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Semiclassical dynamics of a spin- $\frac{1}{2}$ in an arbitrary magnetic field

Adrian Alscher and Hermann Grabert

Fakultät für Physik, Albert-Ludwigs-Universität, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany

Received 17 March 1999

Abstract. The spin coherent state path integral describing the dynamics of a spin- $\frac{1}{2}$ system in a magnetic field of arbitrary time dependence is considered. Defining the path integral as the limit of a Wiener regularized expression, the semiclassical approximation leads to a continuous minimal action path with jumps at the endpoints. The resulting semiclassical propagator is shown to coincide with the exact quantum mechanical propagator. A nonlinear transformation of the angle variables allows for a determination of the semiclassical path and the jumps without solving a boundary-value problem. The semiclassical spin dynamics is thus readily amenable to numerical methods.

1. Introduction

The path integral representation of a quantum system is very helpful to visualize the quantum dynamics in terms of classical concepts. In particular, spin coherent states allow for a representation of a spin as a point on a unit sphere depicting the dynamics in terms of pseudoclassical spin rotations. Unfortunately, in the standard spin coherent state path integral, the action contains no terms quadratic in the velocities, and the typical paths are therefore not continuous, as it is the case with the familiar Feynman configuration space path integral. This problem has attracted considerable attention of mathematical physicists [1–9]. In most of these studies a spin in a constant magnetic field is considered which allows for an explicit solution. Other work [10–15] allowing for time-dependent fields examines the discrete time-lattice version of the path integral, and it is usually concluded [16, 17] that only formal calculations are possible once the continuous path integral is employed.

Here we re-examine the semiclassical propagator of the continuous time path integral starting from Klauder's observation [1] that a Wiener regularized coherent state path integral for the free spin, that is a spin in the absence of a magnetic field, allows for a well-defined stationary phase approximation that turns out to be exact. We will show that essentially the same type of semiclassical approximation leads to the exact propagator also in the presence of a magnetic field of arbitrary time dependence.

The paper is organized as follows. In section 2 we introduce the basic notation and the spin coherent state path integral for a spin- $\frac{1}{2}$ system. We then present, in section 3, a spherical Wiener measure regularizing the path integral and discuss the semiclassical approximation which is shown to become exact. In section 4 we transform the angle variables to variables that allow for a more effective calculation of semiclassical propagators and calculate the spin coherent propagators for two models. Finally, in section 5, we present our conclusions.

2. Spin coherent state path integral

We consider a spin- $\frac{1}{2}$ described by the spin operators S_i , (i = x, y, z) with the two-dimensional Hilbert space spanned, e.g., by the eigenvectors $|\uparrow\rangle$ and $|\downarrow\rangle$ of S_z . For each orientation in real space characterized by a polar angle ϑ and an azimuthal angle φ we may introduce a spin coherent state [18] (we put $\hbar = 1$)

$$|\Omega\rangle \equiv |\vartheta\varphi\rangle = e^{-i\varphi S_z} e^{-i\vartheta S_y} |\uparrow\rangle.$$
⁽¹⁾

These states are not orthogonal but form an overcomplete basis in the Hilbert space. The overlap of two coherent states reads

$$\langle \Omega'' | \Omega' \rangle = \cos\left(\frac{\vartheta''}{2}\right) \cos\left(\frac{\vartheta'}{2}\right) e^{\frac{i}{2}(\varphi'' - \varphi')} + \sin\left(\frac{\vartheta''}{2}\right) \sin\left(\frac{\vartheta'}{2}\right) e^{-\frac{i}{2}(\varphi'' - \varphi')}$$
(2)

and the identity may be represented as

$$I = \frac{1}{2\pi} \int d\cos(\vartheta) \, d\varphi \, |\Omega\rangle \langle \Omega|.$$
(3)

Furthermore, the matrix elements of the spin operators take the form

$$\begin{split} \langle \Omega''|S_{x}|\Omega'\rangle &= \frac{1}{2} \left[\cos\left(\frac{\vartheta''}{2}\right) \sin\left(\frac{\vartheta'}{2}\right) e^{\frac{i}{2}(\varphi''+\varphi')} + \sin\left(\frac{\vartheta''}{2}\right) \cos\left(\frac{\vartheta'}{2}\right) e^{-\frac{i}{2}(\varphi''+\varphi')} \right] \\ \langle \Omega''|S_{y}|\Omega'\rangle &= \frac{1}{2i} \left[\cos\left(\frac{\vartheta''}{2}\right) \sin\left(\frac{\vartheta'}{2}\right) e^{\frac{i}{2}(\varphi''+\varphi')} - \sin\left(\frac{\vartheta''}{2}\right) \cos\left(\frac{\vartheta'}{2}\right) e^{-\frac{i}{2}(\varphi''+\varphi')} \right] \\ \langle \Omega''|S_{z}|\Omega'\rangle &= \frac{1}{2} \left[\cos\left(\frac{\vartheta''}{2}\right) \cos\left(\frac{\vartheta'}{2}\right) e^{\frac{i}{2}(\varphi''-\varphi')} - \sin\left(\frac{\vartheta''}{2}\right) \sin\left(\frac{\vartheta'}{2}\right) e^{-\frac{i}{2}(\varphi''-\varphi')} \right]. \end{split}$$
(4)

Let us consider a spin in a magnetic field of arbitrary time dependence described by the Hamiltonian

$$H(t) = B_{x}(t)S_{x} + B_{y}(t)S_{y} + B_{z}(t)S_{z}$$
(5)

which gives rise to the unitary time evolution operator

$$U(t) = \mathcal{T}_s \exp\left\{-i\int_0^t ds H(s)\right\}$$
(6)

where T_s is the time-ordering operator. U(t) can be shown to be of the form [19]

$$U(t) = \begin{pmatrix} a(t) & b(t) \\ -b^{*}(t) & a^{*}(t) \end{pmatrix} \qquad |a(t)|^{2} + |b(t)|^{2} = 1$$
(7)

where the coefficients obey the linear differential equations

$$\dot{a}(t) = -\frac{1}{2}B_{z}(t)a(t) + \frac{1}{2}[iB_{x}(t) + B_{y}(t)]b^{*}(t)$$

$$\dot{b}(t) = -\frac{i}{2}B_{z}(t)b(t) - \frac{1}{2}[iB_{x}(t) + B_{y}(t)]a^{*}(t).$$
(8)

