

Thermodynamic Parameters of Central Spin Coupled to an Antiferromagnetic Bath: Path Integral Formalism

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Abstract

A path-integral representation of central spin system immersed in an antiferromagnetic environment was investigated. To carry out this study, we made use of the discrete-time propagator method associated with a basic set involving coherent states of Grassmann variables which made it possible to obtain the analytical propagator which is the centerpiece of the study. In this study, we considered that the environment was in the low-temperature and low-excitation limit and was split into 2 subnets that do not interact with each other. The evaluation of our system was made by considering the first neighbor approximation. From the formalism of the path integrals, it is easy to evaluate the partition function and thermodynamic properties followed from an appropriate tracing over Grassmann variables in the imaginary time domain. We show that the energy of the system depends on the number of sites n when $\beta \rightarrow 0$.

Keywords

Path Integral, Grassmann Algebra, Antiferromagnetic Environment, Partition Function

1. Introduction

Since its appearance in the years 1942, the integral of path has become an approach widely used in various fields of physics [1]. From this approach, it is possible to assess several parameters, in this case the mechano-quantum propa-

gator which has gained enormous popularity in recent years [2] [3]. This approach is particularly suitable for the semi-classical evaluation of the transition amplitudes in quantum mechanics and the thermodynamic properties of a system [4]. Numerous attempts have been made to extend the path integrals approach to the operator space with the aim of extracting the information useful during the development of field operators [5], we still notice limits associated to systems with Fermi degrees of freedom formulated in terms of anticommuting fields. In addition to the formalism of the path integrals based on the Lagrangian and the Hamiltonian, Klauder [6], Kuratsuji and Suzuki [7] simultaneously developed the formalism of the integral of the coherent state path, which has proved particularly suitable to the description of Bose quantum dynamics [8] and spin systems [6] [9]. Recently, studies of the time-dependent electronic nuclear dynamics of molecular collision processes have made it possible to study the quasi-classical properties of coherent states in rotation [10]. To overcome this problem, a method based on the representation of discretized coherent states during the study of the dynamics of quantum systems has been developed [11].

Recently, it has been proven that there are fundamental difficulties when using continuous time in the formalism of path integrals of coherent spin states [12]. This difficulty arises when studying a single spin system or when conducting studies in which one takes account of the fluctuations around the “classical path”. Such difficulty is also observed when it comes to the coherent state path integral. An explicit analysis of the origin of its difficulties sufficiently shows that the use of an appropriate discrete time formalism can prove to be effective. Although the coherent state path integral is formally considered as an alternative to the conventional integral phase-space path, the former has a crucial advantage since it can be extended to a wider class of physical systems using “generalized coherent states” [6] [8] [9] [13]. The spin system is one of its fascinating and vital systems whose dynamics are perfectly described using path integrals in the $SU(2)$ (or spin) coherent state representation [14].

In general, the partitioning of Hilbert space into several coherent states makes it possible to introduce invariant functions for several groups, in this case the group $SU(2)$, the study of which made it possible to determine its orbital spaces in representations $j=1/2$ and $j=1$ [15]. Integrals with respect to anticommuting variables have been used to rewrite partition and correlation functions in Ising models in 2D and 3D as theories of fermionic fields [16]. For Ising 2D model, the partition function was discussed and the Grassmann representative was obtained using the transfer matrix method [17]. Pablo G. and Horacio Grinberg used the Short-time propagator algorithms and a discrete time formalism combine with Grassmann variables coherent states to get a many-body analytic propagator to study interacting spin systems and for 1D Ising and XY spin models respectively. There are several spin models to describe the environment in quantum mechanics, which opens up a large field of research that requires investigation.

This article aims to construct a functional integral representation for a central

spin system immersed in an antiferromagnetic environment under the application of an external global magnetic field that involves non-orthogonal Grassmann coherent states integration variables. We will use Grassmann algebra to construct coherent states. The construction of the variables associated with this algebra will be used to evaluate the path integral representation of a transition amplitude and thereby the partition function. The choice of this system does not happen by chance. It has been proven that in some cases, central spin coupled with a spin environment (lattice nuclear spins, Ising spin bath, the device substrates doped with spin impurities) may be more appropriate to represent the actual localized background spins or magnetic defects than the delocalized oscillator bath that is usually used. Such a system was used by Xio-Zhong Yuan *et al.* with the aim of showing how the external magnetic field affect the decoherence of a central spin bathing in an antiferromagnetic environment [18].

This paper is organized as follows: in Section 2, we presented the Hamiltonian model and the spin wave approximation was applied to map the spin operators of the antiferromagnetic environment. Section 3, introduces the propagator in a basis of Grassmann generators of a spin Hamiltonian involving nearest neighbor correlations and assuming a uniform external magnetic field applied in the z-direction. In Section 4, it was shown that the discrete-time formalism and short time algorithms provide a generating function for the given Hamiltonian from which an appropriate tracing in the imaginary time domain leads to the partition function for our models. In Section 5, we evaluated the thermodynamic parameters associated with our system. We concluded in Section 6, with the discussion of result.

