfy the convergence condition. We get

\[
\langle x' | \tilde{K}(t) | x'' \rangle_{sc} = \frac{\lambda}{b\sqrt{\pi}} \frac{e^{\Gamma_0}}{\sqrt{m_{qq} + im_{qp}}} \frac{1}{\sqrt{2\hbar (\Gamma_{qq} \Gamma_{pp} - \Gamma_{pq}^2)}}.
\]

After some simple manipulations, where we used \( \det[m] = 1 \), one obtains

\[
\langle x' | \tilde{K}(t) | x'' \rangle_{sc} = \frac{e^{\Gamma_0}}{b\sqrt{2\pi im_{qp}}},
\]

which presents a pre-factor that is formally identical to that of the van Vleck expression [33]. The argument of the exponential, however, is quite distinct. With the help of the boundary conditions (46) we get the expression

\[
\Gamma_0 = -\frac{1}{2b^2} (x'^2 - q_0^2) + \frac{1}{b^2} \left( \frac{\lambda + 1}{\lambda - 1} \right) (x' - q_0)^2 - \frac{\xi}{2b^2} (x'' - q_t)^2 + \frac{i}{\hbar} [S + p_t (x'' - q_t)].
\]
The final result is then
\[ \langle x''|\hat{K}(t)|x'\rangle_{sc} = \frac{e^{\text{S}}}{\hbar\sqrt{2\pi m_{qp}}} e^{-\frac{1}{2}\hbar(\lambda^2\xi^2) + \frac{\hbar}{2}(\lambda^2)(x'-q_0)^2 - \frac{\hbar}{2}(x''-q_0)^2 + \frac{\hbar}{2}(x''-q_t)} . \] (55)

In general, the application of the above expression to a particular system provides different results for distinct values of \( \lambda \), all semiclassically valid. There are, however, two exceptions: the free particle and the harmonic oscillator, for which all consistent second order semiclassical expressions must coincide with the exact quantum result. In the next subsection we show this explicitly for the free particle.

It is known that, for a general anharmonic system, the van Vleck formula presents spurious divergences when the classical path passes through a caustic \( (m_{qp} = 0) \). Since in our general expression the classical trajectory itself depends on \( \lambda \), the position and time at which a caustic occurs are also \( \lambda \)-dependent. This suggests that one can construct well behaved semiclassical propagator by combining two or more expressions given by the family (55) with different \( \lambda \)'s, conveniently chosen to avoid caustics. The price to be paid is to deal with complex paths and connection conditions.

A clarification is now in order. It might look awkward to have a semiclassical propagator which depends on a parameter that is neither present in the Hamiltonian of the system nor depends on \( h \). However, we must keep in mind that \( \lambda \) is not a physical parameter but, rather, a mathematical one which is present because of the redundancies associated to the coherent-state representation. Our result gives an explicit example of the fact that, very often, there is an infinity of semiclassical formulas corresponding to the same quantity in quantum mechanics. An already classical example is the two forms of the coherent-state path integral given by Klauder and Skagerstam [1]. In the first form the Hamiltonian that determines the paths is \( H(z^*, z) = \langle z|\hat{H}|z\rangle \), while in the second form it is described by \( h(z^*, z) \), with
\[ \hat{H} = \int \frac{d^2z}{\pi} h(z^*, z) |z\rangle\langle z| \]. (56)

The point is that we find \( H \neq h \) [1], although they coincide in the classical limit, i.e., \( H = H_c + \mathcal{O}(h) \) and \( h = H_c + \mathcal{O}(h) \), where \( H_c \) is the classical Hamiltonian. Besides, the function \( h \) is not unique [1]. Another example is given in [2], where the underlying classical dynamics from which the semiclassical coherent-state propagators are derived is governed by an effective Hamiltonian, whose smoothing parameter is arbitrary and may vary continuously. Therefore, the Hamiltonian operator (even with a specific ordering) present in a quantum propagator does not uniquely determines its semiclassical counterpart.