Employing a Trotter decomposition, the propagator may be written as

$$\langle \Omega''|U(t)|\Omega'\rangle = \lim_{\epsilon \to 0} \int \prod_{k=1}^{n} \frac{\mathrm{d}\cos\left(\vartheta_{k}\right) \mathrm{d}\varphi_{k}}{2\pi} \prod_{k=0}^{n} \langle \Omega_{k+1}|\mathcal{T}_{s}\exp\left\{-\mathrm{i}\int_{k\epsilon}^{(k+1)\epsilon} \mathrm{d}s \,H(s)\right\} |\Omega_{k}\rangle \tag{9}$$

where $\epsilon = t/n$, $\Omega_0 = \Omega'$, $\Omega_{n+1} = \Omega''$. Now, for $\epsilon \to 0$ we have

$$\langle \Omega_{k+1} | \mathcal{T}_{s} \exp \left\{ -i \int_{k\epsilon}^{(k+1)\epsilon} ds \, H(s) \right\} | \Omega_{k} \rangle = \langle \Omega_{k+1} | \Omega_{k} \rangle \\ \times \left(1 - i\epsilon \frac{\langle \Omega_{k+1} | H(k\epsilon) | \Omega_{k} \rangle}{\langle \Omega_{k+1} | \Omega_{k} \rangle} \right) + O(\epsilon^{2})$$
(10)

and the right-hand side of equation (9) can be expressed as

$$\lim_{\epsilon \to 0} \int \prod_{k=1}^{n} \frac{\mathrm{d}\cos(\vartheta_k) \,\mathrm{d}\varphi_k}{2\pi} \exp\left\{\sum_{k=0}^{n} \left[\log\left\langle\Omega_{k+1}|\Omega_k\right\rangle - \mathrm{i}\epsilon \frac{\left\langle\Omega_{k+1}|H(k\epsilon)|\Omega_k\right\rangle}{\left\langle\Omega_{k+1}|\Omega_k\right\rangle}\right]\right\}$$

With the assumption that for $\epsilon \to 0$ the paths $\Omega(s)$ remain continuous, we may expand the terms in the exponent as

$$\log \langle \Omega_{k+1} | \Omega_k \rangle = \frac{i}{2} \frac{\cos(\vartheta_{k+1}) + \cos(\vartheta_k)}{2} (\varphi_{k+1} - \varphi_k) - \frac{1}{8} [(\vartheta_{k+1} - \vartheta_k)^2 + \sin^2(\vartheta_k)(\varphi_{k+1} - \varphi_k)^2] + O(\delta\Omega^3)$$
(11)

and

$$\epsilon \frac{\langle \Omega_{k+1} | H(k\epsilon) | \Omega_k \rangle}{\langle \Omega_{k+1} | \Omega_k \rangle} = \epsilon \langle \Omega_k | H(k\epsilon) | \Omega_k \rangle + \mathcal{O}(\epsilon \delta \Omega).$$
(12)

While the term of order $\delta \Omega^2$ in equation (11) has the form of the line element on the sphere, this term does not lead to a Wiener measure in the path integral, since there are no factors of ϵ in the denominator. Hence, the assumption of continuous paths is obsolete, and the resulting continuous path integral

$$\langle \Omega''|U(t)|\Omega'\rangle = \int_{(\vartheta',\varphi')}^{(\vartheta'',\varphi'')} \mathcal{D}\cos(\vartheta)\mathcal{D}\varphi\exp\left\{i\int_{0}^{t} ds\left[\frac{1}{2}\cos(\vartheta)\dot{\varphi} - H(\vartheta,\varphi,s)\right]\right\}$$
(13)

where

$$H(\vartheta,\varphi,t) = \langle \Omega | H(t) | \Omega \rangle$$

= $\frac{1}{2} [B_x(t) \sin(\vartheta) \cos(\varphi) + B_y(t) \sin(\vartheta) \sin(\varphi) + B_z(t) \cos(\vartheta)]$ (14)

has only formal meaning.

3. Wiener regularization and semiclassical approximation

Following Klauder [1] the ill-defined path integral (13) can be turned into a meaningful expression if the propagator is written as

$$\langle \Omega''|U(t)|\Omega'\rangle = \lim_{\nu \to \infty} \int d\mu_{W} \exp\left\{ i \int_{0}^{t} ds \left[\frac{1}{2} \cos(\vartheta) \dot{\varphi} - H(\vartheta, \varphi, s) \right] \right\}$$
(15)

where

$$d\mu_{\rm W} = N \prod_{s=0}^{t} d\cos(\vartheta(s)) \, d\varphi(s) \, \exp\left\{-\frac{1}{4\nu} \int_{0}^{t} ds \left[\dot{\vartheta}^{2} + \sin^{2}(\vartheta)\dot{\varphi}^{2}\right]\right\}$$
(16)

is a Wiener measure on the unit sphere which enforces that only continuous Brownian motion paths contribute to the path integral. This amounts to replacing the action of the spin by

$$S_{\nu}[\Omega(s)] = \int_0^t \mathrm{d}s \,\left\{ \frac{\mathrm{i}}{4\nu} [\dot{\vartheta}^2 + \sin^2(\vartheta)\dot{\varphi}^2] + \frac{1}{2}\cos(\vartheta)\dot{\varphi} - H(\vartheta,\varphi,s) \right\}. \tag{17}$$

In the limit $\nu \to \infty$, the ν -dependent terms in the action vanish, and the previous expression (13) is formally recovered.

Let us now investigate the semiclassical approximation of the path integral. For finite ν the Euler–Lagrange equations following from the action (17) read

$$\frac{1}{2}\sin(\vartheta)\dot{\varphi} + \frac{\partial H}{\partial\vartheta} = -\frac{i}{2\nu}[\ddot{\vartheta} - \sin(\vartheta)\cos(\vartheta)\dot{\varphi}^2]$$

$$\frac{1}{2}\sin(\vartheta)\dot{\vartheta} - \frac{\partial H}{\partial\varphi} = \frac{i}{2\nu}[\sin^2(\vartheta)\ddot{\varphi} + 2\sin(\vartheta)\cos(\vartheta)\dot{\vartheta}\dot{\varphi}].$$
(18)