2. Hamiltonian Model

We consider a central system having a spin $1/2$ which is coupled to an antiferromagnetic environment consisting of $2N$ atoms each having a spin S . A global magnetic field is applied to both the central spin and the antiferromagnetic environment. The Hamiltonian that governs the dynamics of the system reads:

$$H(t) = H_S + H_{SB} + H_B, \quad (1)$$

where H_S , H_B respectively represent the Hamiltonians of the central spin and the environment respectively, and H_{SB} is the interaction Hamiltonian [19] [20]. The Hamiltonian central can be written:

$$H_S = -g\mu_B BS_0^z, \quad (2)$$

where g is the gyro magnetic Lande factor, μ_B is the Bohr magneton and B is a uniform external magnetic field applied in the z -direction. The Hamiltonian of the environments is defined by

$$H_B = -g\mu_B (B + B_A) \sum_i S_{a,i}^z - g\mu_B (B - B_A) \sum_j S_{b,j}^z + J \sum_{i,\delta} S_{a,i} S_{b,i+\delta} + J \sum_{j,\delta} S_{b,j+\delta} S_{a,j+\delta}, \quad (3)$$

We assumed in this study that the spin structure of the environment may be divided into two interpenetrating sublattices (contains N atoms) a and b with the property that all nearest neighbors of an atom on a lie on b , and conversely [19]. At each atom of each sublattices a and b we associate spin operators $S_{a,i}$ ($S_{a,i}$) where the indices i and j label the N atoms, whereas the vectors δ connect atom i or j with its nearest neighbors. J being the exchange interaction and was positive for our environment B_A is the anisotropy field and assume to be positive, which approximates the effect of the crystal anisotropy energy, with the property of tending for positive magnetic moment μ_B to align the spins on sublattice a in the positive z -direction and the spins on sublattice b in the negative z direction [18]. The effects of the next nearest-neighbor interactions in our environment antiferromagnetic are neglected, although they may be important in some real antiferromagnets.

$$H_{SB} = -\frac{J_0 S_0^z}{\sqrt{N}} \sum_i (S_{a,i}^z + S_{b,i}^z), \tag{4}$$

In this work, the Hamiltonian of interaction was of type Ising with J_0 being the coupling constant. The design of the Hamiltonian coupling between our two subsystem has been widely discussed by Rossini and al [21]. In order to diagonalize the Hamiltonian (1), we supposed the environment was in the low-temperature and low-excitation limit which allowed us to approximate the Holstein-Primakov transformations in the following form $S_{a,i}^+ \geq \sqrt{2S} a_i$ and $S_{b,j}^- \geq b_j^\dagger \sqrt{2S}$. This could be justified as in this limit, the number of excitation was small, and the thermal average $\langle a_i^\dagger a_i \rangle$ and $\langle b_i^\dagger b_i \rangle$ was expected to be of the order $O(1/N)$ and can be safely neglected with respect to $2S$ when N is very large [18]. The low excitations correspond to low temperatures, where $T \ll T_N$ is the Nel temperature [22]. Neglecting all the terms containing products of four operators, the Hamiltonians H_B and H_{SB} can then be written in the spin-wave approximation as [21] [23]

$$H_{SB} = -\frac{J_0 S_0^z}{\sqrt{N}} \sum_i (b_i^\dagger b_i - a_i^\dagger a_i) \tag{5}$$

$$H_B = E_0 + \omega_- \sum_i b_i^\dagger b_i + \omega_+ \sum_i a_i^\dagger a_i + 2MSJ \sum_{i,\delta} (a_i b_{i+\delta} + a_i^\dagger b_{i+\delta}^\dagger) \tag{6}$$

where

$$\omega_\pm = (2MSJ - g\mu_B (B \pm B_A))$$

where M is the number of nearest neighbors of an atom and

$$E_0 = -2NMSJ - 2NSg\mu_B B_A.$$

3. Notation and Propagator of a Spin System in Terms of Grassmann Coherent States

The generalized coherent states path integrals over the years has positioned itself as an excellent tool for studying quantum problems in many-body or in which we are dealing with a spin system [6] [7] [8]. In this work, we proposed to de-

velop a functional integral from the propagator associated to a given spin 1/2 Hamiltonian H in terms of a complete set of states $|\xi, \zeta\rangle = |\xi_n \cdots \xi_1, \zeta_n \cdots \zeta_1\rangle$ where $\xi_n \cdots \xi_1$ and $\zeta_n \cdots \zeta_1$ are Grassmann variables. To achieve this goal, we will use the method which consists in partitioning the time interval $[t', t]$ into N intervals by points τ_r with $\tau_0 \equiv t', \tau_N \equiv t$ and $\Delta\tau_r \equiv \tau_{(r+1)} - \tau_r$. Using the partitioning technique the feynman, the propagator that joins two Grassmann coherent states $\langle \xi, \zeta |$ and $|\xi, \zeta\rangle$ takes the form of an infinite product of short-time propagators.

