Memory-dependent Damping in Heisenberg Spin Chain

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We derive the contracted dynamics of a Heisenberg spin coupled to a semi-infinite chain bath of Heisenberg spins. The resulting dynamics mimics the Langevin dynamics observed for oscillators. Whereas in oscillators the dynamics contains a random force and memory-dependent damping, the case for spins results in a random torque and the generalization of the Landau-Lifshitz equation to the memory-dependent damping case. We show that the decay rate of the damping kernel is algebraic and of the same form as the case for oscillators.

I. INTRODUCTION

The Langevin equation[1] is a celebrated equation of physics as it describes dissipative dynamics of open systems. First applied to understanding Brownian motion[2], it allows one to understand the dynamics of open systems through a contracted description. Since its use as a phenomenological equation to describe the dissipative dynamics of a system, there has been a search for a microscopic model that could result in a Langevin equation. For the lattice dynamics of atoms in the context of thermal transport by phonons a recipe has been developed for obtaining a Langevin equation[3]. It is now well known that the effect of an infinite number of particles on a small subsystem coupled is to induce random fluctuations and damping, as correctly predicted by the Langevin equation.

The results for the case of a semi-infinite chain bath of atoms oscillating in one dimension have been derived and yields a Langevin equation with memory dependent damping[4]. In the case of spins, the equation which we wish to generalize is the Landau-Lifshitz (LL) equation[5], which is the phenomenological description of the precession and damping of magnetization in a material. While the LL equation is local in time, the results we obtain show memory dependence for the damping.

The purpose of this work is to derive the analogous results for the case of Heisenberg spins placed on a semi-infinite lattice. The general recipe is to transform to the normal modes using a generating function. From there we solve the diagonalized equation of motion, and then transform back to obtain the dynamics as a functional of the "Brownian" degree of freedom, and the corresponding equation of motion of the Brownian particle will now be a contracted one and of the form of a Langevin equation. The specific organization of the paper is as follows. In Section II we provide a brief derivation for a semi-infinite chain bath of one dimensional oscillators for reference. In Section III we derive the dynamics of the semi-infinite chain spin bath as a functional of the "Brownian" spin. In Section IV, we refer to the Landau-Lifshitz equation describing the precession and damping of magnetization in a material and recognize for our system the generalized memory-dependent damping. In Section V we provide our conclusions from the comparison between the oscillator and spin cases and describe steps moving forward.

II. SEMI-INFINITE CHAIN OSCILLATOR BATH

In this section we provide a brief derivation of the dynamics and Langevin equation from an oscillator chain. Suppose we have a semi-infinite chain of particles of mass m and nearest neighbor spring constant of α, connected to what we will call the zeroth particle. In this case, the Heisenberg equation of motion of our one-dimensional system is described as:

$$m\frac{d^2}{dt^2}\hat{x}_{H_n} = \alpha\left(\hat{x}_{H_{n+1}} + \hat{x}_{H_{n-1}} - 2\hat{x}_{H_n}\right) \quad n \in \mathrm{Z}^+ \tag{1}$$

For simplicity, we define the frequency $\omega \equiv 2\sqrt{\frac{\alpha}{m}}$ and define a non-dimensional time as $\tau = \omega t$. We define the generating function and its inverse transformation to diagonalize the equations of motion:

$$\hat{h}_k(\tau) \equiv \sum_{n=1}^{\infty} \sqrt{\tfrac{2}{\pi}} \sin(kn) \hat{x}_{H_n}(\tau)$$
$$\hat{x}_{H_n}(\tau) = \int_0^{\pi} \sqrt{\tfrac{2}{\pi}} \sin(kn) \hat{h}_k(\tau) dk \qquad (2)$$

Multiplying Eq. 1 by $\sqrt{\tfrac{2}{\pi}} \sin(kn)$ and summing n over the positive integers, we obtain the diagonalized equation of motion:

$$\frac{d^2}{d\tau^2} \hat{h}_k + \hat{h}_k \sin^2\left(\tfrac{k}{2}\right) = \tfrac{1}{4} \sqrt{\tfrac{2}{\pi}} \sin(k) \hat{x}_{H_0} \qquad (3)$$

From this diagonalized equation of motion, we can easily recognize the dispersion to be $\omega_k = \omega \sin\left(\tfrac{k}{2}\right)$. As such, our defined non-dimensional frequency ω is the maximum allowed frequency of the dispersion.