Before closing this work, we illustrate the use of formula (55) along with the boundary conditions (46) in the simple case of a free particle with mass \( m \). This also serves as a test of consistency for our result, since, for this system, we must obtain the exact quantum propagator for any \( \lambda \). We start with the solutions of the equations of motion \( q_t = q_0 + pt/m \) and \( pt = p_0 \), which lead to the following elements for the stability matrix \( m_{qp} = m_{pp} = 1, m_{qp} = \hbar t/mb^2 \), and \( m_{pq} = 0 \). The action integral is simply given by
\[ S = \int f (pdq - Hdt) = \frac{p_0^2}{2m} \cdot t , \] (57)
where \( H \) is the Hamiltonian function. The solutions of the equations of motion along with equations (46) enable us to write \( q_t, q_0 \), and \( p_0 \) in terms of \( x', x'', \) and \( t \). The results are
\[ q_0 = \frac{1}{2\lambda} \left[ (\lambda + 1)x' + i(\lambda - 1)\frac{mb^2}{\hbar t}(x'' - x') \right] , \] (58)
\[ q_t = \frac{1}{2\lambda} \left\{ (\lambda + 1)x'' + i(\lambda - 1) \left[ \frac{mb^2}{\hbar t}(x'' - x') - \frac{\hbar t}{mb^2} x' \right] \right\} , \] (59)
and
\[ p_t = p_0 = \frac{m}{2\lambda} \left[ (\lambda + 1)(x'' - x') - i(\lambda - 1)\frac{\hbar t}{mb^2} x' \right] . \] (60)
Note that we have \( g_0 = x', \ g_1 = x'' \), and \( p_t = p_0 = m(x'' - x')/t \), for \( \lambda = 1 \). Substituting all these quantities in the general expression for \( \Gamma_0 \), equation (53), we simply get \( \Gamma_0 = \frac{\text{im}(x'' - x')^2}{2\hbar t} \). The final result for the semiclassical propagator of the free particle is independent of \( \lambda \) and reads

\[
\langle x'' | \hat{K}(t) | x' \rangle_{\text{sc}} = \sqrt{\frac{m}{2\pi i\hbar t}} e^{\frac{\text{im}}{\hbar t}(x'' - x')^2},
\]

that coincides with the exact quantum result, as expected. Of course, the use of \( \lambda \neq 1 \) in this very simple case only brings extra complications. The point is that, besides the caustic problem, in situations where it is not easy or even possible to determine the classical paths that satisfy the van Vleck boundary conditions, we expect that an appropriate choice of \( \lambda \) may simplify the problem.

V. CONCLUSIONS AND PERSPECTIVES

In this work we presented an off-center coherent-state identity operator, showing that even when the whole phase space is considered, there is no unique representation for the closure relation in terms of the set \( \{ |z \rangle \} \). This property has enabled the development of an alternative way to express the mathematical quantities involved in the Bargmann representation as well as the derivation of extra conditions that the function \( \psi(z) \) has to meet. As a consequence we found a family of reproducing kernels indexed by one continuous parameter \( \lambda \) and an integer \( N \). The potential applicability of relation (19) was illustrated for a simple example in the field of semiclassics, which may enable the construction of well behaved semiclassical position-position propagators. We note that similar arguments can be used to derive yet another form for the semiclassical Feynman propagator starting from relation (19) and the first line of relation (10). In fact, the sort of procedure we used in section III is far from being exhausted. The same technique can be used to generalize semiclassical approximations involving Gaussian states, e.g., the propagator \( \langle x | \hat{K}(t) | z \rangle \), which is of importance in different fields [11, 13, 15]. For this class of propagators the outcome of the stationary exponent method, without any further approximation, always involves complex trajectories and the root search problem [11, 16, 17]. In this context it would be a major simplification if one could adjust the parameter \( \lambda \) in order to get an initial value representation (IVR), or at least, to simplify the root search problem. Finally, it is also possible to use expression (19) in the direct evaluation of propagators via path integrals, in the spirit of references [7, 11]. Some of these topics are presently under investigation.