$$\begin{aligned} & \langle \xi', \zeta' | T \exp\left(-\frac{i}{\hbar} \int_{t'}^t H(\tau) d\tau\right) | \xi, \zeta \rangle \\ &= \lim_{\max \Delta\tau_r \rightarrow 0} \int \left[\prod_{r=0}^{N-1} \langle \xi^{(r)}, \zeta^{(r)} | 1 - \frac{i}{\hbar} H(\tau_r) \Delta\tau_r | \xi^{(r+1)}, \zeta^{(r+1)} \rangle \right] \prod_{r=1}^{N-1} d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) \end{aligned} \tag{7}$$

where, the rule of discarding $\mathcal{O}(\Delta\tau^2)$ terms has been employed. $\xi^{(N)} = \xi, \xi^{(0)} = \xi'$ and $\zeta^{(N)} = \zeta, \zeta^{(0)} = \zeta'$, here T is the Dyson time-ordering operator, and the integration measure is given by:

$$d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) = \prod_{j=1}^n (1 - \bar{\xi}_{n+1-j} \xi_{n+1-j}) (1 - \bar{\zeta}_{n+1-j} \zeta_{n+1-j}) d^n \bar{\xi} d^n \xi d^n \bar{\zeta} d^n \zeta \tag{8}$$

with

$$d^n \bar{\mathcal{L}} = d\bar{\mathcal{L}}_1 d\bar{\mathcal{L}}_2 \cdots d\bar{\mathcal{L}}_n \text{ and } d^n \mathcal{L} = d\mathcal{L}_1 d\mathcal{L}_2 \cdots d\mathcal{L}_n \tag{9}$$

where, $\mathcal{L} = \xi$ or ζ . We therefore considered a system for which the particles can go to n-channels. The system being made up of two subsystems, we assumed that the vacuum state $|0\rangle$ is the product of the vacuum states of the respective subsystems a and b that we defined by $|0_a\rangle$ and $|0_b\rangle$. In this way, the state of the subsystems is defined as follows:

$$|\xi\rangle = \exp(a^\dagger \xi) |0_a\rangle = \exp\left(\sum_{j=1}^n a_j^\dagger \xi_j\right) |0_a\rangle \tag{10}$$

and

$$|\zeta\rangle = \exp(b^\dagger \zeta) |0_b\rangle = \exp\left(\sum_{j=1}^n b_j^\dagger \zeta_j\right) |0_b\rangle \tag{11}$$

Assuming that the different states of each subsystem that makes up the global system are independent of each other, then the final state of the system can take the form $|\xi, \zeta\rangle = |\xi\rangle |\zeta\rangle$. The final state of the all the system can be represent on this form:

$$|\xi, \zeta\rangle = \exp(b^\dagger \zeta) |0_b\rangle = \exp\left[\sum_{j=1}^n (a_j^\dagger \xi_j + b_j^\dagger \zeta_j)\right] |0\rangle \tag{12}$$

where, $|0\rangle = |0_a\rangle |0_b\rangle$ avec $|0_a\rangle$ and $|0_b\rangle$ which respectively represent the fermion vacuum state for the sublattice a and b. For each degree of freedom, that the state for this 2n-site system can be represented by:

$$\begin{aligned}
 |\xi_n \cdots \xi_1, \zeta_n \cdots \zeta_1\rangle &= \prod_{j=1}^n \delta(a_{n+1-j}^\dagger - \xi_{n+1-j}) \delta(b_{n+1-j}^\dagger - \zeta_{n+1-j}) |0\rangle \\
 &= \sum_{m=0}^n A_m B_m |0\rangle
 \end{aligned}
 \tag{13}$$

where, $A_0 = B_0 = 1$ and which can be generalized as follows:

$$A_m = \sum_{\alpha_m > \alpha_{m-1} > \cdots > \alpha_1 = 1} \left(\prod_{i=1}^m a_{m+1-i}^\dagger \right) \xi_{\alpha_1 \cdots \alpha_m} \tag{14}$$

and

$$B_m = \sum_{\beta_m > \beta_{m-1} > \cdots > \beta_1 = 1} \left(\prod_{i=1}^m b_{m+1-i}^\dagger \right) \xi_{\beta_1 \cdots \beta_m} \tag{15}$$

with $(m \geq 1)$. In the expressions [14] and [15], the notations ξ_{jlk} and ζ_{jlk} stands respectively for the products $\xi_j \xi_l \xi_k$ and $\zeta_j \zeta_l \zeta_k$. We see that the state of each sublattice $|\xi_n \cdots \xi_1\rangle$ and $|\zeta_n \cdots \zeta_1\rangle$ contains all possible independent $0, 1, 2, \dots, n$ fermion states. Each of its states being associated with either A_m and B_m or they are included only once and that any permutation of their operators is capable of generating dependent states [17]. The totality of these $2n$ -site states forms a complete set in the sense [12]

