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Path integral for system with spin

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Abstract. A path integral representation for the system with spin is considered. Explicit path integral representations are given in classical phase space for spin realized as the complex Kãhler manifold and as the Grassmann algebra for the spin-$\frac{1}{2}$ case.

1. Introduction

The path integral representation of the wavefunction has the advantage of a clear and compact formulation of quantum theory in terms of classical theory. In some cases, spin effects should be taken into account, for example in the cases of polarized electron beam scattering or studies of magnetic materials.

The works of Klauder [1, 2] are related to this subject. These works use spinor coherent states with the parametrization of spin phase space by spherical coordinates. In the present work we give an explicit path integral representation in classical phase space for spin realized as the complex Kãhler manifold. This form is natural in the case of complex realization of phase space for non-spin variables (the Fock–Bargmann representation of wavefunctions).

The spin-$\frac{1}{2}$ case can be treated in terms of fermi operators. The corresponding path integral representation uses Grassmann variables. Although there are many works devoted to this subject, all of them assume (explicitly or not) that the Hamiltonian is even function of fermions. The path integral representation in Grassmann algebra in the general case of a Hamiltonian of arbitrary parity can be found in [3]. In the present paper we use this result to find an explicit path integral representation in the case of spin-$\frac{1}{2}$.

2. A path integral representation for a system with spin

Spin effects are described by a relativistic Hamiltonian. The relativistic Hamiltonian correct to $1/c$ ($c = 137$ au—the velocity of light), which is known as the Pauly Hamiltonian, is

$$\hat{H} = \frac{1}{2}\left(\hat{\boldsymbol{p}} - \frac{1}{c}\boldsymbol{A}\right)^2 + V - \frac{1}{c}\hat{\boldsymbol{s}}\boldsymbol{B} \tag{2.1}$$

where $\hat{\boldsymbol{s}}$ is the spin operator, $\boldsymbol{B} = \mathrm{rot}\,\boldsymbol{A}$ is the magnetic field with vector potential $\boldsymbol{A}$, (atomic units are used). The corresponding Schrõdinger equation contains the spinor wavefunction ψ.

The Hamiltonian equation (2.1) describes propagation in a magnetic field. In the absence of magnetic field, spin effects of higher order, such as spin–orbit and spin–spin interactions, are distinct. They are described by the relativistic Hamiltonian correct to $1/c^2$ which is known as the Breight Hamiltonian.

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We should write formulae, for instance, of Hamiltonian equation (2.1) only, although all results are valid for an arbitrary Hamiltonian.

The path integral representation may be derived by using generalized coherent state theory [4]. For a system with spin we consider two possible systems of generalized coherent states: (i) Spinor coherent states [1, 4] (section 2.1); (ii) fermion coherent states [5] (section 2.2).

2.1. Spinor coherent states

In this case spin operators $\hat{s}$ are treated as generators of the group $SO(3)$ locally isomorphic to $SU(2)$. The corresponding generalized coherent states are parametrized by elements of some homogeneous space $\mathcal{X}$ of the group $SU(2)$ [4]. The space $\mathcal{X}$ is a Kãhler manifold and may be treated as a classical phase space for spin. It is isomorphic to the sphere S^2 of dimension two and has two standard local coordinate realizations:

(1) by spherical coordinates on S^2;

(2) by stereographic projection of S^2 on complex plane $\mathcal{C}$.

Case (1) was considered in [1, 2]. We consider case (2) and write the coherent state as $|\zeta\rangle$, with complex $\zeta \in \mathcal{C}$, and the adjoint state as $\langle\zeta^*|$.

Coherent states define covariant symbols of the operators [6] as

$$A(\zeta^*, \eta) = \frac{\langle\zeta^*|\hat{A}|\eta\rangle}{\langle\zeta^*|\eta\rangle} \tag{2.2}$$

which may be treated as the corresponding classical values (the correspondence principle).

Coherent states also define covariant symbols of the wavefunctions

$$\psi(\zeta^*) = \frac{\langle\zeta^*|\psi}{\langle\zeta^*|0\rangle} \tag{2.3}$$

where $|0\rangle$ is the vacuum state.

Operators and wavefunctions can be restored by their symbols.

