

Thermodynamic Properties and Decoherence of a Central Electron Spin of Atom Coupled to an Anti-Ferromagnetic Spin Bath

Martin Tchoffo, Georges Collince Fouokeng*, Lukong Cornelius Fai, Mathurin Esouague Ateuafack

Mesoscopic and Multilayer Structures Laboratory, Department of Physics, Faculty of Science,
University of Dschang, Dschang, Cameroon
Email: *fouokengge2012@yahoo.fr

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ABSTRACT

The decoherence of a central electron spin of an atom coupled to an anti-ferromagnetic spin bath in the presence of a time varying B-Field (VBF) is investigated applying the Holstein-Primak off and Bloch transformations approaches. The Boltzmann entropy and the specific heat capacity at a given temperature are obtained and show the correlation of the coupling of the spin bath and the electron spin of the central atom. At low frequencies, the coherence of the coupled system is dominated by the magnetic field intensity. At low VBF intensity, there is decrease in entropy and heat capacity at increase external magnetic field that show the decoherence suppression of the central electron spin atom. The crossing observed in the specific heat capacity corresponds to the critical field point B_C of the system which represents the point of transition from the anti-ferromagnetic system to the ferromagnetic one.

Keywords: Entropy; Specific Heat Capacity; Varying B-Field; Decoherence

1. Introduction

Thermodynamic properties of Quantum systems have become very attractive due to their potential applications in thermoelectric devices [1], tunneling and decoherence [2,3]. Thermodynamic properties of quantum systems now aid in the investigation of the dynamical entropy [4-8]. Recently, different definitions of specific heat are discussed [9] and the entropy for a quantum oscillator in an arbitrary heat bath at finite temperature is examined [10-12]. Experiments [13,14] show the feasibility of processing Quantum Information (QI) via the manipulation of optically excited electron spins [15] in Diamond. Decoherence of electron spins coupled to nuclear spin baths in quantum dots or solid-state impurity centers [16] is crucial in spin-based Quantum Information (QI) processing [17], magnetic resonance spectroscopy [18,19], and magnetometry [20]. Recent quantum technologies show that the relevant environments are of nanometer size [16-19] and therefore their quantum nature is enhanced. Quantum nuclear spin bath, in contrast to classical noises, possessed to a great extent controllability and surprisingly coherence recovery of an electron spin [21-23]. The central-spin model, or Gaudin model, describes one spin coupled to $N - 1$ bath spins via both isotropic and an-

sotropic Heisenberg interactions, including a constant magnetic field [24-27]. Decoherence leads to suppression of spin tunneling in magnetic molecules and nanoparticles [28,29] and also destroys the Kondo effect in a dissipationless manner [30]. Decoherence may be investigated with the help of the spin-echo-like techniques [31] or spin wave approximation. Extension of the spin-echo-like approach to quantum computations is known as the “bang-bang control” [32].

In this paper, our objective is to evaluate the influence of the external parallel VBF on the thermodynamic properties and Decoherence tailoring of a Central electron spin of atom coupled to an anti-ferromagnetic spin bath by the SWA method and compare our results with those obtained via the partition function [4].

The organization of the paper is as follows: in Section 2, we present a brief description of the theoretical approach used and the model for simulation of open many-spin systems. In Section 3, we evaluate the thermodynamic properties of the Central electron spin of atom coupled to an Anti-ferromagnetic spin bath and then conclude our findings in Section 4.

2. Theoretical Approach and the Model Hamiltonian

The theoretical description of decoherence have been

*Corresponding author.

studied numerically [33] and show that the evolution of the central spin system from its initial pure state ψ_0 to the final mixed state, along with the corresponding transformation of the environment, is a very difficult problem of quantum theory. For some more complex models, different approximations can be employed, such as the Markov approximation [34]. A special case of environment consisting of uncoupled oscillators, so-called ‘‘boson bath’’, is also rather well understood theoretically [35]. The boson bath description though applicable for many types of environment [36], is not universal. The boson bath model is not applicable for the decoherence caused by an environment made of spins [33]. The most direct approach to study the spin-bath decoherence is to simulate numerically the evolution of the whole compound system by directly solving the time-dependent Schrödinger equation [33]. This approach allows us to avoid any kind of approximation, except for the obvious limitation on the total number of spins models [33]. To make such simulations feasible, high-performance computational schemes are needed. The simulation method based on the Chebyshev’s polynomial expansion [35,36] was used in [33]. The spin wave approximation method was also used in [26,27]. Both approaches are applicable when the Hamiltonian is not explicitly dependent on time. In this work, we use a spin wave approximation by the Holstein-Primakoff and the Fourier transformation method.

