Semiclassical propagation of spin-coherent states

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The semiclassical propagation of spin-coherent states is considered in complex phase space. For two time-independent systems, we find the appropriate classical trajectories and show that their combined contributions are able to describe quantum interference with great accuracy. Not only the modulus but also the phase of the quantum propagator, both dynamical and geometric terms combined, are accurately reproduced.

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I. INTRODUCTION

The coherent state path integral for spin systems and its semiclassical approximation have appeared simultaneously [1,2], and since then they have been intensively studied. Solari [3], and independently Kochetov [4,5], have shown the existence of an initially unexpected term that is sometimes called the Solari-Kochetov "extra phase," even though it is usually not a phase. Some important applications of spin path integral were in the study of spin tunneling in the semiclassical limit [6–8], even though initially some considered the method to be inaccurate [9]. Stone *et al.* [10] and also Vieira and Sacramento [11] have derived the spin-coherent state semiclassical propagator in detail, paying particular attention to the Solari-Kochetov correction. This correction is related to the difference between the average value of the Hamiltonian in coherent states and its Weyl symbol [12], and has a counterpart in the canonical case [5,13], which has a flat phase space. The semiclassical description of tunneling was reconsidered recently, using the instanton method [14,15].

Recently, a semiclassical quantization condition for one-dimensional spin systems was derived [16], including the first quantum corrections, in the spirit of the Bohr-Sommerfeld formalism. The same quantization condition was reobtained in [17], where the authors also presented a semiclassical expression for the Husimi functions of stationary states. Semiclassical theories for spin-orbit coupling in connection with trace formulas have appeared [18] and recently received renewed attention [19].

It is interesting to note that the coherent state spin path integral is a natural setting for the investigation of geometric phases [20,21], a topic that has not only a fundamental importance in the mathematical structure of quantum theory [22] but also as an ingredient in the implementation of some quantum information protocols [23]. The semiclassical approximation to the spin propagator $K(z_i,\bar{z}_f,T)=\langle z_f|e^{-iHT/\hbar}|z_i\rangle$ may sometimes lead to an expression of the geometric phase in terms only of classical quantities.

In this work, we present a concrete application of the semiclassical spin propagator. In general, the calculation involves a classical trajectory $(z(t),\bar{z}(t))$ that starts at $z=z_i$ and ends at $\bar{z}=z_f^*$ after a time T. Under these too stringent conditions, the only way to find a classical trajectory is by allowing the variable $\bar{z}(t)$ to be different from the complex conjugate of $z(t)$ [which is denoted by $z^*(t)$]. We must therefore find a trajectory in $\mathbb{C}^2$ that satisfies the boundary conditions $z(0)=z_i$ and $\bar{z}(T)=z_f^*$. This is known as the root-search problem. Similar calculations have already appeared for the canonical coherent states [24], even in chaotic cases [25], but so far no numerical example for a spin system has been presented.

The article is divided as follows. In the next section, the semiclassical theory of the spin-coherent states propagator is briefly reviewed. The geometric phase and the tangent matrix associated with classical trajectories are also presented. In Sec. III, we study the simple system $\hat{H}=\hbar^2\nu J_z^2$, which already has nontrivial properties. In Sec. IV, the less symmetrical Hamiltonian $\hat{H}=\hbar^2\nu[J_z^2+\pi J_x^2]$ is considered, and in Sec. V we present the conclusions.

II. THE SEMICLASSICAL PROPAGATOR

Let $|z\rangle$ denote non-normalized spin-coherent states, defined by

$$|z\rangle = \exp\{zJ_+\}|-j\rangle = \sum_{m=-j}^{j}\binom{2j}{m}^{1/2} z^{j+m}|m\rangle, \tag{1}$$

where the states $|m\rangle$ are the usual spin basis, and let

$$K(z_i,\bar{z}_f,T) = \langle z_f|e^{-i\hat{H}T/\hbar}|z_i\rangle \tag{2}$$

be the quantum propagator, where $\hat{H}$ is the spin Hamiltonian and T is the time. It has been shown that, in the semiclassical limit $j\to\infty$, $\hbar=1/j\to 0$, this can be approximated by [10,11]

$$K_{\rm sc}(z_i,\bar{z}_f,T) = \sum_{\rm c.t.}\left(\frac{i}{\hbar}\frac{e^{iB/\hbar j}}{2j}\frac{\partial^2 S}{\partial z_i\partial\bar{z}_f}\right)^{1/2}\exp\left\{\frac{i}{\hbar}\Phi\right\}, \tag{3}$$

where the sum is over different classical trajectories. The exponent is the classical action S plus an extra term, the Solari-Kochetov (SK) correction,

$$\Phi = S + \mathcal{I}_{\rm SK} = S + \int_0^T A(t)dt. \tag{4}$$

It is well known that this semiclassical approximation is exact if the Hamiltonian belongs to the su(2) algebra [4,5,10,11].