The covariant symbols of the spin operator $\hat{s}$ are

$$s_x(\zeta^*, \eta) = \frac{1}{2}\frac{\zeta^* + \eta}{1 + \zeta^*\eta} \qquad s_y(\zeta^*, \eta) = \frac{1}{2i}\frac{\zeta^* - \eta}{1 + \zeta^*\eta} \qquad s_z(\zeta^*, \eta) = -\frac{1}{2}\frac{1 - \zeta^*\eta}{1 + \zeta^*\eta}. \tag{2.4}$$

First, let us formulate the path integral representation for spin motion only. The spinor wavefunction symbol has the following representation:

$$\psi(\zeta^*) = \int \exp(\mathrm{i}S)\psi_{in}(\tilde{\zeta}^*(0))\,\mathrm{d}\tilde{\zeta}^*\,\mathrm{d}\tilde{\zeta}. \tag{2.5}$$

Formula (2.5) assumes integration by all virtual trajectories $\tilde{\zeta}^*$, $\tilde{\zeta}$ in phase space $\mathcal{X}$ with the condition

$$\tilde{\zeta}^*(t) = \zeta^* \tag{2.6}$$

at the final point.

$$S = \int \left(\frac{1}{\mathrm{i}}\partial^* F(\tilde{\zeta}^*, \tilde{\zeta}) - H(\tilde{\zeta}^*, \tilde{\zeta})\,\mathrm{d}t\right)$$

is the classical Hamilton-Kãhler action, where

$$F = \ln(1 + \zeta^*\zeta)$$

is the potential of Kãhler's metrics on $\mathcal{X}$ and

$$\partial^* F = \frac{\zeta\,\mathrm{d}\zeta^*}{1 + \zeta^*\zeta}$$

is the differential 1-form on the complexified cotangent fibration for manifold $\mathcal{X}$.

The continual path integral (2.5) can be treated as the limit of the finite-dimensional approximations [6]

$$\psi(\zeta^*_{l+1}) = \int \exp(\mathrm{i}S_l)\psi_{in}(\zeta^*_0)\,\mathrm{d}\tilde{\zeta}^*\,\mathrm{d}\tilde{\zeta}$$

where $\tilde{\zeta}^* = (\zeta^*_0, \ldots, \zeta^*_{l+1})$, $\tilde{\zeta} = (\zeta_0, \ldots, \zeta_l)$ is the discrete phase trajectory,

$$\mathrm{d}\tilde{\zeta}^*\,\mathrm{d}\tilde{\zeta} = \prod_0^l \mathrm{d}\mu(\zeta^*_k, \zeta_k)$$

where

$$\mathrm{d}\mu(\zeta^*, \zeta) = -\frac{2}{\pi}\frac{\partial^2 F}{\partial\zeta^*\partial\zeta}\mathrm{d}\zeta^* \wedge \mathrm{d}\zeta = -\frac{2}{\pi}\frac{\mathrm{d}\zeta^* \wedge \mathrm{d}\zeta}{(1+\zeta^*\zeta)^2}$$

is the invariant measure on $\mathcal{X}$, and

$$S_l = \sum_{k=0}^{l} \Delta S_k \qquad \Delta S_k = \frac{1}{\mathrm{i}}\Delta^*_k F - \Delta t H(\zeta^*_{k+1}, \zeta_k) \tag{2.7}$$

where

$$\Delta^*_k F = F(\zeta^*_{k+1}, \zeta_k) - F(\zeta^*_k, \zeta_k).$$

The covariant symbol of the Hamilton operator (2.1), $H(\zeta^*_{k+1}, \zeta_k)$, can be expressed by the covariant symbols of the spin operator $\boldsymbol{s}(\zeta^*_{k+1}, \zeta_k)$, equation (2.4).