For given boundary conditions $\Omega(0) = \Omega' \equiv (\vartheta', \varphi'), \Omega(t) = \Omega'' \equiv (\vartheta'', \varphi'')$ and $t \gg 1/\nu$, these equations have for small and intermediate times $s(s \ll t - 1/\nu)$ a solution of the form

$$\cos(\vartheta(s)) = \cos(\bar{\vartheta}(s)) + [\cos(\vartheta') - \cos(\bar{\vartheta}')]e^{-\nu s}$$
⁽¹⁹⁾

and

$$\varphi(s) = \bar{\varphi}(s) + \varphi' - \bar{\varphi}' + \frac{i}{2} \log \left[\frac{1 + \cos(\vartheta')}{1 - \cos(\vartheta')} \right] \\ - \frac{i}{2} \log \left[\frac{1 + \cos(\bar{\vartheta}') + (\cos(\vartheta') - \cos(\bar{\vartheta}'))e^{-\nu s}}{1 - \cos(\bar{\vartheta}') - (\cos(\vartheta') - \cos(\bar{\vartheta}'))e^{-\nu s}} \right]$$
(20)

while for intermediate and large times $s(s \gg 1/\nu)$ the solution becomes

$$\cos(\vartheta(s)) = \cos(\bar{\vartheta}(s)) + [\cos(\vartheta'') - \cos(\bar{\vartheta}'')]e^{-\nu(t-s)}$$
(21)

)

and

$$\varphi(s) = \bar{\varphi}(s) + \varphi'' - \bar{\varphi}'' - \frac{i}{2} \log \left[\frac{1 + \cos(\vartheta'')}{1 - \cos(\vartheta'')} \right] + \frac{i}{2} \log \left[\frac{1 + \cos(\bar{\vartheta}'') + (\cos(\vartheta'') - \cos(\bar{\vartheta}''))e^{-\nu(t-s)}}{1 - \cos(\bar{\vartheta}'') - (\cos(\vartheta'') - \cos(\bar{\vartheta}''))e^{-\nu(t-s)}} \right].$$

$$(22)$$

Here, $\bar{\Omega}(s) \equiv (\bar{\vartheta}(s), \bar{\varphi}(s))$ is a solution of the classical equations of motion

$$\frac{1}{2}\sin(\bar{\vartheta})\dot{\bar{\varphi}} = -\frac{\partial H}{\partial\bar{\vartheta}}$$

$$\frac{1}{2}\sin(\bar{\vartheta})\dot{\bar{\vartheta}} = \frac{\partial H}{\partial\bar{\varphi}}$$
(23)

with the boundary conditions $\overline{\Omega}(0) = \overline{\Omega}' \equiv (\overline{\vartheta}', \overline{\varphi}')$ and $\overline{\Omega}(t) = \overline{\Omega}'' \equiv (\overline{\vartheta}'', \overline{\varphi}'')$. Note that the solutions (19) and (20) describe a jump within the time interval $1/\nu$ from the initial state Ω' to the starting point $\overline{\Omega}'$ of the classical trajectory (23). Likewise, for *s* near *t*, the solution (21) and (22) describes a jump from the endpoint $\overline{\Omega}''$ of the classical trajectory to the final state Ω'' . Now, in order that the short-time and long-time solutions coincide for intermediate times $1/\nu \ll s \ll t - 1/\nu$, the boundary conditions of the classical path must obey the relations

$$\tan\left(\frac{\bar{\vartheta}'}{2}\right)e^{i\bar{\varphi}'} = \tan\left(\frac{\vartheta'}{2}\right)e^{i\varphi'}$$
(24)

$$\tan\left(\frac{\bar{\vartheta}''}{2}\right)e^{-i\bar{\varphi}''} = \tan\left(\frac{\vartheta''}{2}\right)e^{-i\varphi''}.$$
(25)

This determines the size of the jumps of the semiclassical trajectory near the endpoints.

Inserting the semiclassical path (19)–(22) into the action S_{ν} and taking the limit $\nu \to \infty$ one finds

$$\exp\{iS_{\rm cl}[\Omega(s)]\} = \sqrt{\frac{\sin(\vartheta')\sin(\vartheta'')}{\sin(\bar{\vartheta}')\sin(\bar{\vartheta}'')}} \exp\left\{i\int_0^t ds \left[\frac{1}{2}\cos(\bar{\vartheta})\dot{\bar{\varphi}} - H(\bar{\vartheta},\bar{\varphi},s)\right]\right\}.$$
 (26)

Klauder has shown that for $H(\Omega) = 0$ the expression (26) coincides with the overlap $\langle \Omega'' | \Omega' \rangle$, so that this 'dominant stationary phase approximation' [1] without fluctuations becomes exact for a free spin. In general, for a non-vanishing Hamiltonian, Klauder has concluded that (26) 'cannot be expected to provide the correct result by itself'. In fact, in later work [3] he has suggested a different definition of the spin coherent path integral. However, we will prove now that for any Hamiltonian H(t) the exact propagator is given by

$$\langle \Omega'' | U(t) | \Omega' \rangle = \exp\{ i S_{cl}[\Omega(s)] \}.$$
⁽²⁷⁾

First we rewrite the overlap between the initial state and the starting point of the classical trajectory as

$$\begin{split} \langle \bar{\Omega}' | \Omega' \rangle &= \cos\left(\frac{\bar{\vartheta}'}{2}\right) \cos\left(\frac{\vartheta'}{2}\right) e^{\frac{i}{2}(\bar{\varphi}'-\varphi')} + \sin\left(\frac{\bar{\vartheta}'}{2}\right) \sin\left(\frac{\vartheta'}{2}\right) e^{-\frac{i}{2}(\bar{\varphi}'-\varphi')} \\ &= \frac{\sqrt{\sin(\vartheta')\sin(\bar{\vartheta}')} \left[1 + \tan\left(\frac{\bar{\vartheta}'}{2}\right)\tan\left(\frac{\vartheta'}{2}\right) e^{-i(\bar{\varphi}'-\varphi')}\right]}{\sqrt{4\tan\left(\frac{\bar{\vartheta}'}{2}\right)\tan\left(\frac{\vartheta'}{2}\right) e^{-i(\bar{\varphi}'-\varphi')}}}. \end{split}$$
(28)

Making use of the jump condition (24), this overlap can be expressed as

$$\langle \bar{\Omega}' | \Omega' \rangle = \sqrt{\frac{\sin(\vartheta')}{\sin(\bar{\vartheta}')}}.$$
(29)

Likewise, from (25) we find for the jump at the endpoint

$$\langle \Omega'' | \bar{\Omega}'' \rangle = \sqrt{\frac{\sin(\vartheta'')}{\sin(\bar{\vartheta}'')}}.$$
(30)