The function A is given by

$$A = \frac{\partial}{\partial \bar{z}} \frac{1}{4g(z,\bar{z})} \frac{\partial H}{\partial z} + \frac{\partial}{\partial z} \frac{1}{4g(z,\bar{z})} \frac{\partial H}{\partial \bar{z}}, \tag{5}$$

where $H(z,\bar{z}) = \langle z|\hat{H}|z\rangle / \langle z|z\rangle$ plays the role of the classical Hamiltonian and the metric factor is

$$g(z,\bar{z}) = \frac{\partial^2}{\partial z \partial \bar{z}} \ln\langle z|z\rangle = \frac{2j}{(1+z\bar{z})^2}. \tag{6}$$

The classical action is given by

$$S = \int_0^T \left[i\hbar j \frac{\bar{z}\dot{z} - \dot{\bar{z}}z}{1+\bar{z}z} - H(z,\bar{z}) \right] dt + \mathcal{B}, \tag{7}$$

where $\mathcal{B} = -i\hbar j \ln\{[1+\bar{z}_f z(T)][1+\bar{z}(0)z_i]\}$ is a boundary term that takes into account the fact that in general $\bar{z}$ is not the complex conjugate of z.

The integrals in Eqs. (4) and (7) are to be calculated along classical trajectories satisfying the Hamilton equations of motion

$$\dot{\bar{z}} = \frac{i}{\hbar} \frac{1}{g(z,\bar{z})} \frac{\partial H}{\partial z}, \quad \dot{z} = -\frac{i}{\hbar} \frac{1}{g(z,\bar{z})} \frac{\partial H}{\partial \bar{z}}, \tag{8}$$

with boundary conditions

$$z(0) = z_i, \quad \bar{z}(T) = z_f^*. \tag{9}$$

Notice that, in general,

$$z(T) \neq z_f, \quad \bar{z}(0) \neq z_i^*. \tag{10}$$

Since $\bar{z}(t) \neq z^*(t)$, the Hamiltonian $H(z,\bar{z})$, the action, and the SK correction will in general all be complex numbers. Therefore, the term $\exp\{i\hbar^{-1}\Phi(z_i,\bar{z}_f,T)\}$ is usually not just a phase.

If the propagator is written as a modulus times a phase, $K(z_i,\bar{z}_f,T) = |K|e^{i\varphi}$, it is well known that φ contains not just the dynamical term, $-i\int_0^T H dt$, but also the geometric (or Berry) phase φ_g, which depends only on the geometry of the path traced by the state in the Hilbert space [20,22]. This was shown by Berry in the context of Hamiltonians depending on slowly varying cyclic parameters, and later generalized in many different ways, in particular to parameter-independent, nonadiabatic, and noncyclic evolutions such as the one considered here [21]. From Eq. (3) we see that in the semiclassical limit the total phase will result from the interference of many classical trajectories, and that each one of them has an individual phase which is the sum of a dynamical term plus a geometric term given by

$$\varphi_p + \frac{1}{\hbar} \mathrm{Re} \left\{ \mathcal{B} + \int_0^T \left[i\hbar j \frac{\bar{z}\bar{z} - \dot{\bar{z}}z}{1+\bar{z}z} + A(t) \right] dt \right\}, \tag{11}$$

where φ_p is a phase coming from the prefactor.

If we set $z_f = z_i$ in the simplest case $\hat{H} = \nu\hbar J_z$, we have $z(t) = e^{-i\nu t} z_i$ and $\bar{z}(t) = e^{i\nu(t-T)} z_i^*$, and there is only one classical trajectory. The stability matrix element $M_{\bar{z}\bar{z}}$ (see below) in this case is simply $e^{i\nu T}$. For the very particular time $T = 2\pi/\nu$ it happens that $\bar{z}(t) = z^*(t)$ and thus $\mathcal{B}$ is purely imaginary. If we use stereographic coordinates $z = e^{i\phi}\tan(\theta/2)$, then it is easy to see that, since A and φ_p both vanish, the geometric phase reduces to the well known result $\varphi = 2\pi j(1-\cos\theta)$. Generically, i.e., if $\hat{H} = \nu\hbar J_z$ but T is not a multiple of the period, or for more general Hamiltonians, the fact that $\bar{z}(t) \neq z^*(t)$ will introduce additional contributions coming from A, φ_p, and $\mathcal{B}$, even for cyclic evolutions. Besides, more than one classical trajectory will be necessary, as we will see in the next sections.

