Spin-lattice coupling as environmental effect

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Abstract. The exchange constant in a magnetic system results from the overlap of orbitals, so it depends upon the ion distance and yields a coupling with the lattice vibrations: this can strongly influence the statistical mechanics of magnets. As the fast lattice dynamics allows for a rapid thermalization, phonon-induced spin correlations can be reasonably neglected, so that phonons can be regarded as a thermalized environment (or bath) for the spins. It is therefore natural to treat it within a Caldeira-Leggett scheme, i.e., by the influence action obtained after tracing-out the bath’s degrees of freedom, whose contribution can be accounted for within a known semiclassical approach. In this way extended phase diagrams, accounting for the environmental interaction, can be drawn for the magnetic phase transitions.

Real magnetic systems, having the spins sitting on the sites of a crystal lattice, are necessarily interacting with its vibration modes. As the faster dynamics allows for a rapid thermalization of the lattice, one expects that phonons could be considered as a quantum environment (or bath, or reservoir) for each spin. Such a coupled system is naturally approached by the system plus reservoir model [1, 2], in a suitably generalized version including a bath interaction for the momenta [3]. In this way one can study if environmental effects could be displayed by magnetic materials. Although a microscopic derivation of the spin-phonon coupling gives a nonlinear bath-spin interaction, in order to derive a first qualitative picture we consider here the linear case, which gives rise to a quadratic influence action.

The exchange coupling between two spins sitting on neighboring ions arises from the fermionic character of electrons, and is essentially due to the overlap of orbitals, so that its strength \( J = J(r) \) depends on the separation \( r \) of the ions. This dependence is usually neglected when dealing with magnetic models, but in principle it can be very important: for instance, the gain in magnetic energy can even lead to a distorted lattice configuration, as in the spin-Peierls transition [4, 5].

To derive the microscopic form of the coupling, consider the bond connecting lattice sites \( i \) and \( j \),

\[
J(|r_i - r_j|) \approx J + J'(r_i - r_j) ,
\]

where \( d \equiv j - i \) is the equilibrium distance. The overall quantum Hamiltonian must therefore
include the magnetic and the (harmonic) lattice contribution,

\[ \tilde{\mathcal{H}} = - \sum_{(ij)} \left( J \hat{S}_i \hat{S}_j + \tilde{\mathcal{H}}_E^{(ij)} \right) , \quad \tilde{\mathcal{H}}_E^{(ij)} = \frac{1}{2} \sum_\alpha \left[ a_\alpha^2 \hat{p}_\alpha^2 + b_\alpha^2 (\hat{q}_\alpha - \hat{S}_i \cdot \hat{S}_j)^2 \right] , \tag{2} \]

where the conjugated variables \( \{ \hat{p}_\alpha, \hat{q}_\alpha \} \) are suitable normal coordinates for the lattice vibrations. Neglecting phonon-mediated spin correlations, one can regard the above Hamiltonian as containing an independent phonon environment for each bond. The same coupling model was also used to account for environmental effects on quantum phase transitions [6], on thermal-transport anomalies [7], and on the magnetic phase diagrams [8, 9]. The influence action derived from Eq. (2), obtained by tracing-out the environmental variables from the corresponding path integral, turns out to be quartic in the spin operators and its treatment is rather involute [10, 11]. Qualitative insight about the effects of environmental coupling onto a Heisenberg magnet can however be obtained by considering an approximate quadratic influence action,

\[ S_1 = - \frac{J}{2} \sum_\sigma \int_0^\beta \! \! du \, \kappa (u - u') \, S_1^\sigma (u) \, S_1^\sigma (u') , \quad [\sigma = x, y, z] , \tag{3} \]

corresponding, for each spin component, to a bath Hamiltonian

\[ \tilde{\mathcal{H}}_E^{(i\sigma)} = \frac{1}{2} \sum_\alpha \left[ a_\alpha^2 \hat{p}_\alpha^2 + b_\alpha^2 (\hat{q}_\alpha - \hat{S}_i^\sigma)^2 \right] , \tag{4} \]

where \( \{ \hat{p}_\alpha, \hat{q}_\alpha \} \) are the environmental variables. The Matsubara components of the kernel,

\[ J \kappa_n = J \int du \, \kappa (u) \, e^{-i \nu_n u} = \sum_\alpha \frac{b_\alpha^2 \nu_n^2}{\nu_n^2 + a_\alpha^2} = |\nu_n| \, \gamma (\nu = |\nu_n|) , \tag{5} \]

are related [2] to the Laplace transform of the memory function \( \gamma (t) \) which characterizes the dissipative Langevin dynamics [2] of a ‘particle’ whose coordinate is linearly coupled with the environment as in Eq. (4). Eq. (5) connects the microscopic parameters of the bath with the macroscopic system’s response, allowing one to guess a physically meaningful expression for the kernel using what is known for dissipative systems: a typical phenomenological model for the memory function is the Drude one,

\[ \gamma (t) = \theta (t) \, \gamma \, \omega_\nu \, e^{-\omega_\nu t} , \quad \gamma (z) = \frac{\gamma \omega_\nu}{\omega_\nu + z} , \tag{6} \]

which is characterized by the strength \( \gamma \) and the cutoff frequency \( \omega_\nu \), the latter can be assumed of the order of the Debye frequency if the environment is a phonon bath.

While the above approach holds for any spin Hamiltonian, in order to show how it applies let us consider a known system: the two-dimensional easy-axis XXZ magnet,

\[ \hat{\mathcal{H}} = - J \sum_{(ij)} \left[ \mu (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + \hat{S}_i^z \hat{S}_j^z \right] , \tag{7} \]

where \( \mu \in [0, 1) \) is the easy-axis anisotropy. This system displays an Ising phase transition, both in the classical \( (S \to \infty) \) [12, 13] and in the quantum case [14, 15].