Therefore, we have from equation (26)

$$\exp\{iS_{\rm cl}[\Omega(s)]\} = \langle \Omega''|\bar{\Omega}''\rangle \exp\left\{i\int_0^t ds \left[\frac{1}{2}\cos(\bar{\vartheta})\dot{\bar{\varphi}} - H(\bar{\vartheta},\bar{\varphi},s)\right]\right\} \langle \bar{\Omega}'|\Omega'\rangle. \tag{31}$$

Now, the time evolution operator (7) acts on a coherent state (1) as

$$U(t)|\Omega\rangle = \left[\cos\left(\frac{\vartheta}{2}\right)e^{-\frac{i}{2}\varphi}a(t) + \sin\left(\frac{\vartheta}{2}\right)e^{\frac{i}{2}\varphi}b(t)\right]|\uparrow\rangle$$
$$+ \left[-\cos\left(\frac{\vartheta}{2}\right)e^{-\frac{i}{2}\varphi}b^{*}(t) + \sin\left(\frac{\vartheta}{2}\right)e^{\frac{i}{2}\varphi}a^{*}(t)\right]|\downarrow\rangle. \tag{32}$$

Apart from a phase factor, the right-hand side is again a spin coherent state of the form (1). Hence,

$$U(t)|\Omega\rangle = \exp\{i\Phi(t)\}|\Omega(t)\rangle$$
(33)

where $\Omega(t)$ follows from equation (32) as

$$\vartheta(t) = \arccos\{[|a(t)|^2 - |b(t)|^2]\cos(\vartheta) + [a^*(t)b(t)e^{i\varphi} + b^*(t)a(t)e^{-i\varphi}]\sin(\vartheta)\}$$
and
(34)

$$\varphi(t) = -\frac{i}{2} \log \left\{ \frac{a^*(t)b^*(t) - 2[a^*(t)^2 e^{i\varphi} - b^*(t)^2 e^{-i\varphi}] \tan(\vartheta)}{a(t)b(t) - 2[a(t)^2 e^{-i\varphi} - b(t)^2 e^{i\varphi}] \tan(\vartheta)} \right\}$$
(35)

and where the phase takes the form

$$\Phi(t) = \frac{1}{2}\varphi(t) - \frac{i}{2}\log\left[\frac{a(t)\cos(\frac{\vartheta}{2})e^{-i\varphi} + b(t)\sin(\frac{\vartheta}{2})}{a^*(t)\cos(\frac{\vartheta}{2}) + b^*(t)\sin(\frac{\vartheta}{2})e^{-i\varphi}}\right].$$
(36)

In this way we obtain in the spin coherent representation

$$\begin{split} \langle \Omega''|U(t)|\Omega'\rangle &= a(t)\cos\left(\frac{\vartheta''}{2}\right)\cos\left(\frac{\vartheta'}{2}\right)e^{\frac{i}{2}(\varphi''-\varphi')} + a^*(t)\sin\left(\frac{\vartheta''}{2}\right)\sin\left(\frac{\vartheta'}{2}\right)e^{-\frac{i}{2}(\varphi''-\varphi')} \\ &+ b(t)\cos\left(\frac{\vartheta''}{2}\right)\sin\left(\frac{\vartheta'}{2}\right)e^{\frac{i}{2}(\varphi''+\varphi')} - b^*(t)\sin\left(\frac{\vartheta''}{2}\right)\cos\left(\frac{\vartheta'}{2}\right)e^{-\frac{i}{2}(\varphi''+\varphi')}. \end{split}$$
(37)

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Next, let us show that $\Omega(t)$ is a solution of the classical equations of motion (23) with initial condition $\Omega(0) = \Omega$. Inserting equation (8) for the time derivatives of the coefficients a(t) and b(t) we find

$$\frac{\partial \cos(\vartheta(t))}{\partial t} = \frac{i}{2} B_x(t) \{ 2[a^*(t)b^*(t) - a(t)b(t)] \cos(\vartheta) - [a^*(t)^2 + b(t)^2] \sin(\vartheta)e^{i\varphi} + [a(t)^2 + b^*(t)^2] \sin(\vartheta)e^{-i\varphi} \} + \frac{1}{2} B_y(t) \{ 2[a^*(t)b^*(t) + a(t)b(t)] \cos(\vartheta) - [a^*(t)^2 - b(t)^2] \sin(\vartheta)e^{i\varphi} - [a(t)^2 - b^*(t)^2] \sin(\vartheta)e^{-i\varphi} \}.$$
(38)

Now, using equations (34) and (35), the right-hand side simplifies to give

$$\frac{\partial \cos(\vartheta(t))}{\partial t} = B_x(t)\sin(\vartheta(t))\sin(\varphi(t)) - B_y(t)\sin(\vartheta(t))\cos(\varphi(t)).$$
(39)

In the same way one derives

$$\frac{\partial\varphi(t)}{\partial t} = -B_x(t)\frac{\cos(\varphi(t))}{\tan(\vartheta(t))} - B_y(t)\frac{\sin(\varphi(t))}{\tan(\vartheta(t))} + B_z(t).$$
(40)

The equations (39) and (40) are readily shown to coincide with the equations of motion (23). Hence, the time evolution of the labels $\Omega(t)$ is purely classical.

The phase $\Phi(t)$ in equation (33) may be expressed in classical terms as well. In order to do so, let us make use of the Schrödinger equation for the operator U(t). Since $\frac{\partial}{\partial t}U(t) = -iH(t)U(t)$, we find from equation (33)

$$\left\langle \Omega(t) \left| \frac{\partial}{\partial t} \right| \Omega(t) \right\rangle = -i \frac{\partial \Phi(t)}{\partial t} - i \langle \Omega | H(t) | \Omega \rangle.$$
(41)

This gives

$$\Phi(t) = \int_0^t ds \left\langle \Omega(s) \left| i \frac{\partial}{\partial s} - H(s) \right| \Omega(s) \right\rangle$$

=
$$\int_0^t ds \left[\frac{1}{2} \cos(\vartheta) \dot{\varphi} - H(\vartheta, \varphi, s) \right]$$
(42)

where the right-hand side is just the classical action. Since $\overline{\Omega}'' = \overline{\Omega}'(t)$, we have from equations (33) and (42)

$$U(t)|\bar{\Omega}'\rangle = \exp\left\{i\int_0^t ds \left[\frac{1}{2}\cos(\bar{\vartheta})\dot{\bar{\varphi}} - H(\bar{\vartheta},\bar{\varphi},s)\right]\right\}|\bar{\Omega}''\rangle.$$
(43)