In the study of semiclassical spin tunneling, the relevant classical trajectories are instantons with the remarkable property that $\bar{z}(0) = z_i^*$ and $z(T) = z_f$ [14]. This happens because the initial and final points of the instanton minimize the average value of the Hamiltonian, and in that case the calculation is greatly simplified, leading to analytical results. However, as noted in [15], a more realistic description of the system requires the addition of higher-order terms to the Hamiltonian that destroy this simple property and make it necessary to consider the more generic trajectories we have discussed (which have been called "boundary jump instantons" in [15]).

Note that the action (7), with the necessary boundary term, leads to the following Hamilton-Jacobi relations:

$$\frac{i}{\hbar}\frac{\partial S}{\partial \bar{z}_f} = \frac{2jz(t)}{1+\bar{z}_f z(t)}, \quad \frac{i}{\hbar}\frac{\partial S}{\partial z_i} = \frac{2j\bar{z}(0)}{1+\bar{z}(0)z_i}, \tag{12}$$

$$\frac{\partial S}{\partial t} = -H. \tag{13}$$

Note also that if the Hamiltonian is $O(j)$, then S is $O(j)$, but the SK correction is $O(1)$, and therefore it can be considered small in the semiclassical limit.

The prefactor is related to the tangent matrix, or stability matrix, as follows. Small variations in the boundary points δz_i and $\delta\bar{z}_f$ induce variations $\delta z(T)$ and $\delta\bar{z}(0)$. Taking derivatives of the Hamilton-Jacobi relations (12), it is possible to write

$$\begin{pmatrix} [1+\bar{z}_f z(T)]^{-2}\delta z(T) \\ [1+z_i\bar{z}(0)]^{-2}\delta\bar{z}(0) \end{pmatrix} = \begin{pmatrix} A_{zz} & A_{z\bar{z}} \\ A_{\bar{z}z} & A_{\bar{z}\bar{z}} \end{pmatrix} \begin{pmatrix} \delta z_i \\ \delta\bar{z}_f \end{pmatrix}, \tag{14}$$

where all matrix elements can be written in terms of second derivatives of the action (see [13] for an analogous calculation with canonical coherent states). On the other hand, the tangent matrix of a given trajectory $(z(t),\bar{z}(t))$ is defined as the linear application that takes a small initial displacement to a final displacement,

$$\begin{pmatrix} \delta z(T) \\ \delta\bar{z}_f \end{pmatrix} = \begin{pmatrix} M_{zz} & M_{z\bar{z}} \\ M_{\bar{z}z} & M_{\bar{z}\bar{z}} \end{pmatrix} \begin{pmatrix} \delta z_i \\ \delta\bar{z}(0) \end{pmatrix}. \tag{15}$$

Manipulating Eq. (14), one can show that the element $M_{\bar{z}\bar{z}}$ is related to the prefactor in Eq. (3) according to

$$\frac{i}{\hbar}\frac{\partial^2 S}{\partial z_i \partial\bar{z}_f} = \frac{2j}{[1+z_i\bar{z}(0)]^2}\frac{1}{M_{\bar{z}\bar{z}}}. \tag{16}$$

Since the tangent matrix may be numerically integrated together with the coordinates, this expression is very convenient in practice. The phase φ_p may then be followed dynamically, imposing that $K=1(\varphi_p=0)$ for $T=0$.

In practice, one must find all values of $\bar{z}(0)$ for which $\bar{z}(T)=z_f^*$. Notice that these initial values are implicit functions of the time T, and as such they trace out curves, or "branches," in the $\bar{z}(0)$ plane. There will in general exist more than one branch for each value of T, and one must add all contributions coherently. Note, however, that the contribution of a branch may display an erroneous increase and need to be removed for a certain region of the parameter T, because of a phenomenon that is common in asymptotic expansions known as Stokes' phenomenon [26–29]. A discussion of this problem in the context of the one-dimensional semiclassical propagator may be found in [30]. Stokes' phenomenon will not be relevant to the present work.

From Eq. (16), it is clear that the semiclassical approximation fails in the vicinity of points for which $M_{\bar{z}\bar{z}}(T)=0$, which are called phase-space caustics [25,30,31]. Semiclassical uniform approximations that are valid near caustics have been obtained for the canonical coherent state propagator using a conjugate of the Bargmann representation in [32], and a similar calculation is in principle possible for the spin propagator, but here we shall not be concerned with the effect of caustics.