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VI. APPENDIX: ALTERNATIVE IDENTITIES WITH CONDITIONAL CONVERGENCE

In this appendix we analyze the extension of equation (19) when \( \lambda \) is allowed to be complex and a further example of “pathological” representation of the unit operator. We stress that in both cases the resulting operators are not unconditionally convergent. If we use a complex \( \lambda \) in the arguments presented in section II, the integration path in (17) is no longer on the real axis and the extension of the initial variable \( r \) into the complex plane would have to be justified. The possible resolution of unit is

\[
\int \frac{d^2z}{\pi} \lambda e^{\frac{i}{2}(\lambda R^2 + 2\lambda^2)|z|^2} |\lambda z \rangle \langle z|,
\]

with \( \text{Re}(\lambda) > 0 \), \( Q = (\lambda + \lambda^*)q/2 + i(\lambda - \lambda^*)b^2p/\hbar \), and \( P = (\lambda + \lambda^*)p/2 - i(\lambda - \lambda^*)\hbar q/b^2 \). The important point is that in analogy to equation (17) we have \( n!\gamma_n = \gamma(n + 1, \lambda R^2) \), where \( \gamma(a, b) \) is the incomplete Gamma function. However, with the complex argument \( \lambda R^2 \), for a given \( n \), we may have values of \( R \) for which \( \text{Re}(\gamma_n) > 1 \). For definiteness take \( n = 0 \) and \( \lambda = e^{i\pi/4} \), by setting \( R^2 = \sqrt{2\pi} \) we get \( \text{Re}(\gamma_n) = 1 + e^{-\pi} \approx 1.04 \). For the arguments presented in the body of the paper (in the case of real \( \lambda \)) to be valid here we should have necessarily \( 0 < \text{Re}(\gamma_n) \leq 1 \). Thus, unconditional convergence is not guaranteed. As an example of successful application of (62), let us consider the modification of an arbitrary squeezed state \( |w \rangle \), with \( w = q'/\sqrt{2B + iBp'/\sqrt{2\hbar}} \). It is easy to show that [7]

\[
\langle w | z \rangle = \sqrt{\frac{2bB}{b^2 + B^2}} e^{-\frac{1}{2}|w|^2 - \frac{1}{2}|z|^2 + \frac{1}{4}(\frac{w^2 + z^2}{b^2 + B^2})(z^2 - w^*z) + \frac{w^2 - z^2}{2b^2 + 2B^2}} e^{\frac{2bB}{b^2 + B^2}w^*z},
\]

where \( n = 0 \) and \( \lambda = e^{i\pi/4} \), by setting \( R^2 = \sqrt{2\pi} \) we get \( \text{Re}(\gamma_n) = 1 + e^{-\pi} \approx 1.04 \). For the arguments presented in the body of the paper (in the case of real \( \lambda \)) to be valid here we should have necessarily \( 0 < \text{Re}(\gamma_n) \leq 1 \). Thus, unconditional convergence is not guaranteed. As an example of successful application of (62), let us consider the modification of an arbitrary squeezed state \( |w \rangle \), with \( w = q'/\sqrt{2B + iBp'/\sqrt{2\hbar}} \). It is easy to show that [7]
Therefore, if one uses identity (62) the inner product becomes
\[
\langle w|w\rangle = \int \frac{d^2 z}{\pi} \chi^2 |(\lambda z^2 + 2\lambda z^2)|^2 \langle \lambda z|\lambda z\rangle \langle z|w\rangle = \frac{2\lambda B}{b^2 + B^2} e^{-|w|^2 - \frac{1}{2} \left( \frac{4\lambda b^2}{(b^2 + B^2)} |w^2 + w'^2| \right)} \mathcal{J},
\]  
(64)
where
\[
\mathcal{J} = \int \frac{d^2 z}{\pi} e^{-\lambda|z|^2 + \frac{\lambda^2}{2} \left( \frac{2\lambda b^2}{b^2 + B^2} |z| + \frac{\lambda^2}{b^2 + B^2} w^2 + w'^2 \right) \mathcal{J}}.
\]  
(65)
whose convergence is guaranteed if \(2\lambda B^2/(b^2 + B^2)\) and \(2\lambda B^2/(b^2 + B^2)\) have both positive real parts, which is equivalent to \(\text{Re}(\lambda) > 0\). This leads to the correct normalization \(|w|w\rangle = 1\) for all values of the squeezing parameter \(B\). Nevertheless, expression (65) is not convergent, e. g., for matrix elements of non-normalizable kets like \(|x'|x\rangle\). In this case we should satisfy the extra condition \(\text{Re}(\lambda) > \text{Im}(\lambda)\), which shows that the convergence is, in general, only conditional.

