Combined molecular dynamics-spin dynamics simulations of bcc iron

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Abstract.
Using a classical model that treats translational and spin degrees of freedom on an equal footing, we study phonon-magnon interactions in BCC iron with combined molecular and spin dynamics methods. The atomic interactions are modeled via an empirical many-body potential while spin dependent interactions are established through a Hamiltonian of the Heisenberg form with a distance dependent magnetic exchange interaction obtained from first principles electronic structure calculations. The temporal evolution of translational and spin degrees of freedom was determined by numerically solving the coupled equations of motion, using an algorithm based on the second order Suzuki-Trotter decomposition of the exponential operators. By calculating Fourier transforms of space- and time-displaced correlation functions, we demonstrate that the presence of lattice vibrations leads to noticeable softening and damping of spin wave modes. As a result of the interplay between lattice and spin subsystems, we also observe additional longitudinal spin wave excitations, with frequencies which coincide with that of the longitudinal lattice vibrations.

1. Introduction
Computer simulations have played a vital role in advancing our knowledge and understanding of magnetic properties of materials. Investigation of model spin systems with Monte Carlo (MC) methods has revealed a substantial amount of information regarding the static thermodynamic properties of magnetic systems such as phase transitions and critical phenomena [1]. However, as the progression of “time” in these stochastic methods is completely unrelated to the “real time” associated with the true dynamics of the system, they are incapable of probing the deterministic time-dependent properties of the system. A widely used approach for exploring the dynamical behavior of magnetic systems is to numerically solve the classical equations governing the dynamics of magnetic moments at atomic level. This method, generally known as spin dynamics (SD) simulations, has been successfully employed in the past few decades to investigate the time-dependent properties of spin models with continuous degrees of freedom [2]. By choosing exchange interaction parameters determined from experiments or first principle calculations, one can construct realistic models of magnetic materials, where the obtained results can be quantitatively compared with the data from neutron scattering experiments [3, 4].

Recent, rapid advancements in SD simulations were largely due to the emergence of a
novel class of symplectic integrators based on the Suzuki-Trotter (ST) decomposition of the exponential time evolution operator [5, 6]. These algorithms are known to be time reversible, and conserve phase-space volume exactly. In comparison with predictor-corrector schemes, decomposition methods are superior in terms of numerical stability, accuracy as well as efficiency [7].

Much of the theoretical and computational investigations of magnetic materials, by far, has been restricted to lattice-based spin systems, where the locations of the spins are fixed on regular lattice points. A major disadvantage of such simplified models is their lack of capacity to capture the wide range of complex phenomena that occur in real materials due to the coexistence of lattice vibrations (phonons) and spin waves (magnons). For instance, in transition metals, magnitudes of atomic magnetic moments and the strength of their interactions strongly depend on the changing local atomic environment in a non-trivial manner [8, 9]. On the other hand, magnetic interactions themselves play a significant role in determining the structural properties of such systems [10, 11]. Thus, the strong mutual interdependence between the lattice and spin subsystems suggest that any atomistic model designed to provide an accurate description of a real magnetic material should, in principle, facilitate the coupling between these subsystems.

To the best of our knowledge, the first attempt to incorporate the dynamics of translational degrees of freedom into a spin system was made by Omelyan et al. [12], in the context of a simple model for Heisenberg ferrofluids. By taking the exchange interaction as a pairwise function of inter-atomic distance, they presented a dynamical simulation model that could be exploited via combined molecular and spin dynamics simulations. For integrating the coupled equations of motion, Omelyan et al. devised a new algorithm based on the ST decomposition of the full time evolution operator which includes both translational and spin degrees of freedom. Using empirical many-body potentials and an exchange interaction parameterized by first principles calculations, Ma et al. [13] further extended the idea of coupled molecular and spin dynamics into a more realistic model for the treatment of ferromagnetic iron. They further investigated the rate of transfer of energy between lattice and spin subsystems via large-scale microcanonical (NVE) simulations and emphasized the shorter characteristic time scale associated with the dynamics of the spins in comparison to translational degrees of freedom.

Recently, Yin et al. [9] discussed the inadequacy of modeling the exchange interaction for itinerant systems as a simple function of inter-atomic distance since such models fail to describe the longitudinal fluctuations in magnetic moments. By introducing local atomic environmental parameters such as shell number and atomic volume, they developed a many-body-like exchange function for BCC iron based on first principles calculations. However, the proposed exchange function is not suitable for molecular dynamics simulations due to the complications associated with the discontinuity of its derivative at the cut-off distance.