III. FIRST EXAMPLE, $\hat{H}=\hbar^2\nu J_z^2$

We consider a simple Hamiltonian,

$$H=\hbar^2\nu J_z^2 \tag{17}$$

(the constant ν has the appropriate units), and we shall be interested only in the diagonal propagator

$$K(z_i,T)=\langle z_i|e^{-iHT/\hbar}|z_i\rangle, \tag{18}$$

whose squared modulus, after proper normalization, corresponds to the return probability as a function of time. This is given by

$$K(z_i,T)=\sum_{m=-j}^{j}|\langle m|z_i\rangle|^2 e^{-im^2\hbar\nu T}, \tag{19}$$

which for integer j is periodic with period $T_r=2\pi/\hbar\nu$. In the semiclassical limit, the term that contributes the most to this sum [see Eq. (1)] is $m_0=j(|z_i|^2-1)/(|z_i|^2+1)$. If we linearize the exponent in the vicinity of this term, we have

$$K(z_i,\tau)\approx|\langle m_0|z_i\rangle|^2 e^{-im_0^2\tau}\sum_n e^{-2im_0 n\tau}, \tag{20}$$

where we have introduced a scaled time

$$\tau=\hbar\nu T. \tag{21}$$

Notice that expression (20) has a different time scale, $\tau_c=\pi/m_0$. The quantities T_r and $T_c=\tau_c/\hbar\nu$ are usually called revival time and classical time [33].

Let us turn to the semiclassical approximation, which has been analyzed in some previous works [5,10,11]. The classical Hamiltonian is

$$H=\hbar^2\nu j\left(j-\frac{1}{2}\right)\left(\frac{z\bar{z}-1}{z\bar{z}+1}\right)^2+\frac{\hbar^2\nu j}{2}. \tag{22}$$

The classical equations of motion, $\dot{z}=-i\hbar\nu\omega z$ and $\dot{\bar{z}}=i\hbar\nu\omega\bar{z}$ (here a dot denotes derivative with respect to t), together with the boundary conditions $z(0)=z_i$ and $\bar{z}(T)=z_i^*$, have the simple solutions

$$z(t)=e^{-i\hbar\nu\omega t}z(0),\quad \bar{z}(t)=e^{i\hbar\nu\omega t}\bar{z}(0). \tag{23}$$

Notice that

$$\omega=\frac{2\mu}{j}\left(\frac{z\bar{z}-1}{z\bar{z}+1}\right) \tag{24}$$

is a constant of the motion, where $\mu=j(j-1/2)$. Calculating it at the initial and final points, we have the consistency condition

$$\omega=\frac{2\mu}{j}\left(\frac{e^{-i\omega\tau}|z_i|^2-1}{e^{-i\omega\tau}|z_i|^2+1}\right), \tag{25}$$

which in general has an infinite number of solutions. We come back to that later. Notice also that for $z(0)=z_i$ and $\bar{z}(0)=z_i^*$ the motion is periodic with period $2\pi/\hbar\nu\omega$, which in the semiclassical limit becomes T_c.

The action can be easily found to be

$$\frac{S}{\hbar}=-2ij\ln(1+e^{-i\omega\tau}|z_i|^2)+\tau\left[j\omega+\frac{j^2\omega^2}{4\mu}-\frac{j}{2}\right], \tag{26}$$

and the Solari-Kochetov term is also available,

$$A=\hbar^2\nu\left[\frac{j\omega+\mu}{2j}-\frac{j\omega^2}{8\mu}\right]. \tag{27}$$

To find the prefactor, we consider small variations δz_i and $\delta\bar{z}(0)$. The final value of $\bar{z}$ will be changed according to

$$\bar{z}(\tau)+\delta\bar{z}(\tau)=e^{i(\omega+\delta\omega)\tau}[\bar{z}(0)+\delta\bar{z}(0)]\approx\bar{z}(\tau)+M_{\bar{z}\bar{z}}\delta\bar{z}(0), \tag{28}$$

which leads to

$$M_{\bar{z}\bar{z}}=e^{i\omega\tau}\left[1+\frac{4\mu}{j}\frac{i\tau z_i\bar{z}(0)}{[1+z_i\bar{z}(0)]^2}\right]. \tag{29}$$

There are two different phase-space caustics, which can be found by equating $M_{\bar{z}\bar{z}}=0$. They are located, as functions of the scaled time, along the curves $\bar{z}_\pm(0)=-z_i^{-1}(1+i\tau\pm\sqrt{2i\tau-\tau^2})$. We shall not be concerned here with the effect of caustics.