Now let us address the operator involving a ket that is restricted to the unit circle while the bra runs over the entire phase space:
\[
\hat{A} = \int \frac{d^2 z}{\pi} \mu(z, z^*) |z/|z|| \langle z|z\rangle.
\]  
(66)
We have \(f = e^{i\lambda}(z) = e^{i\varphi}\) with \(D\) being the unit circle. Accordingly, \(Q = q (\langle q^2/2b^2 + b^2p^2/2h^2 \rangle)^{-1/2}\) and \(P = p (\langle q^2/2b^2 + b^2p^2/2h^2 \rangle)^{-1/2}\). We will use once more the harmonic oscillator basis in order to determine the appropriate weighting function. We have
\[
A_{n,m} = \int \frac{d^2 z}{\pi} \mu(z, z^*) \langle n|z/|z|| \langle z|m\rangle = \frac{1}{\sqrt{n!m!}} \int \frac{d^2 z}{\pi} \mu e^{-\frac{1}{2} |z|^2} \left( \frac{z}{|z|} \right)^n e^{-\frac{1}{2} |z|^2} z^m.
\]  
(67)
Passing again to polar coordinates one gets
\[
A_{n,m} = \frac{1}{\sqrt{n!m!}} \int \frac{rd\varphi dr}{\pi} \mu e^{-\frac{1}{2} (r^2 + 1)} r^m e^{i\varphi(n-m)} = \frac{2\delta_{n,m}}{\sqrt{n!m!}} \int_0^\infty dr \mu r^{m+1} e^{-\frac{1}{2} (r^2 + 1)}.
\]  
(68)
By setting \(\mu = \frac{1}{r} e^{\frac{i}{2}(r-1)^2}\), we obtain \(A_{n,m} = \delta_{n,m}\). The possible closure relation is then
\[
\int \frac{d^2 z}{\pi} \frac{1}{2|z|} e^{\frac{i}{2} (|z|-1)^2} \frac{|z/|z|| \langle z|}{\langle z|}.
\]  
(69)
Note that there is no actual singularity since \(d^2 z/|z| = d\varphi dr\) as it is clear from the Bargmann representation
\[
\int \frac{d^2 z}{\pi} \left( \frac{1}{2|z|} e^{-|z|/|z|} |z/|z|| \right) = \int \frac{d\varphi dr}{2\pi} e^{-r} \langle e^{i\varphi}|(re^{i\varphi})\rangle.
\]  
(70)
In showing the unconditional convergence of (13) we defined a quantity, see equation (13), that would correspond in the present case to
\[
\int_0^R \int_0^{2\pi} \frac{d\varphi dr}{2\pi} e^{-r} \langle \psi|e^{i\varphi}\rangle(r e^{i\varphi})|\psi\rangle,
\]  
(71)
which is meaningless in the region \(r < 1\), because \(|e^{i\varphi}|\) always has \(r = 1\). Again, the arguments given in the body of the paper cannot be repeated. In fact, it is quite easy to find well behaved quantities that present spurious divergence when (69) is employed. The reader can easily show that application of (69) to the evaluation of \(\langle w|w\rangle\) yields convergent results only if \(B > b\). Thus, expression (69) has very limited convergence properties and must be seen as a formal result that requires a careful analysis to be used in practice. The convergence of \(\langle \psi|\hat{A}|\psi\rangle\) can be guaranteed only if \(|\psi\rangle\) is given either by a finite superposition of number states or coherent states.

We remark that (69) is not directly related to the circle representation given in (13). In the present case the integration still runs over the whole phase space, only the ket \(|z/|z|| = e^{i\varphi}\) being restricted to the unit circle. Nevertheless, the circle representation can be obtained from our result. More specifically, using relation (69) we can write a Fock state as
\[
|n\rangle = \int \frac{d^2 z}{\pi} \frac{1}{2|z|} e^{\frac{i}{2} (|z|-1)^2} \frac{|z/|z|| \langle z|}{\langle z|} = \frac{e^{i\varphi}}{2\pi |n|!} \int_0^{2\pi} d\varphi \left[ \int_0^\infty dr \frac{r^n e^{-r}}{2\pi |n|!} \right] e^{-in\varphi} |e^{i\varphi}\rangle,
\]  
(72)
So,

\[ |n \rangle = \sqrt{\frac{n!}{2\pi}} \int_0^{2\pi} d\phi \ e^{-in\phi}|e^{i\phi}\rangle, \]

which is the unit circle representation of a number state \[ |3, 12 \rangle. \]

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