Solving the equation which mimics a driven harmonic oscillator and inverse transforming back to the real space variables we obtain for the dynamics:

$$x_{H_n}(\tau) = \sum_{j=1}^{\infty} \left(\hat{x}_j \frac{d}{d\tau} + \frac{\hat{p}_j}{m\omega} \right) \left[f_{n-j}(\tau) - f_{n+j}(\tau) \right] + \frac{1}{4} \int_0^{\tau} \hat{x}_{H_0}(\tau') \left[f_{n-1}(\tau - \tau') - f_{n+1}(\tau - \tau') \right] d\tau' \qquad (4)$$

We have defined for simplicity the function:

$$f_n(x) \equiv \frac{1}{\pi} \int_0^{\pi} \cos(kn) \frac{\sin\left[x \sin\left(\tfrac{k}{2}\right)\right]}{\sin\left(\tfrac{k}{2}\right)} dk = \int_0^{x} J_{2n}(y) dy \qquad n \in \mathrm{Z} \qquad (5)$$

which is obtained through a straightforward contour integration.

We now have the dynamics of the semi infinite chain as a functional of the zeroth atom. The force on the zeroth atom due to the semi infinite chain bath is simply:

$$\hat{F}_{H_{bath}} = \alpha\left(\hat{x}_{H_1} - \hat{x}_{H_0}\right) = \hat{F}(\tau) - \int_0^{\tau} \omega K(\tau - \tau') \dot{\hat{x}}_{H_0}(\tau') d\tau' \qquad (6)$$

Where we have explicitly written the result we expect of fluctuation and dissipation from a heat bath. Utilizing the dynamics of the first bath particle, the one that couples to the zeroth, we obtain for these terms:

$$\hat{F}(\tau) = \alpha \sum_{n=1}^{\infty} \left(\hat{x}_n \frac{d}{d\tau} + \frac{\hat{p}_n}{m\omega} \right) \frac{8n}{\tau} J_{2n}(\tau)$$
$$K(\tau) = \frac{\alpha}{\omega} \frac{2}{\tau} J_1(\tau) \qquad (7)$$

The asymptotic expansion of the friction kernel for large times is:

$$K(\tau \to \infty) \propto \tau^{-\frac{3}{2}} \sin\left(\tau - \frac{\pi}{4}\right) \qquad (8)$$

As described, we obtain memory dependent damping with algebraic decay with oscillatory behavior. The frequency of oscillations is ω, the cutoff frequency of the phonon dispersion.

III. DYNAMICS OF A SEMI-INFINITE SPIN CHAIN

Our Hamiltonian for the semi-infinite spin chain we take as the three dimensional spin XXX model with an external magnetic field to allow for a single, non-degenerate ground state energy:

$$\hat{H} = -J \sum_{n=0}^{\infty} \hat{\vec{\sigma}}_n \cdot \hat{\vec{\sigma}}_{n+1} - \alpha \sum_{n=0}^{\infty} \hat{\sigma}_{n,z} \qquad (9)$$

where $J, \alpha > 0$. We will take $\alpha \to 0^+$ so that the external field does not affect the dynamics other than providing a non-degenerate ground state for the spins.

Utilizing the commutator of the Pauli spin operators, we obtain for the equation of motion of the Heisenberg operators:

$$\frac{d}{dt} \hat{\vec{\sigma}}_{H_n}(t) = \frac{2J}{\hbar} \hat{\vec{\sigma}}_{H_n} \times \left(\hat{\vec{\sigma}}_{H_{n-1}} + \hat{\vec{\sigma}}_{H_{n+1}} \right) \qquad (10)$$

Unlike the phonon case, the dynamics of this system is nonlinear, due to the fact that the commutation relations for the position and momentum for the phonon system was a scalar, whereas for the spin case the commutator is itself a spin operator.