The corresponding expressions for both the spin and orbital motions are as follows. For a continual path integral

$$\psi(\zeta^*, q) = \int \exp(\mathrm{i}S)\psi_{in}(\tilde{\zeta}^*(0), \tilde{q}(0))\,\mathrm{d}\tilde{\zeta}^*\,\mathrm{d}\tilde{\zeta}\,\mathrm{d}\tilde{q}\,\mathrm{d}\tilde{p}$$

with virtual trajectories with the conditions of equation (2.6) and

$$\tilde{q}(t) = q \tag{2.8}$$

at the final point, and

$$S = \int \left(\frac{1}{\mathrm{i}}\partial^* F(\tilde{\zeta}^*, \tilde{\zeta}) + \mathrm{d}\tilde{q}\,\tilde{p} - H(\tilde{\zeta}^*, \tilde{\zeta}, \tilde{q}, \tilde{p})\,\mathrm{d}t\right).$$

For finite-dimensional approximations

$$\psi(\zeta^*_{l+1}, q_{l+1}) = \int \exp(\mathrm{i}S_l)\psi_{in}(\zeta^*_0, q_0)\,\mathrm{d}\tilde{\zeta}^*\,\mathrm{d}\tilde{\zeta}\,\mathrm{d}\tilde{q}\,\mathrm{d}\tilde{p}$$

where S_l has the form of equation (2.7) with

$$\Delta S_k = \frac{1}{\mathrm{i}}\Delta^*_k F + \Delta q_k p_k - \Delta t H(\zeta^*_{k+1}, \zeta_k, q_{k+1}, p_k). \tag{2.9}$$

The covariant symbol of the Hamilton operator (2.1) correct to $1/c$ is

$$\begin{aligned} H(\zeta^*_{k+1}, \zeta_k, q_{k+1}, p_k) &= \frac{1}{2}p_k^2 - \frac{1}{c}p_k\boldsymbol{A}(q_{k+1}) - \frac{\mathrm{i}}{2c}\mathrm{div}\,\boldsymbol{A}(q_{k+1}) + V(q_{k+1}) \\ &\quad -\frac{1}{c}\boldsymbol{s}(\zeta^*_{k+1}, \zeta_k)\boldsymbol{B}(q_{k+1}). \end{aligned} \tag{2.10}$$

It should be noted that the path integral in complex Kãhler phase space for spin is natural in the case of complex realization of phase space for non-spin variables (the Fock–Bargmann representation of wavefunctions). We have a complex total phase space.

With

$$z^* = \frac{1}{\sqrt{2}}(q - \mathrm{i}p) \qquad z = \frac{1}{\sqrt{2}}(q + \mathrm{i}p)$$

the corresponding continual path integral is

$$\psi(\zeta^*, q) = \int \exp(\mathrm{i}S)\psi_{in}(\tilde{\zeta}^*(0), \tilde{z}^*(0))\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}\, \mathrm{d}\tilde{z}^*\, \mathrm{d}\tilde{z}$$

with virtual trajectories with the conditions of equation (2.6) and

$$\tilde{z}^*(t) = z^*$$

at the final point, and

$$S = \int \left(\frac{1}{\mathrm{i}} \partial^* F(\tilde{\zeta}^*, \tilde{\zeta}) + \frac{1}{\mathrm{i}} \mathrm{d}\tilde{z}^* \tilde{z} - H(\tilde{\zeta}^*, \tilde{\zeta}, \tilde{z}^*, \tilde{z})\, \mathrm{d}t \right).$$

For finite-dimensional approximations

$$\psi(\zeta_{l+1}^*, z_{l+1}^*) = \int \exp(\mathrm{i}S_l)\psi_{in}(\zeta_0^*, z_0^*)\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}\, \mathrm{d}\tilde{z}^*\, \mathrm{d}\tilde{z}$$

where S_l has the form of equation (2.7) with

$$\Delta S_k = \frac{1}{\mathrm{i}} \Delta_k^* F + \frac{1}{\mathrm{i}} \Delta z_k^* z_k - \Delta t H(\zeta_{k+1}^*, \zeta_k, z_{k+1}^*, z_k).$$

2.2. Fermions coherent states

In the case of spin-$\frac{1}{2}$ operators $\hat{s}$ may be treated in terms of two operators $\hat{s}_+, \hat{s}_-$

$$\hat{s}_x = \frac{1}{2}(\hat{s}_+ + \hat{s}_-) \qquad \hat{s}_y = \frac{1}{2\mathrm{i}}(\hat{s}_+ - \hat{s}_-) \qquad \hat{s}_z = \frac{1}{2}[\hat{s}_+, \hat{s}_-]$$

where [,] is the commutator.