In Ref. [14] the quantum XXZ magnet was studied by the pure-quantum self-consistent harmonic approximation (PQSCHA) [16], an approach that and can be naturally extended to account for environmental coupling, yielding an effective classical Hamiltonian for the magnet.
The procedure involves the use of a spin-boson transformation, such as the Holstein-Primakoff (HP) one,
\[ \hat{S}_x^i + i\hat{S}_y^i = (2S - \hat{a}_i^\dagger\hat{a}_i)^{1/2}\hat{a}_i, \quad \hat{S}_z^i = S - \hat{a}_i^\dagger\hat{a}_i, \]
and the PQSCHA recipe is applied for the phase space variables \((\hat{p}_i, \hat{q}_i)\) defined by \(\hat{a}_i = (\hat{S}/2)^{1/2}(\hat{q}_i + i\hat{p}_i)\). The final outcome is the effective Hamiltonian
\[ \mathcal{H}_{\text{eff}} = E(T) - J\tilde{S}^2 \sum_{\langle ij \rangle} \left[ \mu_{\text{eff}}(\hat{s}_i^x\hat{s}_j^x + \hat{s}_i^y\hat{s}_j^y) + \hat{s}_i^z\hat{s}_j^z \right], \]
in terms of classical spins \(|s_i| = 1\), where \(\tilde{S} = S + \frac{1}{2}\) is the bare classical spin value and \(E(T)\) is a uniform contribution to the free-energy. Using the reduced temperature \(t \equiv T/J\tilde{S}^2\), in Refs. [14] it is shown that the effective exchange \(j_{\text{eff}}(t, \mu, S) = \theta_1^2\) and anisotropy \(\mu_{\text{eff}}(t, \mu, S) = \mu \theta_2/\theta_1\) depend on the parameters
\[ \theta_1 = 1 - \frac{1}{N} \sum_k (1 - \mu \gamma_k) \mathcal{L}(a_k, b_k), \quad \theta_2 = 1 - \frac{1}{N} \sum_k (1 - \mu^{-1} \gamma_k) \mathcal{L}(a_k, b_k), \]
to be evaluated self-consistently with the quantities \(a_k^2 = 4(\theta_1 - \mu \theta_2 \gamma_k)\) and \(b_k^2 = 4(\theta_1 \pm \mu \theta_2 \gamma_k)\) (+ antiferromagnet, − ferromagnet), where \(\gamma_k = (\cos k_x + \cos k_y)/2\) and the function
\[ \mathcal{L}(a, b) = \frac{1}{2\tilde{S}} \frac{a}{b} \left( \coth \frac{ab}{2t\tilde{S}} - \frac{2t\tilde{S}}{ab} \right); \]

**Figure 1.** Phase diagram of the easy-axis Heisenberg antiferromagnet (AFM, left panel) and ferromagnet (FM, right panel). The dotted line is the classical result, and the other curves refer to the spin values 5/2 (upper curves) and \(S = 1\) (lower curves) with different environmental coupling strengths \(\Gamma = 0\) (-----), 0.2 (-- -- --), 0.5 (-- · ·), 1 (-- · · --). The Drude cutoff frequency is fixed to \(\Omega = 10\).
the subtracted large-$S$ asymptotic term evidences that only pure-quantum fluctuations of the spins contribute to renormalizing the effective interaction parameters.

When the influence action (3), expressed in terms of the HP coordinates \( S_i \approx \tilde{S}(q_i, p_i, 1-\gamma^2 q_i^2) \), is included in the system’s action, it immediately appears that the z-components give rise to negligible quartic contributions, and one deals with the influence action

\[
S_1 = -\frac{1}{2t} \sum_{i,n} \kappa_n (q_{in}q_{i-n} + p_{in}p_{i-n}) = -\frac{1}{2t} \sum_{k,n} \kappa_n \left( p_{k\nu}p_{-k\nu} + q_{k\nu}q_{-k\nu} \right),
\]

so that it is easy to obtain that the above renormalization scheme is modified just by replacing Eq. (11) with

\[
\mathcal{L}(a, b) = 2t \sum_{n=1}^{\infty} \frac{a^2 + \kappa_n}{\nu_n^2 + (a^2 + \kappa_n)(b^2 + \kappa_n)},
\]

where \( \nu_n = 2\pi T S n \) is the dimensionless Matsubara frequency. Assuming the phenomenological Drude memory function, Eqs. (5) and (6), the corresponding kernel is

\[
\kappa_n = \frac{1}{J} \frac{\gamma \omega_D \nu_n}{\omega_{in} + \nu_n} = \Gamma \frac{\Omega \nu_n}{\Omega + \nu_n},
\]

where \( \Gamma = \gamma S^2 \) and the dimensionless cutoff \( \Omega \equiv \omega_{in}/J S^2 \) is of the order of the ratio between the Debye and the Curie temperature: for real magnets it can take values \( \Omega = 0.1 \div 100 \).

The resulting typical environmental effect upon the phase diagram for the Ising transition in the easy-axis XXZ magnet, calculated as in Ref. [14], is reported in Fig 1. It appears that the transition temperature decreases for increasing environmental coupling: substantially, the environment enhances the pure-quantum magnetic fluctuations. This effect switches on rapidly with the coupling intensity \( \Gamma \), but is less and less sensitive to its further increase.

Although the assumption of linear environmental coupling (4) makes these observations qualitative, the established phonon-induced decrease of the transition temperature in a magnetic model is a nontrivial and somewhat unexpected result, as for instance the normal-superconducting transition in Josephson junction arrays [17] has the opposite behavior.

The extension of the semiclassical approach in order to treat the more realistic quartic influence action obtained from Eq. (2) is currently under investigation.

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