The problem now is to find the values of $\bar{z}(0)$ for which $\bar{z}(T)=z_i^*$. These points form curves in the plane $\bar{z}(0)$ that we call branches and denote $\bar{z}_\tau(0)$, since they are parametrized by the time. We note again that even for a fixed time there may exist many branches. The method used for finding them was the following: for a fixed value of time, τ_0, a regular grid is placed on the $\bar{z}(0)$ plane, and each point is taken as an initial condition. Those points for which $\bar{z}(\tau_0)$ is close to z_i^* are then used as initial guesses for a root-finding procedure. For $\tau=\tau_0\pm\delta\tau$, the previously obtained solutions serve as ini-

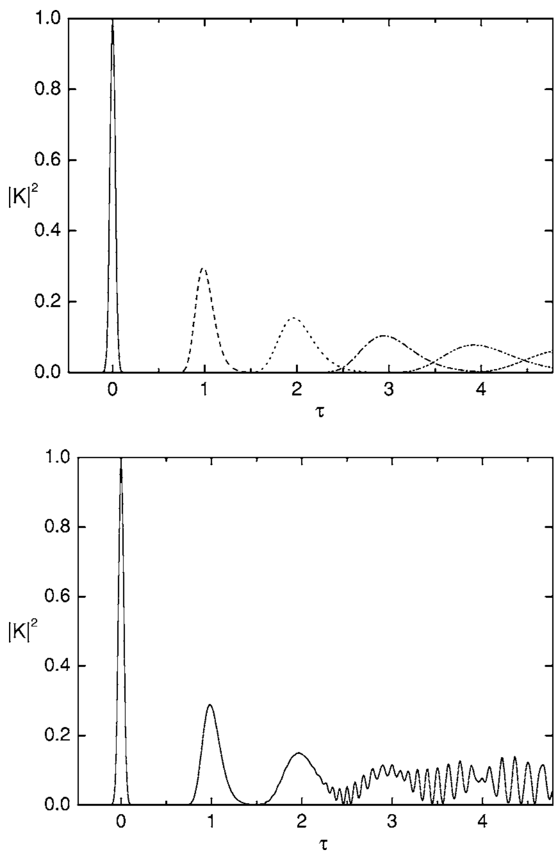

FIG. 1. The normalized propagator as a function of scaled time $\tau = \hbar \nu T$ (in units of the classical period τ_c) for $z_i = 0.5$ and $j = 50$. In (a) we see the separate contributions of six branches (each peak is due to a different branch). When they are added coherently we get (b), which is indistinguishable from the exact result, including the fast oscillations.

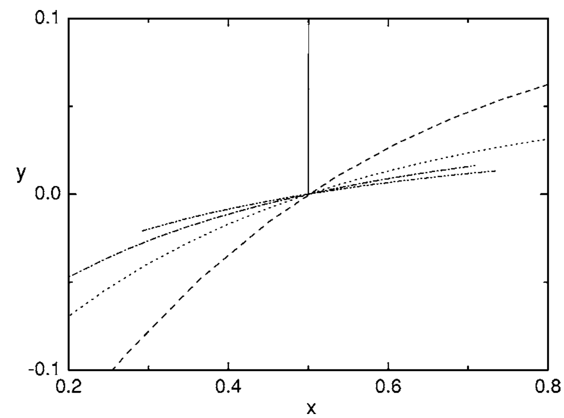

FIG. 2. The different branches in the $\bar{z}(0) = x + iy$ plane contributing to the semiclassical return probability, for the same parameters as in the previous figure (quantities are dimensionless). These curves as parametrized by the time, and each one of them passes through the point (0.5, 0) at a different instant. Only the vicinity of this point is shown, for the sake of visibility.

tial guesses, and no grid is used. This way the branches may be obtained rapidly and exhaustively. Of course the point $\bar{z}(0) = z_i^*$ is a solution for $\tau = 0$, and thus it must be contained in one of the branches.

As an example, let us consider $z_i = 0.5$ and a very semiclassical regime, $j = 50$ (which gives $\hbar = 0.02$). For the time interval of five classical periods, we have found six different branches. The squared modulus of each of their normalized contributions is shown in Fig. 1(a), with different line styles. We see that each peak in the return probability is due to a different branch. The appearance of the classical time scale τ_c, which comes from $m_0 = -30$, is very clear. For $\tau \approx 0$, the branch depicted by the solid line is in the vicinity of the point z_i^*, and as τ approaches the integer multiples of τ_c, each one of the other branches approaches this point, generating a peak in the return probability. The behavior of the different branches can be seen in Fig. 2. After the third peak, the contributions start to overlap, and therefore we must add them coherently to get interference effects. When this is done, the result is as shown in Fig. 1(b). The exact calculation is easy to perform, and it is indistinguishable from the semiclassical one at this scale. Even the fast oscillations for $\tau > 2.5\tau_c$ are reproduced.