Operators $\hat{s}_+, \hat{s}_-$ satisfy canonic anticommutation relations

$$\hat{1} = [\hat{s}_+, \hat{s}_-]_- \qquad \hat{0} = [\hat{s}_+, \hat{s}_+]_- \qquad \hat{0} = [\hat{s}_-, \hat{s}_-]_-$$

where $[\ ,\ ]_-$ is the anticommutator.

So they are Fermi operators and generators of the Heisenberg–Weyl supergroup and define the corresponding set of generalized coherent states [4, 5].

It should be noted that coherent states of the fermions introduced in [5] do not exist in the usual space of wavefunctions but only in its extension by Grassmann algebra. Nevertheless, these states can be used in calculations and give correct results.

The classical phase space for fermions is the Grassmann algebra $\mathcal{G}$ with involution *.

We write the coherent state as $|\zeta\rangle$ and the adjoint state as $\langle\zeta^*|$, where $\zeta, \zeta^* \in \mathcal{G}$ are Grassmann algebra generators.

The important difference with usual phase spaces is in the fact that the Grassmann algebra is not commutative and hence the corresponding symbols of operators are also not commutative in the general case. This leads to some peculiarities in the path integral representation as was shown in [3].

The covariant symbols are defined similar to those in equations (2.2) and (2.3).

As in section 2.1 let us consider first the spin motion for 'frozen' orbital motion. The spinor wavefunction symbol has a continual path integral representation similar by form to equation (2.5)

$$\psi(\zeta^*) = \int \exp(\mathrm{i}S)\psi_{in}(\tilde{\zeta}^*(0))\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}. \tag{2.11}$$

Formula (2.11) assumes integration by all virtual trajectories $\tilde{\zeta}^*, \tilde{\zeta}$ in phase space $\mathcal{G}$ with a condition similar to equation (2.6) at the final point and

$$S = \int \left(\frac{1}{\mathrm{i}}\, \mathrm{d}\tilde{\zeta}^* \tilde{\zeta} - H(\tilde{\zeta}^*, \tilde{\zeta})\, \mathrm{d}t - \frac{1}{\mathrm{i}} O\, \mathrm{d}t \right) \tag{2.12}$$

where the term O according to [3] is

$$O = H^{\mathrm{o}}(\tilde{\zeta}^*, \tilde{\zeta}) \int_0^t H^{\mathrm{o}}(\tilde{\zeta}^*, \tilde{\zeta})\, \mathrm{d}t'. \tag{2.13}$$

and H^{o} is the odd part of H in the Grassmann algebra $\mathcal{G}$.

Without the term in equation (2.13), equation (2.12) has the same form as the Hamilton–Kãhler action for commutative variables. It is valid for the even Hamilton function ($H^{\mathrm{o}} = 0$). The nonlinear Hamiltonian H term in equation (2.13) is the specific feature of the path integral representation in the Grassmann algebra in the general case of the Hamiltonian symbol with arbitrary Grassmann parity [3].

It should be noted that the Pauli Hamiltonian equation (2.1) has no definite parity and it is essential to take into account the nonlinear term in equation (2.13).

The continual path integral equation (2.11) is treated as the limit of the finite-dimensional approximations

$$\psi(\zeta^*_{l+1}) = \int \exp(\mathrm{i}S_l)\psi_{in}(\zeta^*_0)\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}$$

where $\tilde{\zeta}^* = (\zeta^*_0, \ldots, \zeta^*_{l+1})$, $\tilde{\zeta} = (\zeta_0, \ldots, \zeta_l)$ is the discrete phase trajectory,

$$\mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta} = \prod_0^l \mathrm{d}\zeta^*_k \zeta_k$$

and with integration in the Grassmann algebra [6]. The term S_l has the form of equation (2.7) with

$$\Delta S_k = \frac{1}{\mathrm{i}} \Delta\zeta^*_k \zeta - \Delta t H(\zeta^*_{k+1}, \zeta_k) - \Delta t \frac{1}{\mathrm{i}} O_k$$

where

$$O_k = H^{\mathrm{o}}(\zeta^*_{k+1}, \zeta_k)\Delta t \sum_{j=0}^{k} H^{\mathrm{o}}(\zeta^*_{j+1}, \zeta_j).$$