With the external magnetic field in the positive z-direction, the degeneracy of the ground state is broken. At zero temperature, the system's state will be such that it will prefer to point upwards, so that $\left\langle \hat{\vec{\sigma}}_{H_n}(t) \right\rangle = \vec{e}_z$. We are interested in low temperature excitations, and so we expand our Heisenberg operators in a small expansion about this equilibrium point: $\hat{\vec{\sigma}}_{H_n}(t) = \vec{e}_z + \hat{\vec{s}}_n(t)$, where $\hat{\vec{s}}_n(t)$ is a two-dimensional vector operator in the xy plane.

Inputting this and linearizing, we obtain:

$$\frac{d}{dt}\hat{\vec{s}}_n = \frac{2J}{\hbar}\vec{e}_z \times \left\{ \hat{\vec{s}}_{n-1} + \hat{\vec{s}}_{n+1} - 2\hat{\vec{s}}_n \right\} \tag{11}$$

Defining for convenience the frequency $\omega \equiv \frac{8J}{\hbar}$, and the non-dimensional time $\tau = \omega t$, we now have a first order differential vector equation that has similar nearest neighbor structure as the oscillator chain.

Defining the following generating function and its inverse transformation:

$$\begin{aligned} \hat{\vec{g}}_k(\tau) &\equiv \sum_{n=1}^{\infty} \sqrt{\frac{2}{\pi}} \sin(kn)\hat{\vec{s}}_n(\tau) \\ \hat{\vec{s}}_n(\tau) &= \int_0^{\pi} \sqrt{\frac{2}{\pi}} \sin(kn)\hat{\vec{g}}_k(\tau)\,dk \end{aligned} \tag{12}$$

We can multiply our equation our motion by $\sqrt{\frac{2}{\pi}}\sin(kn)$ and sum n over the positive integers to obtain the diagonalized equation of motion:

$$\frac{d}{d\tau}\hat{\vec{g}}_k = \frac{1}{4}\vec{e}_z \times \sqrt{\frac{2}{\pi}}\sin(k)\hat{\vec{s}}_0 - \frac{1}{2}\left[1-\cos(k)\right]\vec{e}_z \times \hat{\vec{g}}_k \tag{13}$$

This can be understood as an oscillatory equation causing the two dimensional vector to rotate with a dispersion $\omega_k = \omega \sin^2\left(\frac{k}{2}\right)$. Thus our defined frequency ω is the maximum cutoff frequency of the dispersion. Notice the dispersion for these oscillations (magnons) is the square of the case for phonons. One important difference is that the group velocity of the magnon dispersion vanishes at zero wavevector whereas it is finite for the case of phonons. Thus the magnon dispersion is quadratic for small wavevector whereas the phonon dispersion is linear.

We can represent the cross product with the z-direction vector acting on a two dimensional vector in the xy plane as a matrix operation so that our differential equation in matrix form becomes:

$$\frac{d}{d\tau}\hat{\vec{g}}_k = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} i \left\{ \frac{\omega_k}{\omega}\hat{\vec{g}}_k - \frac{1}{4}\sqrt{\frac{2}{\pi}}\sin(k)\hat{\vec{s}}_0 \right\} \tag{14}$$