$$\underbrace{\int \cdots \int}_{2n} \int \cdots \int_{2n} |\xi_n \cdots \xi_1, \zeta_n \cdots \zeta_1\rangle \langle \xi_n \cdots \xi_1, \zeta_n \cdots \zeta_1 | d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) = 1 \tag{16}$$

where, its evaluation used the standard properties of integration of Grassmann variables namely:

$$\int d\bar{\mathcal{L}}_j \mathcal{L}_j (1 - \bar{\mathcal{L}}_j \mathcal{L}_j) \begin{pmatrix} \bar{\mathcal{L}}_j \mathcal{L}_j \\ \bar{\mathcal{L}}_j \\ \mathcal{L}_j \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{17}$$

Consider two coherent Grassmann states, by definition they are not orthogonal and therefore overlap is given by:

$$\begin{aligned}
 \langle \xi', \zeta' | \xi, \zeta \rangle &= \sum_{m=0}^n \langle 0_a | A_m^{\dagger} A_m | 0_a \rangle \langle 0_b | B_m^{\dagger} B_m | 0_b \rangle \\
 &= \prod_{k=1}^n (1 + \bar{\xi}'_k \xi_k) (1 + \bar{\zeta}'_k \zeta_k)
 \end{aligned}
 \tag{18}$$

with the fact that the matrix elements between states in the Fock space and coherent states contain Grassmann numbers, by imposing anti-periodic boundary conditions, it follows that the trace is worth.

$$\underbrace{\int \cdots \int}_{2n} \int \cdots \int_{2n} d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) \langle -\xi', -\zeta' | \xi, \zeta \rangle = 2^{2n} \tag{19}$$

As expected, Equation (19) clearly represents the dimension of the Grassmann space with $2n$ generators, which corresponds to the number of all possible mixtures of up and down spins. By defining the matrix elements of rank $m \times m$ is:

$$t_{\theta_1 \dots \theta_m} = \begin{cases} 1, & \text{if } \theta_1 > \theta_2 > \dots > \theta_m \\ 0, & \text{otherwise} \end{cases} \quad \theta_i = \alpha_i \text{ or } \beta_i, \quad i = 1, \dots, m \quad (20)$$

this allows the elimination of restrictions in the sums of the Equation (18) which makes it possible to give the overlap of the two states the following form:

$$\langle \xi', \zeta' | \xi, \zeta \rangle = 1 + \sum_{m=0}^n \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}} \bar{\xi}_{\alpha_m \dots \alpha_1}^{(r)} \xi_{\alpha_m \dots \alpha_1}^{(r+1)} \bar{\zeta}_{\beta_m \dots \beta_1}^{(r)} \zeta_{\beta_m \dots \beta_1}^{(r+1)} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \quad (21)$$

4. Fermionic Path Integral for a the Spin Hamiltonian

In this section, we planned to study the spin system in interaction with the environment via the path integral by using these Grassmann variables as a basis set. In quantum mechanics, all the information for the evaluation of a system can be stored in the propagator between an initial state $|\xi, \zeta\rangle$ and a final state $\langle \xi', \zeta'|$ at a time $t = t_f - t_i$. This propagator as a function of the Grassmann variables can be written:

$$\begin{aligned} & \langle \xi', \zeta' | \exp\left(-\frac{i\Delta\tau}{\hbar} H\right) | \xi, \zeta \rangle \\ &= \lim_{\max \Delta\tau_r \rightarrow 0} \int \dots \int \left[\prod_{r=0}^{N-1} \langle \xi^{(r)}, \zeta^{(r)} | 1 - \left(\frac{i\Delta\tau}{\hbar}\right) H | \xi^{(r+1)}, \zeta^{(r+1)} \rangle \right] \prod_{r=1}^{N-1} d^{2n} \mu(\bar{\xi}^{(r)}, \xi^{(r)}) d^{2n} \mu(\bar{\zeta}^{(r)}, \zeta^{(r)}) \end{aligned} \quad (22)$$