The covariant symbol of the Hamilton operator equation (2.1), $H(\zeta^*_{k+1}, \zeta_k)$, can be expressed by the covariant symbols of the spin operator $\boldsymbol{s}(\zeta^*_{k+1}, \zeta_k)$, which are

$$s_x(\zeta^*, \eta) = \frac{1}{2}(\zeta^* + \eta) \qquad s_y(\zeta^*, \eta) = \frac{1}{2\mathrm{i}}(\zeta^* - \eta) \qquad s_z(\zeta^*, \eta) = \zeta^*\eta - \frac{1}{2}. \tag{2.14}$$

The symbols s_x, s_y are odd and s_z is even in Grassmann algebra.

For both the spin and orbital motions the corresponding expressions are as follows. For the continual path integral

$$\psi(\zeta^*, q) = \int \exp(\mathrm{i}S)\psi_{in}(\tilde{\zeta}^*(0), \tilde{q}(0))\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}\, \mathrm{d}\tilde{q}\, \mathrm{d}\tilde{p}$$

with virtual trajectories with the conditions of equation (2.6) and (2.8) at the final point and the superaction

$$S = \int \left(\frac{1}{\mathrm{i}}\, \mathrm{d}\tilde{\zeta}^* \tilde{\zeta} + \mathrm{d}\tilde{q}\, \tilde{p} - H(\tilde{\zeta}^*, \tilde{\zeta}, \tilde{q}, \tilde{p})\, \mathrm{d}t - \frac{1}{\mathrm{i}} O\, \mathrm{d}t \right)$$

where

$$O = H^{\mathrm{o}}(\tilde{\zeta}^*, \tilde{\zeta}, \tilde{q}, \tilde{p}) \int_0^t H^{\mathrm{o}}(\tilde{\zeta}^*, \tilde{\zeta}, \tilde{q}, \tilde{p})\, \mathrm{d}t'$$

and H^{o} is the odd part of H in the Grassmann algebra $\mathcal{G}$.

For finite-dimensional approximations

$$\psi(\zeta^*_{l+1}, q_{l+1}) = \int \exp(\mathrm{i}S_l)\psi_{in}(\zeta^*_0, q_0)\, \mathrm{d}\tilde{\zeta}^*\, \mathrm{d}\tilde{\zeta}\, \mathrm{d}\tilde{q}\, \mathrm{d}\tilde{p}$$

where S_l has the form of equation (2.7) with

$$\Delta S_k = \frac{1}{\mathrm{i}}\Delta\zeta^*_k\zeta_k + \Delta q_k p_k - \Delta t H(\zeta^*_{k+1}, \zeta_k, q_{k+1}, p_k) - \Delta t \frac{1}{\mathrm{i}} O_k$$

where $\Delta\zeta^*_k = \zeta^*_{k+1} - \zeta^*_k$ and

$$O_k = H^{\mathrm{o}}(\zeta^*_{k+1}, \zeta_k, q_{k+1}, p_k)\Delta t \sum_{j=0}^{k} H^{\mathrm{o}}(\zeta^*_{j+1}, \zeta_j, q_{j+1}, p_j).$$

The covariant symbol of the Hamilton operator equation (2.1) correct to $1/c$ is similar in form to equation (2.9) with equation (2.14) for the spin operator symbols.

3. Conclusions

There can exist different realizations of the classical phase space for spin and corresponding different path integral representations. Although the realization of phase space as a sphere of dimension two with natural spherical coordinates is widely used, other possible realizations, such as the complex Kãhler manifold and the Grassmann algebra for spin-$\frac{1}{2}$, have certain advantages.

The path integral in complex Kãhler phase space for spin is natural in the case of complex realization of phase space for non-spin variables (the Fock–Bargmann representation of wavefunctions).

In the case of Grassmann algebra the nonlinear Hamiltonian term in equation (2.13) is a specific feature of the path integral representation in the general case of the Hamiltonian symbol with arbitrary Grassmann parity.

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