Now, we are in the position to rewrite the semiclassical propagator (26). Combining equations (29), (30) and (43) we find

$$\exp\{iS_{cl}[\Omega(s)]\} = \langle \Omega'' | \bar{\Omega}'' \rangle \langle \bar{\Omega}'' | U(t) | \bar{\Omega}' \rangle \langle \bar{\Omega}' | \Omega' \rangle.$$
(44)

On the other hand, using equation (43) one obtains

$$\langle \Omega | U(t) | \bar{\Omega}' \rangle = \langle \Omega | \bar{\Omega}'' \rangle \langle \bar{\Omega}'' | U(t) | \bar{\Omega}' \rangle.$$
(45)

Likewise, with $U(t) = U(-t)^{\dagger}$ one finds

$$\langle \bar{\Omega}'' | U(t) | \Omega \rangle = \langle \bar{\Omega}'' | U(t) | \bar{\Omega}' \rangle \langle \bar{\Omega}' | \Omega \rangle$$
(46)

and equation (44) finally becomes

$$\exp\{iS_{\rm cl}[\Omega(s)]\} = \langle \Omega'' | U(t) | \Omega' \rangle. \tag{47}$$

This shows that the dominant stationary phase approximation gives the exact spin propagator.

To elucidate this point further, we demonstrate that the semiclassical propagator obeys the Schrödinger equation. From equation (26) we find for the time rate of change

$$\frac{\partial}{\partial t} \exp\{iS_{cl}[\Omega(s)]\} = \frac{1}{2} \left\{ \frac{\cos(\bar{\vartheta}')}{\sin^{2}(\bar{\vartheta}')} \frac{\partial\cos(\bar{\vartheta}')}{\partial t} + \frac{\cos(\bar{\vartheta}'')}{\sin^{2}(\bar{\vartheta}'')} \frac{\partial\cos(\bar{\vartheta}'')}{\partial t} + i\cos(\bar{\vartheta}'') \frac{\partial\bar{\varphi}(s,t)}{\partial s} \right|_{s=t} - 2iH(\bar{\vartheta}'',\bar{\varphi}'',t) + i\int_{0}^{t} ds \left[-\sin(\bar{\vartheta}(s,t)) \frac{\partial\bar{\vartheta}(s,t)}{\partial t} \frac{\partial\bar{\varphi}(s,t)}{\partial s} + \cos(\bar{\vartheta}(s,t)) \frac{\partial^{2}\bar{\varphi}(s,t)}{\partial t\partial s} - 2\frac{\partial H}{\partial\bar{\vartheta}} \frac{\partial\bar{\vartheta}(s,t)}{\partial t} - 2\frac{\partial H}{\partial\bar{\varphi}} \frac{\partial\bar{\varphi}(s,t)}{\partial t} \right] \exp\{iS_{cl}[\Omega(s)]\}.$$
(48)

Now, the jump conditions (24) and (25) give

$$\cos(\bar{\vartheta}') = \frac{[1 + \cos(\vartheta')]e^{2i\bar{\varphi}'} - [1 - \cos(\vartheta')]e^{2i\varphi'}}{[1 + \cos(\vartheta')]e^{2i\bar{\varphi}'} + [1 - \cos(\vartheta')]e^{2i\varphi'}}$$
(49)

and a similar relation for $\cos(\bar{\vartheta}'')$. These relations can be used to re-write the first two terms on the right-hand side of equation (48) as

$$\frac{\cos(\bar{\vartheta}')}{\sin^2(\bar{\vartheta}')}\frac{\partial\cos(\bar{\vartheta}')}{\partial t} = i\cos(\bar{\vartheta}')\frac{\partial\bar{\varphi}'}{\partial t}$$
(50)

and

$$\frac{\cos(\bar{\vartheta}'')}{\sin^2(\bar{\vartheta}'')}\frac{\partial\cos(\bar{\vartheta}'')}{\partial t} = -i\cos(\bar{\vartheta}'')\frac{\partial\bar{\varphi}''}{\partial t}.$$
(51)

Then, after an integration by parts, equation (48) becomes

$$\frac{\partial}{\partial t} \exp\{iS_{cl}[\Omega(s)]\} = \left\{ i \int_{0}^{t} ds \left[\frac{1}{2} \sin[\bar{\vartheta}(s,t)] \frac{\partial \vartheta(s,t)}{\partial s} - \frac{\partial H}{\partial \bar{\varphi}} \right] \frac{\partial \bar{\varphi}(s,t)}{\partial t} - i \int_{0}^{t} ds \left[\frac{1}{2} \sin[\bar{\vartheta}(s,t)] \frac{\partial \bar{\varphi}(s,t)}{\partial s} + \frac{\partial H}{\partial \bar{\vartheta}} \right] \frac{\partial \bar{\vartheta}(s,t)}{\partial t} - i H(\bar{\vartheta}'', \bar{\varphi}'', t) \right\} \\ \times \exp\{iS_{cl}[\Omega(s)]\}.$$
(52)

Therefore, with the equations of motions (23), we obtain the Schrödinger equation

$$\frac{\partial}{\partial t} \exp\{iS_{\rm cl}[\Omega(s)]\} = -iH(\bar{\vartheta}'', \bar{\varphi}'', t) \exp\{iS_{\rm cl}[\Omega(s)]\}.$$
(53)

Note that the matrix element of the Hamiltonian at the endpoint $\overline{\Omega}''$ of the classical trajectory generates the time rate of change of the semiclassical propagator and not the matrix element at the final state Ω'' . The semiclassical propagator may thus be written as

$$\exp\{\mathrm{i}S_{\mathrm{cl}}[\Omega(s)]\} = \exp\left\{-\mathrm{i}\int_{0}^{t}\mathrm{d}s\,H(\bar{\vartheta}''(s),\bar{\varphi}''(s),s)\right\}\langle\Omega''|\Omega'\rangle.\tag{54}$$

To demonstrate that the Schrödinger equation (53) generates the exact quantum dynamics, we start from the equation of motion of U(t)

$$\frac{\partial}{\partial t} \langle \Omega'' | U(t) | \Omega' \rangle = -i \langle \Omega'' | H(t) U(t) | \Omega' \rangle.$$
(55)