$\xi^{(r)}$ and $\zeta^{(r)}$ in the equation (22), stands for the state $(\xi_n^{(r)} \dots \xi_1^{(r)})$ and $(\zeta_n^{(r)} \dots \zeta_1^{(r)})$. To simplify the notation, we have assumed $\Delta t = (t - t')/N \equiv \Delta\tau/N = \Delta\tau_r$ where the superscript r designates the Grassmann complex variables. For convenience, rewriting our Hamilton (3) in the form:

$$H = H^{(0)} + H^{(1)} + H^{(2)} \quad (23)$$

where $H^{(0)}$ and $H^{(1)}$ have the follow form:

$$H^{(0)} = -g\mu_B B S_0^z + E_0, \quad (24)$$

and

$$H^{(1)} = \omega_1 \sum_i a_i^\dagger a_i + \omega_2 \sum_i b_i^\dagger b_i, \quad (25)$$

with

$$\omega_{1,2} = 2MSJ - 2g\mu_B (B \pm B_A) \pm \frac{gS_0^z}{\sqrt{N}},$$

$$\omega = \omega_1 + \omega_2 = 4MSJ - 2g\mu_B B$$

and

$$H^{(2)} = 2MSJ \sum_{i,\delta} (a_i b_{i+\delta} + a_i^\dagger b_{i+\delta}^\dagger) \quad (26)$$

We easily find that each short-time propagator involved in Equation (22) can be expressed as

$$\begin{aligned} & \left\langle \xi^{(r)}, \zeta^{(r)} \left| 1 - \frac{i\Delta t}{\hbar} H \right| \xi^{(r+1)}, \zeta^{(r+1)} \right\rangle \\ &= \left\langle \xi^{(r)}, \zeta^{(r)} \left| \xi^{(r+1)}, \zeta^{(r+1)} \right\rangle - \frac{i\Delta t}{\hbar} \sum_{m=0}^n \left(H_{mm}^{0(r,r+1)} + H_{mm}^{1(r,r+1)} + H_{mm}^{2(r,r+1)} \right) \end{aligned} \tag{27}$$

For its evaluation, it is now a question of calculating the following matrix elements:

$$\left\langle \xi^{(r)}, \zeta^{(r)} \left| H^\gamma \right| \xi^{(r+1)}, \zeta^{(r+1)} \right\rangle = \sum_{m=0}^n \langle 0 | B_m^{\dagger(r)} A_m^{\dagger(r)} H^\gamma A_m^{(r+1)} B_m^{(r+1)} | 0 \rangle = \sum_{m=0}^n H_{mm}^{\gamma(r,r+1)} \tag{28}$$

with $\gamma = 0, 1, 2$. $A_m^{(r)}$ and $B_m^{(r)}$ are given by Equations (14) and (15), corresponds to the r^{th} point of the time partition. Knowing that $A_0 = B_0 = 1$, the calculation of the zero-th order matrix elements $H_{mm}^{0(r,r+1)}$ give

$$\begin{aligned} H_{00}^{0(r,r+1)} &= H^0, \\ H_{11}^{0(r,r+1)} &= H^0 \sum_{j=1}^n \bar{\xi}_j^{(r)} \xi_j^{(r+1)} \bar{\zeta}_j^{(r)} \zeta_j^{(r+1)}, \\ H_{22}^{0(r,r+1)} &= H^0 \sum_{l>j=1}^n \bar{\xi}_{jl}^{(r)} \xi_{lj}^{(r+1)} \bar{\zeta}_{jl}^{(r)} \zeta_{lj}^{(r+1)}, \\ H_{33}^{0(r,r+1)} &= H^0 \sum_{k>l>j=1}^n \bar{\xi}_{jlk}^{(r)} \xi_{klj}^{(r+1)} \bar{\zeta}_{jlk}^{(r)} \zeta_{klj}^{(r+1)} \end{aligned}$$

By recurrence, we get the general form of order m,

$$H_{mm}^{0(r,r+1)} = H^0 \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}}^n \bar{\xi}_{\alpha_m \dots \alpha_1}^{(r)} \xi_{\alpha_m \dots \alpha_1}^{(r+1)} \bar{\zeta}_{\beta_m \dots \beta_1}^{(r)} \zeta_{\beta_m \dots \beta_1}^{(r+1)} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \quad (m \geq 1) \tag{29}$$

Analogously, the first-order matrix elements $H_{mm}^{1(r,r+1)} = 0$ gave us:

$$H_{mm}^{1(r,r+1)} = m\omega \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}}^n \bar{\xi}_{\alpha_m \dots \alpha_1}^{(r)} \xi_{\alpha_m \dots \alpha_1}^{(r+1)} \bar{\zeta}_{\beta_m \dots \beta_1}^{(r)} \zeta_{\beta_m \dots \beta_1}^{(r+1)} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \quad (m \geq 1) \tag{30}$$

where, $H_{00}^{1(r,r+1)} = 0$ for $k < 0$. Taking into account that $\langle 0 | a_i b_{i+\delta} | 0 \rangle = \langle 0 | a_i^\dagger b_{i+\delta}^\dagger | 0 \rangle = 0$ then the thrid-order matrix elements $H_{mm}^{2(r,r+1)} = 0$. Thus, it follows from Equations ((29), (30)) that the sum of the diagonal matrix elements of the Hamiltonian (23) can be expressed as:

$$\begin{aligned} & \left\langle \xi^{(r)}, \zeta^{(r)} \left| 1 - \frac{i\Delta t}{\hbar} H \right| \xi^{(r+1)}, \zeta^{(r+1)} \right\rangle \\ &= 1 + \sum_{m=0}^n \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}}^n \bar{\xi}_{\alpha_m \dots \alpha_1}^{(r)} \xi_{\alpha_m \dots \alpha_1}^{(r+1)} \bar{\zeta}_{\beta_m \dots \beta_1}^{(r)} \zeta_{\beta_m \dots \beta_1}^{(r+1)} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \left(1 - \frac{i\Delta t}{\hbar} (H^0 + m\omega) \right) \end{aligned} \tag{31}$$

