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Quantum thermal expectation values from an effective atomistic spin dynamics model using path integrals.

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In previous work, we have developed a method to approximate quantum thermal expectation values of spin systems using a path integral approach in the framework of atomistic spin dynamics. In the present work, we extend this model from a single spin coupled to a constant magnetic field, to the more general case of a system of spins coupled by isotropic Heisenberg interaction, in a potentially time-dependent magnetic field. In a first approximation, the classical atomistic model is extended by an effective field which for every interaction pair, depends only on the two interacting spins. This implies that we have a straightforward generalisation from 2 to N interacting spins. We compare our results to exactly solvable cases using exact diagonalisation for two-spins.

***Index Terms*—Atomistic spin dynamics, Path-integrals, Quantum spin systems, Stochastic simulations.**

I. Introduction

IN CONDENSED MATTER physics, it can be a useful trick to map a classical system onto a quantum equivalent one, which can sometimes be more easily solved. As a rule of thumb, however, solving quantum problems is more tricky because of the exponential scaling of the Hilbert space with the size of systems. Hence a more popular approach is to map, or at least to build an approximation method from the initial quantum problem to a more readily solvable classical one. This is often called classicalisation and is used in the context of quantum optics where one can approximate a quantum system in contact with a thermostat as a classical but stochastic system, depending on the bath properties [1]. Following this idea, and inspired by path integral molecular dynamics [2], we have developed an approach in the context of atomistic spin dynamics [3] for deriving quantum thermal expectation values of quantum spin systems using a path integral approach. In the present work, we have extended our former model from a single spin interacting with a constant magnetic field [4], to a system of two spins coupled by Heisenberg interaction and a more general - potentially time-dependent - magnetic field.

II. The quantum system at hand

We begin with two quantum spins defined by their joint state $|QS\rangle \equiv |s_1, m_1; s_2, m_2\rangle$ and the action of the operators $\hat{\vec{S}}^{(i)}$ and $\hat{S}_z^{(i)}$ on these states

$$\begin{cases} \left(\hat{\vec{S}}^{(i)}\right)^2 |s_1, m_1; s_2, m_2\rangle = s_i(s_i+1)\,|s_1, m_1; s_2, m_2\rangle \\ \hat{S}_z^{(i)}\,|s_1, m_1; s_2, m_2\rangle = m_i\,|s_1, m_1; s_2, m_2\rangle\,. \end{cases} \quad (1)$$

As mentioned in the introduction, they are coupled to each other by isotropic Heisenberg exchange and to an external field by a Zeeman interaction

$$\hat{\mathcal{H}} = -\frac{g\mu_B}{\hbar}\vec{B}\cdot\left(\hat{\vec{S}}_1 + \hat{\vec{S}}_2\right) - \frac{J}{\hbar^2}\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2 \quad (2)$$

where g is the electronic lande g-factor, μ_B is the Bohr magneton, $\hbar$ is Planck's reduced constant and J is the exchange constant. This yield a partition function defined as the following trace

$$\mathcal{Z} = \sum_{(m_1,m_2)=-(s_1,s_2)}^{(s_1,s_2)} \langle QS|\, e^{-\beta\hat{\mathcal{H}}}\,|QS\rangle \quad (3)$$

where $\beta = \frac{1}{k_B T}$, k_B is Boltzmann's constant and T is the temperature. For $\vec{B}$ constant, one can always choose the quantisation axis such that only B_z is non-zero and it is then always possible (in principle) to exactly solve by diagonalisation of the Hamiltonian [5]. This is useful to provide a reference to compare to the approximated scheme, which we will derive in the next section and which can be used more generally.

III. Effective Hamiltonian derivation procedure

A. From a discrete to a continuous description

The first step is always, as was the case in our previous work, to use spin coherent states [6] labeled as $|z_1; z_2\rangle$, defined as

$$|z_1; z_2\rangle = \frac{\left(1+|z_1|^2\right)^{-s}}{\left(1+|z_1|^2\right)^{s}} \exp\left(\frac{z_1}{\hbar}\hat{S}_-^{(1)} + \frac{z_2}{\hbar}\hat{S}_-^{(2)}\right)|0\rangle \quad (4)$$

where $|0\rangle \equiv |s_1, s_1; s_2, s_2\rangle$ and z_1 and z_2 are complex. Using these spin coherent states, we recover a continuous description in terms of an integral partition function, rather than a sum

$$\mathcal{Z} = \int d\mu(z_1) d\mu(z_2)\,\langle z_1; z_2|\, e^{-\beta\hat{\mathcal{H}}}\,|z_1; z_2\rangle \quad (5)$$

where the integration measures are required to ensure the resolution of unity. Up to this point, the method is exact. To go further, we need to be able to compute an approximation of the expectation value contained in (5).