When the value of z_i corresponds to a point along the equator of the Bloch sphere, i.e., when $|z_i| = 1$, the calculation may be simplified. In that case, there exists a very particular classical trajectory: the one for which $z(t) = z_i$ and $\bar{z}(t) = z_i^*$. In this case it is easy to see that $\omega = 0$ and there is no movement. Let us call this the static trajectory. Each different value of $\bar{z}_\tau(0)$ determines a certain ω, and the final expression for the normalized propagator is

$$K_{\mathrm{sc}}(z_i,\tau) = \sum_{\omega} \left[1 - \frac{i\tau}{4\mu j}(\omega^2 j^2 - 4\mu^2) \right]^{-1/2} \times \cos^{2j}\left(\frac{\omega\tau}{2}\right) \exp\left\{ \frac{i\tau j}{2} \left(\frac{\omega^2}{2j} + \frac{\mu}{j^2} - 1 \right) \right\}, \quad (30)$$

where we have used Eq. (24) and the fact that $z\bar{z}$ is a constant in time. It is easy to see that each term in this sum [as well as Eq. (25)] is even in ω, and therefore that trajectories must come in pairs. The net effect is that we may search only for ω's with a positive real part, and once a certain trajectory is found its contribution must be doubled, except for the static one, which gives

$$|K_{\mathrm{st}}(z_i,\tau)|^2 = \left[1 + \tau^2 \left(j - \frac{1}{2} \right)^2 \right]^{-1/2}. \quad (31)$$

For short times, we may approximate

$$|K_{\mathrm{st}}(z_i,\tau)|^2 \approx 1 - \frac{\tau^2}{2} \left(j - \frac{1}{2} \right)^2, \quad (32)$$

and comparing this with the exact short-time return probability

$$|K(z_i,\tau)|^2 \approx 1 - (\langle H^2 \rangle - \langle H \rangle^2) T^2/\hbar^2 = 1 - \frac{\tau^2}{2} j \left(j - \frac{1}{2} \right), \quad (33)$$

(where $\langle\ \rangle = \langle z_i | \, | z_i \rangle$), we see that in the semiclassical limit the short-time regime is well described by the static trajectory alone.

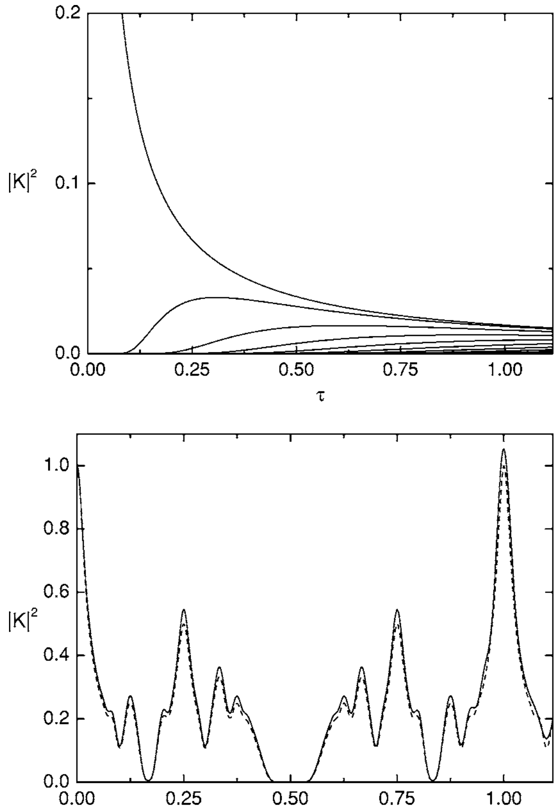

FIG. 3. The normalized propagator as a function of scaled time (in units of τ_r) for $z_i=1$ and $j=10$. In (a) we see the separate contributions of 11 branches (all of them except one must be counted twice, see text). When they are added coherently we get the solid line in (b). The dashed line is the exact result.

As a concrete example, we have considered $z_i=1$ and $j=10$, so that higher-order quantum effects may become more visible. In this case, 11 branches were found that contributed to the final result. Their separate contributions to the normalized propagator can be seen in Fig. 3(a) as functions of time (in units of the revival time τ_r). Because of the even parity in ω, each one of them was considered twice, except for the static one. When we add them coherently, we get the solid line in Fig. 3(b), which is to be compared with the exact result, the dashed line. We see that the latter is reproduced with an extraordinary accuracy, including the quantum revival.

We do not show the branches in the $\bar{z}(0)$ plane, but their behavior is quite simple. The static branch lies in the point $\bar{z}(0)=1$ for all times. For short times, all other branches are at the vicinity of -1, but their contribution to the propagator is negligible. As time passes, they move away from this point and toward 1. The most important thing to note is that all branches have appreciable contributions at the period $\tau=2\pi$, so the phase of the propagator is determined by their coherent superposition and has no simple expression.