Let us consider a system of N quantum spins described by H and initially described by H_0 :

$$H = H_S + H_{SB} + H_B \quad (2.1)$$

where

$$H_S = -g\mu_B B S_0^z \quad (2.2)$$

the Hamiltonian of the central spin atom,

$$H_{SB} = -\frac{J_0}{\sqrt{N}} S_0^z \sum_i (S_{a,i}^z + S_{b,i}^z) \quad (2.3)$$

the Hamiltonian of the interaction of the central spin with the spin bath

$$H_B = J \sum_{i,\delta} S_{a,i} S_{b,i+\delta} + \sum_{j,\delta} S_{b,j} S_{a,j+\delta} - g\mu_B (B + B_A) \sum_i S_{a,i}^z - g\mu_B (B - B_A) \sum_j S_{b,j}^z \quad (2.4)$$

The spin-bath Hamiltonian; g is the gyromagnetic factor, μ_B the Bohr magneton, J_0 the coupling constant, J the exchange interaction and $B = B_0 \cos(\theta)$ is the VBF applied in the z -direction and $\theta = \omega \cdot t$ the pulsation of the VBF. The effects of the next nearest neighbor interactions are neglected. We assumed that the spin structure of the environment may be divided into two interpenetrating sub-lattices a and b with the property that all nearest neighbors of an atom on a lie on b

and vice versa. $S_{a,i}$ and $S_{b,i}$ represents the spin operators of i^{th} and j^{th} atom on sub-lattice a and b . The field B_A is anisotropic and assumed to be positive which approximates the effect of the crystal anisotropy of the energy with the property of tending for positive magnetic moment μ_B to align the spins on sub-lattice a in the positive z^+ direction and spins on sub-lattice b in the negative z^- direction. Using the reduce Holstein-Primakoff and Bogoliubov transformations [17], we have the reduced Hamiltonian

$$H_S = -g\mu_B B S_0^z \quad (2.5)$$

$$H_{SB} = -\frac{J_0}{\sqrt{N}} S_0^z \sum_k (m_k - n_k) \quad (2.6)$$

$$H_B = E_0 + \sum_k \omega_k^+ (n_k) + \sum_k \omega_k^- (m_k) \quad (2.7)$$

where ω_k is the frequency of the magnon in the system and E_0 the energy of a central spin atom. The factors $m_k = \beta_k^+ \beta_k$ and $n_k = \alpha_k^+ \alpha_k$ are respectively the total number of magnons on the branch b and a . From Equation (2.6), we see that if the two branches of the Network have the same number of magnons, the Hamiltonian H_{SB} vanish then there will be no coupling between the Network a and the Network b . In this case the behavior of the system depends totally on the driven external field.

3. Thermodynamic Properties of a Central Electron Spin of Atom Coupled to an Anti-Ferromagnetic Spin Bath

In this section, we find the Boltzmann entropy and the specific heat capacity to show the influence of the anisotropy of the field that characterize the anti-ferromagnetic environment and the VBF on the dynamic of the central electron spin system. We suppose that our system is in a canonical ensemble [37]. To attempt to evaluate the dynamical properties of the considered system, the statistical sum is needed. Let E'_0 be the zero-point energy of the system obtained considering the harmonic approximation given by,

$$E'_0 = \hbar \sum_{i=1}^K m_k \omega_k^+ + \frac{\hbar}{2} \sum_{i=1}^K \omega_k^+ \quad (3.8)$$

with k the mode of vibrations and m_k the atom mass of the crystal, the statistical sum of the system has the form:

$$Z = \exp\{-E'_0 / K_B T\} \quad (3.9)$$

where K_B is the Boltzmann constant and T the absolute temperature. With the help of the Helmholtz free energy F ,

$$F = -K_B T \ln Z \quad (3.10)$$

We find the Boltzmann entropy S as

$$S = -(\partial F / \partial T)_V \quad (3.11)$$

And the specific heat capacity at a constant volume

$$C_v = (T \partial S / \partial T)_V \quad (3.12)$$

The indicated sum in (3.9) is easily done if $N \rightarrow \infty$; then the modes become closer together. In the canonical distribution, according to the thermodynamic principle (from which the entropy of a system depends on disorder such as temperature...), of course using the Spin wave approximation, the Boltzmann entropy and the specific heat Capacity is evaluated respectively as:

$$S = -\frac{2E'_0}{T} + \frac{g\mu_B B}{T} + \sum_k D_1/D_2 + \sum_k D_3/D_4 - \sum_k \ln(D_2 \cdot D_4) \quad (3.13)$$

and

$$C_v = \sum_k \frac{(1/T) \cdot D_1 \cdot D_5}{D_2^2} + \sum_k \frac{(1/T) \cdot D_3 \cdot D_6}{D_4^2} \quad (3.14)$$

where

$$D_1 = (-\omega_k^+ / T) \cdot \exp\{-\omega_k^+ / T\} \quad (3.15.a)$$

$$D_2 = 1 - \exp\{-\omega_k^+ / T\} \quad (3.15.b)$$

$$D_3 = (\omega_k^- / T) \cdot \exp\{-\omega_k^- / T\} \quad (3.15.c)$$

$$D_4 = (1 - \exp\{-\omega_k^- / T\}) \quad (3.15.d)$$

$$D_5 = -1 + 2 \exp\{-\omega_k^+ / T\} \quad (3.15.e)$$

$$D_6 = -1 + 2 \exp\{-(1/T) \cdot (\omega_k^-)\} \quad (3.15.f)$$

From the analytical results obtained in Equation (3.13) we have the plots in **Figures 1** and **2** describing the behavior of the Boltzmann entropy under the influence of the external VBF. From the expression in Equation (3.14) we have the plots in **Figures 3** and **4** describing the behavior of the specific heat capacity under the influence of the external VBF.

It is shown that the Boltzmann entropy (**Figure 1**) increases respectively with increase temperature and decreases as a function of the increase of the paralleled time dependent external VBF intensity (see **Figure 2**). The specific heat capacity in **Figures 3** and **4** show the crossing point for different temperatures and for different external VBF intensity. This crossing point corresponds to the critical magnetic field (B_c) whose expression is given Equation (17), [26]. This represents transition point of the state of the crystal. Tending the entropy to zero show that the external VBF brings the central spin system to its coherent state. From the external VBF, the plot of the Boltzmann entropy in (**Figure 5**) and of the specific heat capacity in (**Figure 6**) show that the

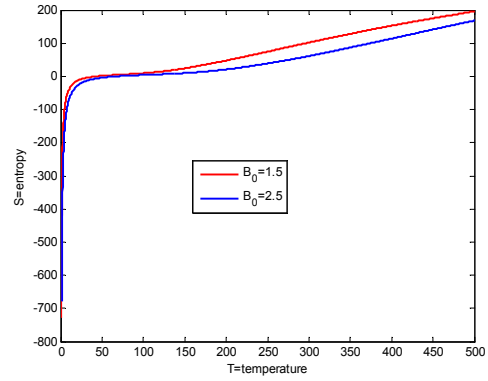


Figure 1. Boltzmann entropy versus temperature for different external VBF intensity with $B_A = 0.14, g = 2$ and $M = 6$.

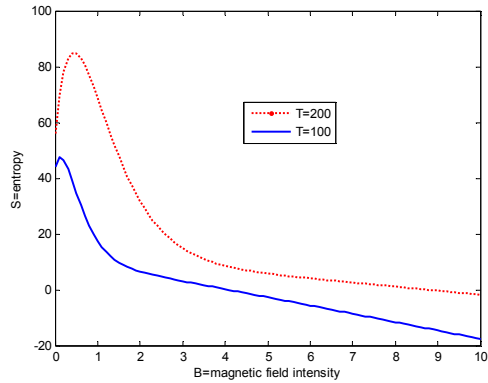


Figure 2. Boltzmann entropy versus the external VBF intensity for different values of temperature with $B_A = 0.14, g = 2$ and $M = 6$.