The evaluation of $I_1(\bar{\xi}^{(r)}, \bar{\zeta}^{(r)}, \xi^{(2)}, \zeta^{(2)})$ which represents the propagator between the states $\bar{\mathcal{L}}^{(r)}, \mathcal{L}^{(2)}$ allows to evaluate the proponent of our system which is given in Equation (24).

$$\begin{aligned} I_1(\bar{\xi}^{(r)}, \bar{\zeta}^{(r)}, \xi^{(2)}, \zeta^{(2)}) &= \underbrace{\int \dots \int}_{2n} \left\langle \xi^{(1)}, \zeta^{(1)} \left| 1 - \frac{i\Delta t}{\hbar} H \right| \xi^{(1)}, \zeta^{(1)} \right\rangle \\ &\quad \times \left\langle \xi^{(1)}, \zeta^{(1)} \left| 1 - \frac{i\Delta t}{\hbar} H \right| \xi^{(2)}, \zeta^{(2)} \right\rangle d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) \end{aligned} \tag{32}$$

Using integration properties of Grassmann variables (17) you have:

$$\begin{aligned} & \langle \xi', \zeta' | 1 - \frac{i\Delta t}{\hbar} H | \xi, \zeta \rangle \\ &= 1 + \sum_{m=0}^n \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}} \xi_{\alpha_m \dots \alpha_1}^{(2)} \zeta_{\beta_m \dots \beta_1}^{(2)} \bar{\xi}'_{\alpha_m \dots \alpha_1} \bar{\zeta}'_{\beta_m \dots \beta_1} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \left(1 - \frac{i\Delta t}{\hbar} (H^0 + m\omega) \right)^2 \end{aligned} \quad (33)$$

By carrying out $N - 1$ integrations of this type and by making repeated use of the completeness relation (16), the propagator (22) can easily be expressed in the following manner:

$$\begin{aligned} & \langle \xi', \zeta' | 1 - \frac{i\Delta t}{\hbar} H | \xi, \zeta \rangle \\ &= \lim_{\Delta t \rightarrow 0} \left[1 + \sum_{m=0}^n \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}} \xi_{\alpha_m \dots \alpha_1} \zeta_{\beta_m \dots \beta_1} \bar{\xi}'_{\alpha_m \dots \alpha_1} \bar{\zeta}'_{\beta_m \dots \beta_1} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \left(1 - \frac{i\Delta t}{\hbar} (H^0 + m\omega) \right)^N \right] \end{aligned} \quad (34)$$

Thus, in the limit $N \rightarrow \infty$ and $\Delta t = \Delta \tau / N$ we get

$$\begin{aligned} & \langle \xi', \zeta' | 1 - \frac{i\Delta t}{\hbar} H | \xi, \zeta \rangle \\ &= 1 + \sum_{m=0}^n \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}} \xi_{\alpha_m \dots \alpha_1} \zeta_{\beta_m \dots \beta_1} \bar{\xi}'_{\alpha_m \dots \alpha_1} \bar{\zeta}'_{\beta_m \dots \beta_1} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} \exp \left(1 - \frac{i\Delta t}{\hbar} (H^0 + m\omega) \right) \end{aligned} \quad (35)$$

The expression (35) represents the propagator of our Hamiltonian from the path integrals assuming discrete time. Insofar as we consider N , time can be assumed to be continuous. This consideration should not sow confusion with the formalism which takes into account continuous time [12].

5. Thermodynamic Parameter

In order to express the imaginary time partition function, involving the antiperiodic boundary condition $-\mathcal{L}_k^{(0)} (\equiv -\mathcal{L}_k^t) = \mathcal{L}_k^{(N)} (\equiv \mathcal{L}_k)$ ($k = 1, 2, \dots, n$) performing an analytic continuation to Euclidean times through the Wick rotation, $\Delta \tau \rightarrow -i\Delta \tau$, and, the subsequent substitution $\Delta \tau / \hbar \rightarrow \beta (\equiv 1/kT)$, the trace formula therefore makes it possible to define the partition function in the following manner:

$$\begin{aligned} Z &= T_r \exp(-\beta H) \\ &= \underbrace{\int \dots \int}_{2n} \langle -\xi, -\zeta | -\beta H | \xi, \zeta \rangle d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta), \end{aligned} \quad (36)$$