In view of (45) we have

$$\langle \Omega''|H(t)U(t)|\Omega' \rangle = \langle \Omega''|H(t)|\bar{\Omega}'' \rangle \langle \bar{\Omega}''|U(t)|\Omega' \rangle = \frac{\langle \Omega''|H(t)|\bar{\Omega}'' \rangle}{\langle \Omega''|\bar{\Omega}'' \rangle} \langle \Omega''|U(t)|\Omega' \rangle$$
(56)

where the first factor in the second line can also be written as

$$\frac{\langle \Omega''|H(t)|\Omega''\rangle}{\langle \Omega''|\bar{\Omega}''\rangle} = \langle \bar{\Omega}''|H(t)|\bar{\Omega}''\rangle = H(\bar{\vartheta}'',\bar{\varphi}'',t).$$
(57)

To show this, we represent the matrix elements (4) of the spin operators in the form

$$\langle \Omega''|S_{x}|\bar{\Omega}''\rangle = \frac{1}{2} \frac{\tan\frac{\vartheta''}{2}e^{i\bar{\varphi}''} + \tan\frac{\vartheta''}{2}e^{-i\varphi''}}{1 + \tan\frac{\vartheta''}{2}e^{i\bar{\varphi}''} - \tan\frac{\bar{\vartheta}''}{2}e^{i\bar{\varphi}''}} \langle \Omega''|\bar{\Omega}''\rangle$$

$$\langle \Omega''|S_{y}|\bar{\Omega}''\rangle = -\frac{i}{2} \frac{\tan\frac{\bar{\vartheta}''}{2}e^{i\bar{\varphi}''} - \tan\frac{\vartheta''}{2}e^{-i\varphi''}}{1 + \tan\frac{\vartheta''}{2}e^{i\bar{\varphi}'' - \varphi''}} \langle \Omega''|\bar{\Omega}''\rangle$$

$$\langle \Omega''|S_{z}|\bar{\Omega}''\rangle = \frac{1}{2} \frac{1 - \tan\frac{\vartheta''}{2}\tan\frac{\vartheta''}{2}e^{i\bar{\varphi}'' - \varphi''}}{1 + \tan\frac{\vartheta''}{2}\tan\frac{\bar{\vartheta}''}{2}e^{i\bar{\varphi}'' - \varphi''}} \langle \Omega''|\bar{\Omega}''\rangle$$

$$(58)$$

and insert the jump condition (25) to yield

$$\langle \Omega'' | S_x | \bar{\Omega}'' \rangle = \frac{1}{2} \sin \bar{\vartheta}'' \cos \bar{\varphi}'' \langle \Omega'' | \bar{\Omega}'' \rangle \langle \Omega'' | S_y | \bar{\Omega}'' \rangle = \frac{1}{2} \sin \bar{\vartheta}'' \sin \bar{\varphi}'' \langle \Omega'' | \bar{\Omega}'' \rangle$$

$$\langle \Omega'' | S_z | \bar{\Omega}'' \rangle = \frac{1}{2} \cos \bar{\vartheta}'' \langle \Omega'' | \bar{\Omega}'' \rangle.$$

$$(59)$$

Then, from equation (5), the relation (57) is readily shown, and equations (55) and (56) combine again to the Schrödinger equation (53).

4. Calculation of semiclassical propagators

In the semiclassical theory described in the previous section the starting and endpoints $\overline{\Omega}'$ and $\overline{\Omega}''$ of the classical trajectory $\Omega(s)$ need to be determined by solving a boundary value problem. This usually requires some effort. The same problem arises for the coherent state propagator of a simple harmonic oscillator [1] and there it is useful to rewrite the propagator in terms of the complex Glauber variables [20]. Here, we present a nonlinear transformation of the angle variables of the semiclassical spin which allows for an explicit calculation of the spin coherent state propagator by solving only an initial value type problem. Let us introduce the variables [18]

$$\zeta = \tan\left(\frac{\vartheta}{2}\right) e^{i\varphi}$$

$$\eta = \tan\left(\frac{\vartheta}{2}\right) e^{-i\varphi}.$$
(60)

For real angles ϑ and φ one has $\eta = \zeta^*$, and the transformation corresponds to a stereographic projection from the south pole of the unit sphere onto the equatorial plane.

However, usually the semiclassical trajectories (19)–(22) become complex and ζ and η are independent variables. Using the inverse transformation

$$\vartheta = \arccos\left[\frac{1-\zeta\eta}{1+\zeta\eta}\right]$$

$$\varphi = \arctan\left[\frac{\zeta-\eta}{i(\zeta+\eta)}\right]$$
(61)

the Hamiltonian (14) takes the form

$$H(\zeta,\eta,t) = \frac{1}{2} \left[B_x(t) \frac{\zeta+\eta}{1+\zeta\eta} - \mathbf{i} B_y(t) \frac{\zeta-\eta}{1+\zeta\eta} + B_z(t) \frac{1-\zeta\eta}{1+\zeta\eta} \right]$$
(62)

and the classical action becomes

$$\exp\{iS_{cl}[\Omega(s)]\} = \sqrt{\frac{(1+\zeta(0)\eta(0))(1+\zeta(t)\eta(t))}{(1+\zeta'\eta')(1+\zeta''\eta'')}} \left(\frac{\zeta'\eta'\zeta''\eta''}{\zeta(0)\eta(0)\zeta(t)\eta(t)}\right)^{\frac{1}{4}} \\ \times \exp\left\{\int_{0}^{t} ds \left[\frac{(1-\zeta\eta)(\dot{\zeta}\eta-\zeta\dot{\eta})}{4\zeta\eta(1+\zeta\eta)} - iH(\zeta,\eta,s)\right]\right\}.$$
(63)

The time integral in the exponent may be rewritten as

$$\int_0^t ds \left[\frac{(1-\zeta\eta)(\dot{\zeta}\eta-\zeta\dot{\eta})}{4\zeta\eta(1+\zeta\eta)} - iH(\zeta,\eta,s) \right] \\= i \int_0^t ds \left[\frac{i}{2} \left(\frac{\dot{\zeta}\eta-\zeta\dot{\eta}}{1+\zeta\eta} - \frac{1}{2} \frac{\partial}{\partial s} \log\left[\frac{\zeta}{\eta} \right] \right) - H(\zeta,\eta,s) \right]$$

and the jump conditions (24) and (25) transform into the simple boundary conditions

$$\zeta(0) = \zeta'$$

$$\eta(t) = \eta''.$$
(64)