Concerning the phase in Eq. (30), notice that it can be written as $i\tau(\omega^2-1)/4$ because μ/j^2-1 is actually equal to $-1/2j$. Since τ is of order $\hbar$, the second term vanishes in the semiclassical limit, but the first one remains because $\omega^2\sim j^2$. However, we have observed numerically that the

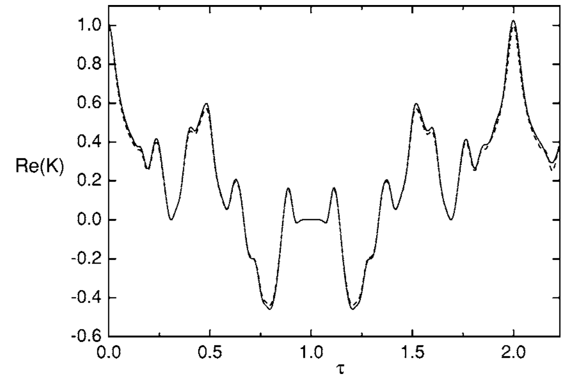

FIG. 4. The semiclassical (solid) and the exact (dashed) calculations of the real part of the normalized propagator, for $z_i=1$ and $j=10$. The imaginary part is also reproduced with great accuracy. Therefore the total phase, dynamical plus geometrical terms, can be recovered from the semiclassical expressions.

factor $e^{-i\tau/4}$, which is common to all branches (and thus has no relevance to the modulus), destroys the correspondence with the exact result. Once this term is removed, which is equivalent to the semiclassically acceptable approximation

$$\mu = j(j-1/2) \approx j^2, \tag{34}$$

the agreement is excellent, as we can see from Fig. 4, where the real part of the normalized propagator is shown (the imaginary part is also very accurate). This approximation must not be done in the prefactor, where we have used $\mu=j(j-1/2)$.

We therefore conclude that expression (3) is able to reproduce both modulus and total phase, dynamical and geometric terms combined, of the quantum propagator with great accuracy in the semiclassical limit. It involves a coherent sum over classical trajectories, and thus it is not possible to extract the geometric phase from it in a closed form. As noted in the previous section, the geometric phase will be given by Eq. (11) only in the simplest cases, when a single classical trajectory is involved. Even then it will in general be different from the simple formula $\int_0^T ijdt(\bar{z}\dot{\bar{z}}-z\dot{\bar{z}})/(1+z\bar{z})$.

Stone *et al.* have analyzed the case $\hat{H}=J_z^2$ in detail [10]. They have shown the formal equivalence of the semiclassical and exact (non-normalized) propagators up to order j^0, and also that for $|z_i|=1$ the result for a massive particle constrained to move on a ring is recovered as $j\rightarrow\infty$. However, in [10] no numerical calculation has been done, and the fact that replacing μ by j^2 in the phase improves the result was not noticed.

IV. SECOND EXAMPLE, $\hat{H}=\hbar^2\nu[J_z^2+\pi J_x^2]$

As a second example, we choose the less symmetrical Hamiltonian $\hat{H}=\hbar^2\nu[J_z^2+\kappa J_x^2]$, which has been considered in [6,11]. We have chosen the irrational value $\kappa=\pi$, in order to avoid too much simplicity. The exact calculation of the return probability can be done by direct diagonalization of the Hamiltonian in the J_z basis. The initial state was taken as a complex number out of the equator, $z_i=1+i$. For very large

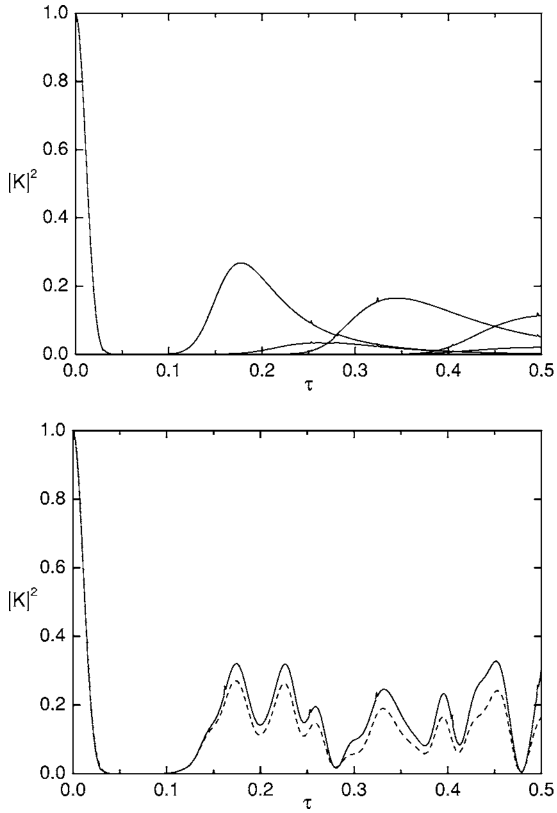

FIG. 5. The normalized propagator as a function of scaled time (in arbitrary units) for $z_i=1+i$ and $j=10$ in the second example. In (a) we see the separate contributions of six branches. When they are added coherently we get the solid line in (b). The dashed line is the exact result.

values of j, the return probability is very similar to what we see in Fig. 1(b), but for more moderate values it is much less regular.