In this paper, we present a compressible magnetic model for BCC iron, which is readily applicable for both Monte Carlo and combined molecular-spin dynamics simulations. We also discuss the generalization of the Suzuki-Trotter deposition method used for solving the coupled equations of motion for translational and spin degrees of freedom. Finally, by computing space-time Fourier transforms of correlation functions, we present solid evidence that indicate direct coupling between phonons and magnons.

2. Model and methods

2.1. Hamiltonian and equations of motion

Let us consider a system of \( N \) magnetic atoms of mass \( m \), described by the classical Hamiltonian

\[
H = \sum_{i=1}^{N} \frac{mv_i^2}{2} + U(\{r_i\}) - \sum_{i<j} J(r_{ij})\mathbf{e}_i \cdot \mathbf{e}_j,
\]
where \( \{ \mathbf{r}_i \} \) and \( \{ \mathbf{v}_i \} \) are positions and velocities respectively and \( \{ \mathbf{e}_i \} \) are the unit vectors representing the directions of atomic spins \( \{ \mathbf{s}_i \} \). \( U(\{ \mathbf{r}_i \}) \) is the many-body atomic interaction term described by the Finnis-Sinclair potential for iron [14, 15]. The magnitudes of the spins \( \mathbf{s}_i \) and \( \mathbf{s}_j \) are absorbed into the exchange interaction \( J(r_{ij}) \), for which we take the same functional form and parameterization as used by Ma et al. [13].

Classical Hamilton equations yield the familiar equations of motion for positions and velocities as

\[
\begin{align*}
\frac{d\mathbf{r}_i}{dt} &= \mathbf{v}_i, \\
\frac{d\mathbf{v}_i}{dt} &= \frac{\mathbf{f}_i}{m},
\end{align*}
\]

where \( \mathbf{f}_i = -\nabla_{\mathbf{r}_i} U_i + \sum_{j \neq i} dJ(r_{ij})/dr_{ij} \left( \mathbf{e}_i \cdot \mathbf{e}_j \right) \) is the force acting the \( i^{th} \) atom. Using the Poisson brackets method for the spin-dependent term of the Hamiltonian, one can obtain an equation for the precessional motion of the spins as,

\[
\frac{d\mathbf{e}_i}{dt} = \left( \frac{g \mu_B}{\hbar M_i} \right) \mathbf{H}_i^{eff} \times \mathbf{e}_i
\]

Here, \( \mathbf{H}_i^{eff} = -\sum_{j \neq i} J(r_{ij}) \mathbf{e}_j \) is the effective field on the \( i^{th} \) spin, \( g \) is the electron g-factor, and \( \{ M_i \} \) are the magnitudes of atomic magnetic moments. A detailed discussion of the derivation of this formula can be found in Ref. [13].

Although the magnitudes of the moments are not considered as explicit phase variables in this model, they are allowed to vary dynamically via the dependence between the moment and the local atomic environment. Thus, whenever the atomic configuration changes during the simulation, moments \( \{ M_i \} \) are re-evaluated from a regression relationship between the moment and the local Voronoi volume of the atom, established via Locally Self Consistent Multiple Scattering (LSMS) first principles method [16].

2.2. Time integration algorithm

According to the Liouville formalism of classical mechanics, equations of motion can be represented as

\[
\frac{dy(t)}{dt} = \hat{L}y(t),
\]

where \( y(t) = \{ \mathbf{r}_i(t), \mathbf{v}_i(t), \mathbf{e}_i(t) \} \) denotes the complete set of phase variables consisting of positions, velocities and directions of the spins at time \( t \). The Liouville operator \( \hat{L} \) takes the form,

\[
\hat{L} = \sum_{i=1}^{N} \left( \mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \frac{\mathbf{f}_i}{m_i} \cdot \frac{\partial}{\partial \mathbf{v}_i} + \left( \frac{g \mu_B}{\hbar M_i} \right) \left( \mathbf{H}_i^{eff} \times \mathbf{e}_i \right) \cdot \frac{\partial}{\partial \mathbf{e}_i} \right).
\]