By entering (14) and (15) and using Equation (17) the evaluation of the 4n-dimensional integrals of the Equation (36) gives us:

$$\begin{aligned} & \underbrace{\int \dots \int}_{2n} \sum_{\substack{\alpha_j=1; 1 \leq j \leq m \\ \beta_j=1; 1 \leq j \leq m}} \xi_{\alpha_m \dots \alpha_1} \zeta_{\beta_m \dots \beta_1} \bar{\xi}'_{\alpha_m \dots \alpha_1} \bar{\zeta}'_{\beta_m \dots \beta_1} t_{\alpha_1 \dots \alpha_m} t_{\beta_1 \dots \beta_m} d^{2n} \mu(\bar{\xi}, \xi) d^{2n} \mu(\bar{\zeta}, \zeta) \\ &= \binom{n}{m}^2, \end{aligned} \quad (37)$$

It therefore becomes obvious to write the imaginary time partition function in the following simplified form:

$$Z(n) = 1 + \sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \tag{38}$$

which allows us to have the expression of free energy in the following form

$$E = \frac{\sum_{m=0}^n \binom{n}{m}^2 (m\omega + H^0) \exp[-\beta(m\omega + H^0)]}{k \left(1 + \sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right)} \tag{39}$$

within the limit of very high temperatures $\beta \rightarrow 0$ and assuming that

$1 \ll \sum_m \binom{n}{m}^2$, the energy of the system gives

$$E(n) = n\omega \binom{2n-1}{n-1} \binom{n}{m}^{-1} + H^0 \tag{40}$$

In the thermodynamic limit, $\beta \rightarrow \infty$, the energy in our system is zero. Several other parameters can be determined from this partition function. The magnetization is

$$M = \frac{\mathcal{N} \beta g \mu_B}{nZ(n)} \sum_{m=0}^n \binom{n}{m}^2 (2m + S_0^z) \exp[-\beta(m\omega + H^0)] \tag{41}$$

with \mathcal{N} represents the number of spins per unit volume. From magnetization we easily deduce the isothermal susceptibility:

$$\chi_T \sim \frac{\mathcal{N}}{n} \left(\frac{\beta g \mu_B}{Z(n)} \right)^2 \prod_{i=0}^2 \left((-1)^{i+1} \sum_{m=0}^n \binom{n}{m}^2 2m \exp[-\beta(m\omega + H^0)] \right) + (iZ(n) - 1) S_0^z + (i-1) mZ(n) \tag{42}$$

Usually for a spin system without interaction this susceptibility is normalized to the Curie value. Considering Equation (38), we found that the Helmholtz free energy can be found from the statistical mechanical definition:

$$F = -T k_B \ln \left(1 + \sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right) \tag{43}$$

We find the Boltzmann entropy as S

$$S = \frac{\sum_{m=0}^n \binom{n}{m}^2 (m\omega + H^0) \exp[-\beta(m\omega + H^0)]}{T \left(1 + \sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right)} \tag{44}$$

and the specific heat capacity at a constant volume

$$C_v = \frac{S^2}{k_B} + \frac{\sum_{m=0}^n \binom{n}{m}^2 (m\omega + H^0) \exp[-\beta(m\omega + H^0)]}{k_B T^2 \left(1 + \sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right)} \quad (45)$$

From the results obtained, we observe that all the thermodynamic parameters of our system depend fundamentally on the parameter

$\left(\sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right)$ which is an exponential function which depends on the number of particles which constitute the system.

$\left(\sum_{m=0}^n \binom{n}{m}^2 \exp[-\beta(m\omega + H^0)] \right)$ then represents a control parameter of our system.

6. Conclusion

In this article, we have developed a formalism based on path integrals to study the dynamics of a central spin coupled to an antiferromagnetic environment together bathing in an external magnetic field. To achieve this objective, we made use of the discrete-time propagator method associated with a basic set involving coherent states of Grassmann variables which made it possible to obtain the analytical propagator. In the study, Hamiltonian was expressed in quadratic form using the creation and annihilation operators. From this transformation, the environment was split into two subnets. The quadratic form involved in the model was diagonalized and naturally led us to a complete set of states from which it was evident by using the coherent states of the Grassmann variables to evaluate the propagator. Thanks to the propagator, it becomes obvious to evaluate the partition function as well as the thermodynamic parameters. Since the partition function Z extends over all quantum states. The evaluation of this partition function Z shows that it extends over all quantum states. Grassmann's coherent states positioned itself as a perfect tool for studying open quantum system consisting of spin. Our study shows that the energy of our system depends on the number of atom sites that make up the system when $\beta \rightarrow 0$.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

References

- [1] Schulman, L.S. (2012) *Techniques and Applications of Path Integration*. Wiley Interscience, New York.
- [2] Campolieti, G. and Brumer, P. (1994) Semiclassical Propagation: Phase Indices and the Initial-Value Formalism. *Physical Review A*, **50**, 997-1018.
<https://doi.org/10.1103/PhysRevA.50.997>