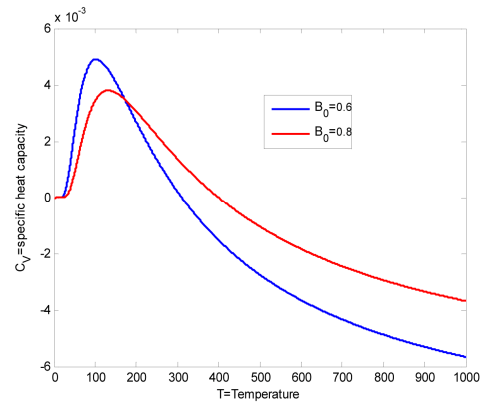


Figure 3. Specific heat capacity versus the temperature for different values of external VBF intensity with the constants $B_A = 0.14, g = 2$ and $M = 6$.

presence of the anisotropic field creates a dephasing: this describes decoherence phase observation in a coupled central spin system. Thus the action of the temperature (T) and of the external VBF are both opposite effects.

The decoherence of the spin of the central atom due to

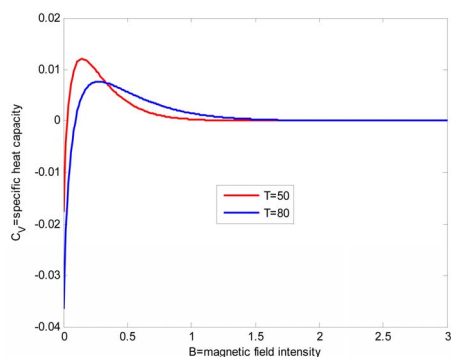


Figure 4. Specific heat capacity versus the external VBF intensity for different values of temperature with $B_A = 0.14$, $g = 2$ and $M = 6$.

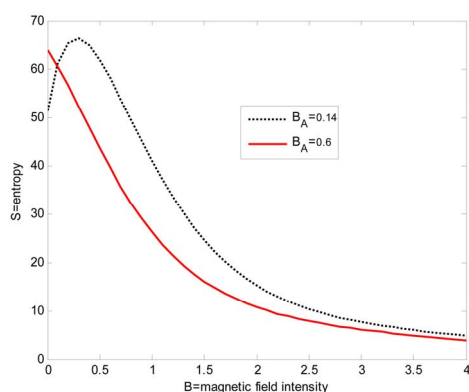


Figure 5. Boltzmann entropy versus the external VBF for different anisotropy field intensity with the given $T = 150$, $g = 2$ and $M = 6$.

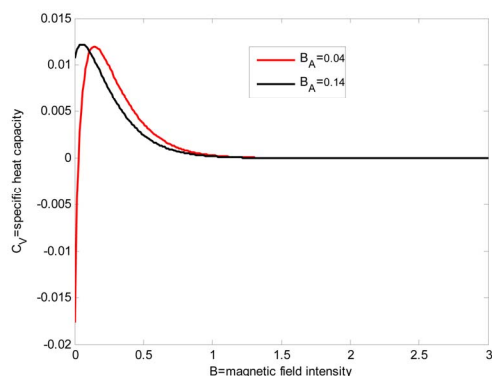


Figure 6. Specific heat capacity versus the external VBF intensity for different anisotropy field intensity with the given $T = 150$, $g = 2$ and $M = 6$.

the anisotropy of the field of the anti-ferromagnetic environment or by the temperature is thus reduced by the increased of the external VBF intensity.

4. Conclusions

In this paper, we have investigated the thermodynamic

properties of quantum multistate-coupled systems. We present the influence of the external VBF on the decoherence of the spin of the central atom coupled to an anti-ferromagnetic spin bath where the number of environmental atom vanishes. A Formalism is developed, using Holstein-Primakoff and Bloch transformations approaches from where the density of state of the system, the statistical sum and the free energy of a central electron spin are found. It is shown that the effect of the external systems in such formalism can always be included in some general classes of Functions (statistical sum and free energy). The resulting specific heat capacity approaches the classical (Pettit-Dulong law) result for high temperatures and goes to zero for vanishing temperature. The entropies of both systems also obey the second law of thermodynamics as well as the third law of thermodynamics.

We observed that both specific heat capacity and entropy decreased with increased intensity of the external VBF and decrease temperature. This shows that the decoherence aspect of the central electron spin atom observed at the coupling with the anti-ferromagnetic spin bath is reduced. We observe the numerical results for the central spin of atom coupled to an anti-ferromagnetic spin bath and confirm the results using the partition function methods [4]. Due to the frequency of the VBF, the evolution of the system is controllable in time. This process is very important in the efforts of suppressing decoherence in spin bath coupled system [21].

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