Thus, we obtain from equation (63)

$$\exp\{iS_{cl}[\Omega(s)]\} = \sqrt{\frac{(1+\zeta'\eta(0))(1+\zeta(t)\eta'')}{(1+\zeta'\eta')(1+\zeta''\eta'')}} \left(\frac{\zeta''\eta'}{\zeta'\eta''}\right)^{\frac{1}{4}} \\ \times \exp\left\{i\int_{0}^{t} ds \left[\frac{i}{2}\frac{\dot{\zeta}\eta-\zeta\dot{\eta}}{1+\zeta\eta} - H(\zeta,\eta,s)\right]\right\}.$$
(65)

The classical equations of motion (23) read in terms of the new variables

$$\dot{\zeta} = -i(1+\zeta\eta)^2 \frac{\partial H}{\partial \eta}$$

$$\dot{\eta} = i(1+\zeta\eta)^2 \frac{\partial H}{\partial \zeta}.$$
(66)

These equations coincide with the Euler-Lagrange equations of the action

$$S'[\zeta(s),\eta(s)] = \int_0^t \mathrm{d}s \left[\frac{\mathrm{i}}{2} \frac{\dot{\zeta}\eta - \zeta\dot{\eta}}{1 + \zeta\eta} - H(\zeta,\eta,s) \right]. \tag{67}$$

This action and the associated classical equations of motion have been studied by several authors [2, 7, 11, 13, 16]. It is important to note that the action (67) evaluated along the trajectories solving equations (66) with boundary conditions (64) does not yield the exact quantum mechanical propagator through a relation of the form (27).

Using the explicit form (62) of the Hamlitonian the equations (66) decouple and read explicitly

$$\dot{\zeta} = -\frac{i}{2}B_x(1-\zeta^2) + \frac{1}{2}B_y(1+\zeta^2) + iB_z\zeta$$

$$\dot{\eta} = \frac{i}{2}B_x(1-\eta^2) + \frac{1}{2}B_y(1+\eta^2) - iB_z\eta.$$
(68)

Since the solution has to satisfy the conditions (64), we see that the boundary-value problem is now reduced to an initial- or final-value problem. Moreover, the two equations of motion are complex conjugate. Inserting the equations of motion (68) into the exponent of equation

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(65), the time integral simplifies and we finally obtain

$$\exp\{iS_{cl}[\Omega(s)]\} = \sqrt{\frac{(1+\zeta'\eta(0))(1+\zeta(t)\eta'')}{(1+\zeta'\eta')(1+\zeta''\eta'')}} \left(\frac{\zeta''\eta'}{\zeta'\eta''}\right)^{\frac{1}{4}} \\ \times \exp\left\{-\frac{i}{4}\int_{0}^{t} ds \left[B_{x}(\zeta+\eta) - iB_{y}(\zeta-\eta) + 2B_{z}\right]\right\}.$$
(69)

To illustrate the theory we apply it to two specific models. As a first example we treat the propagator of a two-state system with Hamiltonian

$$H = \Delta S_x + \epsilon S_z \tag{70}$$

which describes a variety of systems. The Hamiltonian (70) corresponds to a spin- $\frac{1}{2}$ in a timeindependent magnetic field $B = (\Delta, 0, \epsilon)$. With the method presented above, we express this Hamiltonian as

$$H(\zeta,\eta) = \frac{\Delta}{2} \frac{\zeta+\eta}{1+\zeta\eta} + \frac{\epsilon}{2} \frac{1-\zeta\eta}{1+\zeta\eta}.$$
(71)

In accordance with the boundary conditions (64), the equations of motion (68) are solved by

$$\zeta(s) = -\frac{\epsilon}{\Delta} - i\frac{\omega}{\Delta} \tan\left\{\omega\frac{s}{2} + \arctan\left[\frac{i(\epsilon + \Delta\zeta')}{\omega}\right]\right\}$$

$$\eta(s) = -\frac{\epsilon}{\Delta} - i\frac{\omega}{\Delta} \tan\left\{\omega\frac{t-s}{2} + \arctan\left[\frac{i(\epsilon + \Delta\eta'')}{\omega}\right]\right\}$$
(72)

where $\omega = \sqrt{\Delta^2 + \epsilon^2}$. The unspecified boundary values may be written as

$$\zeta(t) = \frac{\omega \zeta' \cos\left(\frac{\omega t}{2}\right) + i(\epsilon \zeta' - \Delta) \sin\left(\frac{\omega t}{2}\right)}{\omega \cos\left(\frac{\omega t}{2}\right) - i(\Delta \zeta' + \epsilon) \sin\left(\frac{\omega t}{2}\right)}$$
(73)

and

$$\eta(0) = \frac{\omega \eta'' \cos\left(\frac{\omega t}{2}\right) + i(\epsilon \eta'' - \Delta) \sin\left(\frac{\omega t}{2}\right)}{\omega \cos\left(\frac{\omega t}{2}\right) - i(\Delta \eta'' + \epsilon) \sin\left(\frac{\omega t}{2}\right)}.$$
(74)

Now, the time integral in equation (69) can be readily solved

$$\exp\left\{-\frac{\mathrm{i}}{2}\int_{0}^{t}\mathrm{d}s\left[\frac{1}{2}\Delta(\zeta(s)+\eta(s))+\epsilon\right]\right\} = \frac{1}{\omega}\left[\omega\cos\left(\frac{\omega t}{2}\right)-\mathrm{i}(\Delta\zeta'+\epsilon)\sin\left(\frac{\omega t}{2}\right)\right]^{\frac{1}{2}} \times \left[\omega\cos\left(\frac{\omega t}{2}\right)-\mathrm{i}(\Delta\eta''+\epsilon)\sin\left(\frac{\omega t}{2}\right)\right]^{\frac{1}{2}}.$$
(75)

Combining these relations we obtain from equation (69)

$$\exp\{\mathrm{i}S_{\mathrm{cl}}[\Omega(s)]\} = \frac{\left(\frac{\zeta''\eta'}{\zeta'\eta'}\right)^{\frac{1}{4}}}{\sqrt{(1+\zeta'\eta')(1+\zeta''\eta'')}} \\ \times \left[(1+\zeta'\eta'')\cos\left(\frac{\omega t}{2}\right) - \frac{\mathrm{i}(\epsilon - \epsilon\zeta'\eta'' + \Delta\zeta' + \Delta\eta'')}{\omega}\sin\left(\frac{\omega t}{2}\right)\right].$$
(76)

With the inverse transformation the semiclassical propagator takes the form of the right-hand side of equation (37) with

$$a(t) = \cos\left(\frac{\omega t}{2}\right) - \frac{i\epsilon}{\omega}\sin\left(\frac{\omega t}{2}\right)$$
(77)

and

$$b(t) = -\frac{i\Delta}{\omega}\sin\left(\frac{\omega t}{2}\right) \tag{78}$$

which coincides with the exact quantum mechanical result.