In Fig. 5(a), we see the separate contribution of six branches, each of which has only one peak. This time the classical trajectories, the tangent matrix, the action, and the SK correction all had to be determined through a numerical integration, using the Runge-Kutta method. The coherent superposition of the individual contributions is the solid line in Fig. 5(b), and the dashed line is the exact result. Even though the dynamics does not show any periodicity or regularity in the considered time interval, the semiclassical approximation works very well. Notice that we have used the same scaled time as in the previous example, $\tau=\hbar\nu T$.

The phase of the propagator is again recovered with great precision, as we see in Fig. 6, where the real part of both the semiclassical and the exact calculations is shown (again the imaginary part is reproduced with the same accuracy). This time no approximation of the kind (34) was made to the phase, which was obtained numerically.

V. CONCLUSIONS

A numerical evaluation of the semiclassical spin-coherent state propagator has been presented. We have considered two different systems as examples, namely the quantum rotor$\hat{H}=\hbar^2\nu J_z^2$ and the less symmetrical Hamiltonian $\hat{H}=\hbar^2\nu[J_z^2+\pi J_x^2]$. In the first case, the exact calculation of the return probability is very simple, and is reproduced by the semiclassical one with excellent precision for $j=50$. For the smaller value $j=10$, the accuracy of the approximation is still remarkable.

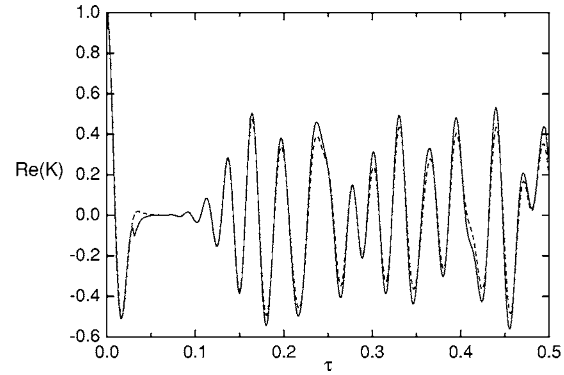

FIG. 6. The semiclassical (solid) and the exact (dashed) calculations of the real part of the normalized propagator, in the same situation as the previous figure. Once again the phase is accurately reproduced.

We have made the numerical observation that a factor $-i\hbar\nu T/4$ must be removed from the semiclassical phase in order to reproduce the exact quantum phase for the rotor (the modulus is not affected). We have no rigorous explanation for this fact, except that this term vanishes in the semiclassical limit and that its removal corresponds to the replacement $j(j-1/2)\rightarrow j^2$. Since phases are defined modulo 2π, we believe this limit must be considered with great care. Since no such adjustment had to be made for the second Hamiltonian studied, we conclude that geometric phases are adequately reproduced by semiclassical calculations. However, they generally do not have a simple closed formula, but result from the interference of many classical paths.

The most important difficulty in the implementation of the semiclassical spin propagator in practice is finding the relevant classical trajectories, i.e., those values of $\bar{z}(0)$ for which the boundary condition at time T is satisfied, $\bar{z}(T)=z_f^*$. We have done this by first propagating for a time T a grid in the $\bar{z}(0)$ plane, thus finding initial rough estimates for the relevant points. These were then used to feed a root-finding procedure. The whole process is rather artisanal and hard to automatize, making it almost impossible to tackle problems in which a large number of trajectories is necessary. The same kind of difficulty is found in the case of canonical coherent states.

Another problem, which we have not considered, is the existence of caustics, initial conditions for which the prefactor diverges at time T. We have seen that for $\hat{H}=\hbar^2\nu J_z^2$ there are two such points, but they did not have any influence in the cases we have analyzed. For systems with higher nonlinearities, it is reasonable to expect a larger number of caustics, which could also hinder the practical application of the semiclassical approximation. In [32], the authors have developed an approach to treat the vicinity of caustics in the canonical coherent states propagator, which makes use of a certain dual of the Bargmann representation. This could in principle be generalized to the spin case.

The main virtue of the semiclassical propagator is its weak dependence on the dimension of the representation, $2j+1$. If this is too large, a direct diagonalization of the Hamiltonian may become impracticable, while the difficulty with the semiclassical method is basically the same. Therefore, an excellent approximation to the exact result, at least for short times, would be easily available.

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