- [3] Kay, K.G. (1994) Integral Expressions for the Semiclassical Time Dependent Propagator. *The Journal of Chemical Physics*, **100**, 4377. <https://doi.org/10.1063/1.466320>
- [4] Maranon, J. and Grinberg, H. (1984) Feynman Path Integral and the Hückel Model. *The Journal of Chemical Physics*, **81**, 4537. <https://doi.org/10.1063/1.447425>
- [5] Bochicchio, H.R.C. (1990) Feynman Path-Integral Representation of Field Operators and Memory Superoperators in a Liouville Space. *Physical Review A*, **41**, 5814-5819. <https://doi.org/10.1103/PhysRevA.41.5814>
- [6] Klauder, J.R. (1979) Path Integrals and Stationary Phase Approximations. *Physical Review D*, **19**, 2349-2356.
- [7] Kuratsuji, H. and Suzuki, T. (1980) Path Integral in the Representation of SU(2) Coherent State and Classical Dynamics in a Generalized Phase Space. *Journal of Mathematical Physics*, **21**, 472-476. <https://doi.org/10.1103/PhysRevC.24.1740>
- [8] Blaizot, J.P. and Orland, H. (1981) Path Integrals for the Nuclear Many-Body Problem. *Physical Review C*, **24**, 1740.
- [9] Kuratsuji, H. and Suzuki, T. (1980) Coherent States: Applications in Physics and Mathematical. *Journal of Mathematical Physics*, **21**, 472.
- [10] Anderson, L.M. (2001) Quantum Dynamics Using a Discretized Coherent State Representation: An Adaptive Phase Space Method. *The Journal of Chemical Physics*, **115**, 1158-1165.
- [11] Shibata, J. and Takagi, S. (1999) A Note on Spin Coherent State Path Integral. *International Journal of Modern Physics B*, **13**, 107-140.
- [12] Grinberg, H. (2003) Path Integral of Spin Models. *Physics Letters A*, **311**, 133-144. [https://doi.org/10.1016/S0375-9601\(03\)00464-X](https://doi.org/10.1016/S0375-9601(03)00464-X)
- [13] Anicich, P.G.O. and Grinberg, H.J. (2003) Grassmann Coherent States for Spin Systems. *Journal of Molecular Structure: THEOCHEM*, **9**, 621. [https://doi.org/10.1016/S0166-1280\(02\)00528-6](https://doi.org/10.1016/S0166-1280(02)00528-6)
- [14] Kuratsuji, H. and Mizobuchi, Y. (1981) A Semiclassical Treatment of Path Integrals for the Spin System. *Journal of Mathematical Physics*, **22**, 757. <https://doi.org/10.1063/1.524980>
- [15] Zyczkowski, K. and Slomczynski, W. (2001) The Monge Metric on the Sphere and Geometry of Quantum States. *Journal of Physics A: Mathematical and General*, **34**, 6689-6722. <https://doi.org/10.1088/0305-4470/34/34/311>
- [16] Samuel, S.J. (1980) The Use of Anticommuting Variable Integrals in Statistical Mechanics. I. The Computation of Partition Functions. *Journal of Physics A: Mathematical and General*, **21**, 2806. <https://doi.org/10.1063/1.524404>
- [17] Anicich, P.G.O. and Grinberg, H. (2002) Grassmann Coherent States Representation of the Path Integral: Evaluation of the Generating Function for Spin Systems. *International Journal of quantum Chemistry*, **90**, 1562-1576. <https://doi.org/10.1002/qua.10342>
- [18] Yuan, H.X.Z. and Zhu, K.D. (2007) Influence of an External Magnetic Field on the Decoherence of a Central Spin Coupled to an Antiferromagnetic Environment. *New Journal of Physics*, **9**, 219. <https://doi.org/10.1088/1367-2630/9/7/219>
- [19] Yuan, X.-Z., Zhu, K.-D. and Wu, Z.-J. (2005) Two-Qubit Entanglement in an Antiferromagnetic Environment. *The European Physical Journal D*, **33**, 129-132. <https://doi.org/10.1140/epjd/e2005-00023-y>
- [20] Brouard, J.S. (2004) Decoherence of Trapped-Ion Internal and Vibrational Modes: The Effect of Fluctuating Magnetic Fields. *Physical Review A*, **70**, Article ID: 013413.

<https://doi.org/10.1103/PhysRevA.70.013413>

- [21] Rossini, D., Calarco, T., *et al.* (2007) Decoherence Induced by Interacting Quantum Spin Baths. *Physical Review A*, **75**, Article ID: 032333.
- [22] Yosida, K. (1996) Theory of Magnetism. Springer Series in Solid-State Sciences 5.
- [23] Madelung, O. (1980) Introduction to Solid-State Theory. Springer, Berlin.