As a second example, we consider the Landau–Zener problem [21]

$$H = \omega S_x - \gamma^2 t S_z \tag{79}$$

which corresponds to a spin- $\frac{1}{2}$ in the time-dependent magnetic field $B = (\omega, 0, -\gamma^2 t)$. The Hamiltonian now reads

$$H(\zeta,\eta,t) = \frac{\omega}{2} \frac{\zeta+\eta}{1+\zeta\eta} - \frac{\gamma^2 t}{2} \frac{1-\zeta\eta}{1+\zeta\eta}.$$
(80)

The equations of motion (68) are of Riccati form, and for the present model the transformation $r^*(x) = r^*(x)$

$$\zeta(s) = \frac{a^*(s)\zeta - b^*(s)}{b(s)\zeta + a(s)}$$
(81)

leads to Weber equations for a(s) and b(s) [22] which are solved in terms of confluent hypergeometric functions $\Phi(\alpha, \beta, z)$ [23]. Accordingly, the solutions read

$$\zeta(s) = \frac{D(s)\zeta' + C(s)}{B(s)\zeta' + A(s)}$$

$$\eta(s) = \frac{[D(t)A(s) - C(t)B(s)]\eta'' - [A(t)B(s) - B(t)A(s)]}{[C(t)D(s) - D(t)C(s)]\eta'' + [A(t)D(s) - B(t)C(s)]}$$
(82)

where

$$A(s) = \Phi\left(-\frac{i}{8}\frac{\omega^2}{\gamma^2}, \frac{1}{2}, -\frac{i}{2}\gamma^2 s^2\right)$$

$$B(s) = -\frac{i}{2}\omega s \Phi\left(-\frac{i}{8}\frac{\omega^2}{\gamma^2} + \frac{1}{2}, \frac{3}{2}, -\frac{i}{2}\gamma^2 s^2\right)$$

$$C(s) = -\frac{i}{2}\omega s \Phi\left(-\frac{i}{8}\frac{\omega^2}{\gamma^2} + 1, \frac{3}{2}, -\frac{i}{2}\gamma^2 s^2\right)$$

$$D(s) = \Phi\left(-\frac{i}{8}\frac{\omega^2}{\gamma^2} + \frac{1}{2}, \frac{1}{2}, -\frac{i}{2}\gamma^2 s^2\right).$$

(83)

Now, the unspecified boundary values become

$$\zeta(t) = \frac{D(t)\zeta' + C(t)}{B(t)\zeta' + A(t)}$$

$$\eta(0) = \frac{D(t)\eta'' + B(t)}{C(t)\eta'' + A(t)}.$$
(84)

To solve the time integral in equation (69) we make use of analytic properties of $\Phi(\alpha, \beta, z)$ [23] yielding

$$\frac{d}{ds}A(s) = -\frac{i}{2}\omega C(s)$$

$$\frac{d}{ds}B(s) = -\frac{i}{2}\omega D(s)$$

$$\frac{d}{ds}C(s) = -\frac{i}{2}\omega A(s) - i\gamma^2 s C(s)$$

$$\frac{d}{ds}D(s) = -\frac{i}{2}\omega B(s) - i\gamma^2 s D(s).$$
(85)

We then obtain

$$\exp\left\{-\frac{\mathrm{i}}{4}\omega\int_0^t \mathrm{d}s\left[\zeta(s)+\eta(s)\right]\right\} = \sqrt{B(t)\zeta'+A(t)}\sqrt{C(t)\eta''+A(t)}.$$
(86)

Inserting the results into (69) and expressing the final and initial states again in terms of angles, the semiclassical propagator takes the form (37) where

$$a(t) = \exp\left\{\frac{i}{4}\gamma^2 t^2\right\} A(t)$$
(87)

and

$$b(t) = \exp\left\{\frac{\mathrm{i}}{4}\gamma^2 t^2\right\} B(t).$$
(88)

This is again the exact quantum mechanical result.

5. Conclusions

We have analysed the spin coherent state path integral for a spin- $\frac{1}{2}$ in a magnetic field of arbitrary time dependence. To obtain a path integral that may be evaluated with conventional methods, we have introduced a Wiener regularization. Then, the semiclassical approximation was shown to be well defined leading to a classical trajectory with jumps at the endpoints. The action of this trajectory determines the exact quantum mechanical propagator. Hence, the dominant stationary phase approximation without fluctuations was shown to become exact for a spin- $\frac{1}{2}$ system in an arbitrary time-dependent magnetic field. A nonlinear transformation related to the stereographic projection from the south pole onto the equatorial plane was found to simplify the explicit determination of the minimal action trajectory. The method was illustrated by applying it to two specific models.

The theory presented has a straightforward extension to spin systems with quantum numbers $s > \frac{1}{2}$ provided the Hamiltonian remains of the form (5) which is, however, no longer the most general spin Hamiltonian in this case. For other Hamiltonians, for $s > \frac{1}{2}$, the dominant stationary phase approximation cannot be expected to remain exact. An interesting extension of this paper would be the investigation of the semiclassical dynamics of a spin coupled to other degrees of freedom, e.g., boson modes. With a proper c-number representation of these modes, the problem can be described as a spin- $\frac{1}{2}$ in a fluctuating field, and the method presented here can be applied. This will be studied in future work.

Acknowledgments

The authors would like to thank Joachim Ankerhold, Andreas Lucke, Phil Pechukas, Gerhard Stock and Simone Warzel for valuable discussions. AA is grateful to the Department of Chemistry of Columbia University, New York, for hospitality during an extended stay. This work was supported by the Deutsche Forschungsgemeinschaft (Bonn) through the Schwerpunktprogramm 'Zeitabhängige Phänomene und Methoden in Quantensystemen der Physik und Chemie'. Additional support was provided by the Deutscher Akademischer Austauschdienst (DAAD).

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