B. Approximating expectation values

We now we expand the exponential as

$$\langle z_1; z_2| e^{-\beta\hat{\mathcal{H}}} |z_1; z_2\rangle = 1 - \beta \langle z_1; z_2| \hat{\mathcal{H}} |z_1; z_2\rangle + \frac{\beta^2}{2} \langle z_1; z_2| \hat{\mathcal{H}}^2 |z_1; z_2\rangle + \dots \tag{6}$$

where the first corrections appear in the term $\frac{\beta^2}{2} \langle z_1; z_2| \hat{\mathcal{H}}^2 |z_1; z_2\rangle$. Depending on the desired order N of approximation, one needs to compute $\frac{\beta^N}{N} \langle z_1; z_2| \hat{\mathcal{H}}^{N+1} |z_1; z_2\rangle$ which yields an approximate expression of the form

$$\langle z_1; z_2| e^{-\beta\hat{\mathcal{H}}} |z_1; z_2\rangle \approx F[\beta, z_1, \bar{z}_1, z_2, \bar{z}_2] \tag{7}$$

Here again the spin coherent states prove useful as there is a mapping from the spin coherent states, in terms of complex z_1 and z_2, to unit vectors $\vec{n}_1$ and $\vec{n}_2$ such that

$$F[\beta, z_1, \bar{z}_1, z_2, \bar{z}_2] = F[\beta, \vec{n}_1, \vec{n}_2] \tag{8}$$

It is this expression that is used to derive an effective classical Hamiltonian.

C. Mapping to classical Hamiltonian

Once we have an expression in terms of classical vectors, we need to rewrite the approximated form (8) as an exponential. Taking the exponential of the logarithm, we have

$$F[\beta, \vec{n}_1, \vec{n}_2] = \exp(\ln(F[\beta, \vec{n}_1, \vec{n}_2])) \tag{9}$$

and we know that $F[\beta, \vec{n}_1, \vec{n}_2] = 1 + f[\beta, \vec{n}_1, \vec{n}_2]$ where $f[\beta, \vec{n}_1, \vec{n}_2] \to 0$ as $\beta \to 0$. Hence we can perform a Taylor expansion as $\beta \to 0$ for the logarithm, and we finally end up with an expression of the required form

$$\mathcal{Z}_{\text{app}} = \int d\vec{n_1} d\vec{n_2} e^{\beta \mathcal{H}_{\text{eff}}[\beta, \vec{n_1}, \vec{n_2}]}. \tag{10}$$

where the effective Hamiltonian is temperature dependent. We will now use this effective Hamiltonian for atomistic spin dynamics simulations

IV. Atomistic simulations

Using the standard method of atomistic spin dynamics, we can derive an effective field from the Hamiltonian as

$$\vec{B}^{(i)}_{\text{eff}} = -\frac{1}{g\mu_B s} \frac{\partial \mathcal{H}_{\text{eff}}}{\partial \vec{n}_i} \tag{11}$$

where $\vec{n}$ is our normalised magnetic moment, which is then dynamically sampled with the Landau-Lifshitz-Gilbert equation

$$\dot{\vec{n}}^{(i)} = -\frac{\gamma}{1+\alpha^2} \left(\vec{n}^{(i)} \times \vec{B}^{(i)}_{\text{eff}} + \alpha \vec{n}^{(i)} \left(\vec{n}^{(i)} \times \vec{B}^{(i)}_{\text{eff}} \right) \right) \tag{12}$$

where γ is the gyromagnetic ratio and α is the Gilbert damping parameter.

We have performed atomistic simulations of (12) using a symplectic integration scheme, for the exactly solvable case of 2-spins in a constant magnetic field along the z-direction. Results are displayed in Fig. 1 along with exact diagonalisation results as a reference.

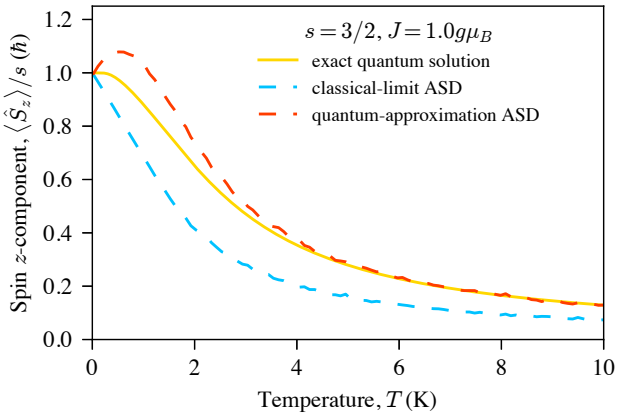

Fig. 1. Total spin z-component normalised expectation value as a function of temperature for $s = 3/2$ and $J = g\mu_B$. Dashed curves are results from atomistic simulations for the classical limit (blue) and first quantum correction (red) as $\langle \hat{S}_z \rangle / s = n_z = 0.5 \left(n_z^{(1)} + n_z^{(2)} \right)$. The yellow line is obtained by exact diagonalisation.

The results show that for very low temperatures, our model struggles to capture the correct expectation value and grows above the value of the normalisation (we would like to emphasize that the expectation values require a normalisation factor for reasons specified in [4]). However, the quantum corrected model very quickly moves towards the exact quantum solution and around $T = 3K$ we obtain results very close to the quantum expectation value with our approximate method, significantly improving on the classical model.

V. Conclusion

We have shown that it is possible to approximate quantum thermal expectation values of interacting quantum systems using a path-integral approach in the framework of atomistic spin dynamics simulations. In this method, the underlying quantum nature of the spins is translated into an effective field which contains both the classical limit, as well as additional terms which represent quantum fluctuations in an effective way. Moreover, in a first approximation, the effective field depends only on the interacting pair and can thus straightforwardly be generalised to N interacting spins, providing a way to efficiently simulate quantum thermal expectation values for very large interacting spin systems.

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