Solving this first order vector differential equation by diagonalizing the Hermitian matrix, we obtain:

$$\begin{aligned} \hat{\vec{g}}_k(\tau) &= R\left(-\tfrac{\omega_k}{\omega}\tau\right)\hat{\vec{g}}_k(0) + \\ &\frac{1}{4}\sqrt{\frac{2}{\pi}}\sin(k)\int_0^{\tau} R\left(\tfrac{\pi}{2} - \tfrac{\omega_k}{\omega}(\tau - \mathrm{T})\right)\hat{\vec{s}}_0(\mathrm{T})\,d\mathrm{T} \end{aligned} \tag{15}$$

where we use the two-dimensional rotation matrix:

$$R(\theta) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \tag{16}$$

Transforming back to the spin variables from this generating function, we obtain:

$$\begin{aligned} \hat{\vec{s}}_n(\tau) &= \sum_{\ell=1}^{\infty} \int_0^{\pi} \tfrac{2}{\pi}\sin(kn)\sin(k\ell)R\left(-\tfrac{\omega_k}{\omega}\tau\right)dk\,\hat{\vec{s}}_{\ell}(0) + \\ &\int_0^{\tau}\int_0^{\pi} \tfrac{1}{2\pi}\sin(kn)\sin(k)R\left(\tfrac{\pi}{2} - \tfrac{\omega_k}{\omega}(\tau - \tau')\right)dk\,\hat{\vec{s}}_0(\tau')\,d\tau' \end{aligned} \tag{17}$$

Out of convenience, we define the function:

$$\begin{aligned} f_n(x) &\equiv \frac{1}{\pi}\int_0^{\pi} \cos(kn) e^{i\frac{\omega_k}{\omega}x}\,dk \qquad n \in \mathrm{Z} \\ &= e^{i\frac{x-\pi n}{2}} J_n\left(\tfrac{x}{2}\right) \end{aligned} \tag{18}$$

which is straightforward to calculate through contour integration. Using this function, we can write our final solution as:

$$\begin{aligned} \hat{\vec{s}}_n(\tau) &= \sum_{\ell=1}^{\infty} R\left(\tfrac{\pi(\ell-n)-\tau}{2}\right)\left[J_{\ell-n}\left(\tfrac{\tau}{2}\right) + (-1)^{n-1} J_{\ell+n}\left(\tfrac{\tau}{2}\right)\right]\hat{\vec{s}}_{\ell}(0) + \\ &\int_0^{\tau} R\left(\tfrac{\pi n - (\tau-\tau')}{2}\right)\frac{n}{\tau - \tau'} J_n\left(\tfrac{\tau-\tau'}{2}\right)\hat{\vec{s}}_0(\tau')\,d\tau' \end{aligned} \tag{19}$$

Thus we obtain the dynamics of the bath spins as a functional of the zeroth spin in order to be able to give a contracted description of the effect of the spin bath on the zeroth spin.

IV. LANDAU-LIFSHITZ EQUATION WITH MEMORY-DEPENDENT DAMPING

In this section we provide the connection between the microscopic dynamics of Sec. III and the macroscopic description of the LL equation and demonstrate memory-dependent damping analogous to the Langevin equation obtained for oscillating atoms on a lattice from Sec. II.

The dynamics of the zeroth spin in dimensional form is:

$$\frac{\hbar}{2}\frac{d}{dt}\hat{\hat{s}}_0 = J\vec{e}_z \times \left(\hat{\hat{s}}_1 - \hat{\hat{s}}_0\right) \tag{20}$$

From this dynamical equation we can see that the net bath torque is:

$$\hat{\hat{\mathrm{T}}}_{bath} = J\vec{e}_z \times \left(\hat{\hat{s}}_1 - \hat{\hat{s}}_0\right) \tag{21}$$

To understand the damping force, we refer to the Landau-Lifshitz equation for a spin in an effective magnetic field with damping:

$$\frac{\hbar}{2}\frac{d}{dt}\hat{\hat{\sigma}}_H = -\vec{B}_{eff} \times \hat{\hat{\sigma}}_H - \lambda\hat{\hat{\sigma}}_H \times \left(\hat{\hat{\sigma}}_H \times \vec{B}_{eff}\right) \tag{22}$$

where λ is the dimensionless damping parameter. If we linearize as before $\vec{m} = \vec{e}_z + \vec{s}$ in the presence of an infinitesimal external magnetic field in the positive z-direction, we obtain for the two dimensional representation:

$$\frac{\hbar}{2}\frac{d}{dt}\hat{\hat{s}} = -\gamma\vec{e}_z \times \hat{\hat{s}} - \gamma\lambda\hat{\hat{s}} \tag{23}$$

This is the case for damping with no memory effects. If we generalize to the case of memory dependent damping, we expect the convolution:

$$\frac{\hbar}{2}\frac{d}{dt}\hat{\hat{s}} = -\gamma\vec{e}_z \times \hat{\hat{s}} - \gamma\int_0^{\tau} K\left(\tau-\tau'\right)\hat{\hat{s}}\left(\tau'\right)d\tau' \tag{24}$$

Where $K(t)$ is the memory-dependent damping kernel, which is in general a tensor now. Thus we can rewrite the net bath torque in terms of the non-dimensional random bath torque and damping torque as:

$$\hat{\hat{\mathrm{T}}}_{bath}\left(\tau\right) = J\left(\hat{\hat{\mathrm{T}}}\left(\tau\right) - \vec{e}_z \times \hat{\hat{s}}_0 - \int_0^{\tau} K\left(\tau-\tau'\right)\hat{\hat{s}}_0\left(\tau'\right)d\tau'\right) \tag{25}$$

Utilizing the solution of the first bath spin, we identify the non-dimensional random bath torque and memory dependent friction kernel:

$$\begin{aligned}\hat{\hat{\mathrm{T}}}\left(\tau\right) &= \sum_{n=1}^{\infty} R\left(\frac{\pi n}{2} - \frac{\tau}{2}\right)\frac{4n}{\tau}J_n\left(\tfrac{\tau}{2}\right)\hat{\hat{s}}_n\left(0\right)\\ K\left(\tau\right) &= R\left(-\frac{\tau}{2}\right)\frac{1}{\tau}J_1\left(\frac{\tau}{2}\right)\end{aligned} \tag{26}$$

Eq. 25 and Eq. 26 are the fundamental equations of this work, as they provide the connection between the microscopic dynamics of the spins on the lattice with the contracted macroscopic description of the LL equation analogous to the Langevin equation for the oscillator chain. Taking the asymptotic expansion of the friction kernel for large times:

$$\begin{aligned}K\left(\tau \to \infty\right) &\propto \tau^{-\frac{3}{2}}\sin\left(\frac{\tau}{2} - \frac{\pi}{4}\right)R\left(-\frac{\tau}{2}\right)\\ &\propto \tau^{-\frac{3}{2}}\left(R\left(\frac{3\pi}{4} - \tau\right) - R\left(\frac{\pi}{4}\right)\right)\end{aligned} \tag{27}$$

Once more we see memory dependent damping that has algebraic decay with an oscillatory pattern similar to Eq. 8. The decay rate is the same and even the frequency of oscillation is analogously the cutoff frequency of the magnon dispersion.

V. CONCLUSIONS

We have derived a memory dependent friction kernel for a semi-infinite chain of Heisenberg spins. By solving for the dynamics and referring to the Landau-Lifshitz equation, we observed that the effect of a semi-infinite chain bath of spins upon a single spin was to provide a random bath torque as well as the typical rotation and damping terms of the LL equation. In our case the damping has memory effects and decays like a Bessel function, as a power law for large times.

More specifically, the memory kernel for both cases shows an algebraic decay of $\tau^{-\frac{3}{2}}$ in amplitude for large times as can be seen from Eq. 8 and Eq. 27, with oscillatory behavior with a frequency equal to the respective dispersion cutoff frequency. Therefore, although we showed two different physical systems that have different normal modes of oscillation (dispersion), we obtained similar dynamics and behavior in their memory-dependent damping kernels.

Future study to solidify the similarity between these two systems would involve deriving the fluctuation dissipation relation showing the dependence of the random bath torque autocorrelation upon the damping kernel as has been show for the case for phonons. With this established, thermal transport by spin waves (magnons) at low temperatures can be calculated in a formalism similar to phonons[6].

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