The formal solution to Eq. 4 is

\[
y(t + \tau) = e^{L\tau} y(t),
\]

where \( \tau \) is the time step, and \( e^{L\tau} \) is the exponential operator which fully determines the time evolution of the microscopic phase variables. Unfortunately this operator cannot be evaluated exactly, thus one has to rely on approximate solutions which involve the decomposition of the operator into a series of sub-operators, where the respective operations are trivial enough to be evaluated analytically. As the first step, we write the Liouville operator \( \hat{L} \) as a sum of three terms,

\[
\hat{L} = \hat{L}_r + \hat{L}_v + \hat{L}_s,
\]
where $\hat{L}_r = \sum_i \mathbf{v}_i \cdot \partial / \partial \mathbf{r}_i$ which only acts on positions, $\hat{L}_v = \sum_i \mathbf{f}_i / m_i \cdot \partial / \partial \mathbf{v}_i$ which only acts on velocities, and $\hat{L}_s = \sum_i (g \mu_B / \hbar M_i) (\mathbf{H}_{eff}^s \times \mathbf{e}_i) \cdot \partial / \partial \mathbf{e}_i$ which only operates on spin orientations. The solution given by Eq. 6 now takes the form,

$$y(t + \tau) = e^{(\hat{L}_v + \hat{L}_v + \hat{L}_s)\tau} y(t).$$

(8)

Grouping the operators $\hat{L}_r$ and $\hat{L}_s$ together as a single operator, one can use the second order Suzuki-Trotter formula [5] to decompose the exponential evolution operator as

$$e^{(\hat{L}_v + (\hat{L}_v + \hat{L}_s))\tau} = e^{\hat{L}_v\tau/2} e^{(\hat{L}_v + \hat{L}_s)\tau/2} e^{\hat{L}_v\tau/2} + \mathcal{O}(\tau^3),$$

which can be further decomposed by factorizing $e^{(\hat{L}_v + \hat{L}_s)\tau}$ in a similar manner to yield

$$e^{(\hat{L}_v + \hat{L}_v + \hat{L}_s)\tau} = e^{\hat{L}_v\tau/2} e^{\hat{L}_s\tau/2} e^{\hat{L}_v\tau/2} + \mathcal{O}(\tau^3).$$

(9)

Operators $\hat{L}_v\tau$ and $\hat{L}_s\tau$ merely shift the positions and velocities of the atoms as [6]

$$\begin{align*}
\left\{ e^{\hat{L}_v\tau} y = \{ \mathbf{r}_i + \mathbf{v}_i \tau, \mathbf{v}_i, \mathbf{e}_i \} \right. \\
\left. e^{\hat{L}_s\tau} y = \{ \mathbf{r}_i, \mathbf{v}_i + \frac{\mathbf{f}_i}{m}, \mathbf{e}_i \} \right. \\
\end{align*}$$

(10)

Since the the effective field $\mathbf{H}_{eff}^s$ acting on each spin depends on all other spins that fall within its interaction range, a similar analytical form doesn’t exist for the operator $e^{\hat{L}_s\tau}$. Therefore, one has to follow a ST decomposition scheme to find an approximate solution for $e^{\hat{L}_s\tau}$.

Krech et al. [7] and Tsai et al. [6] discuss the decomposition of the spin evolution operator $e^{\hat{L}_s\tau}$ for lattice-based spin systems by separating the lattice into a set of non-interacting sublattices. However, such decompositions cannot be directly applied to off-lattice spin systems where the neighbors of the spins are subjected to change with time. Therefore, following the method proposed by Omelyan et al. [12], we write the operator $e^{\hat{L}_s\tau}$ in terms of individual spin evolution operators as

$$e^{\hat{L}_s\tau} = \exp \left( \tau \sum_i \hat{L}_{s_i} \right)$$

where $\hat{L}_{s_i} = (g \mu_B / \hbar M_i) (\mathbf{H}_{eff}^s \times \mathbf{e}_i) \cdot \partial / \partial \mathbf{e}_i$, and apply the second order ST decomposition iteratively to obtain

$$e^{\hat{L}_s\tau} = e^{\hat{L}_{s_1}\tau/2} \ldots e^{\hat{L}_{s_N-1}\tau/2} e^{\hat{L}_{s_N}\tau} e^{\hat{L}_{s_{N-1}}\tau/2} \ldots e^{\hat{L}_{s_1}\tau/2} + \mathcal{O}(\tau^3),$$

(11)

where the operator $\hat{L}_{s_i}\tau$ rotates the spin $\mathbf{s}_i$ by an angle $|\mathbf{H}_{eff}^s|\tau$ around $\mathbf{H}_{eff}^s$ while keeping all other spins fixed. Thus the operation $e^{\hat{L}_v\tau} y$ is performed as a series of spin rotations, strictly following the order specified by Eq. (11), which thereby leads to the exact conservation of spin lengths [7, 6].

2.3. Dynamic structure factor

In MD and SD simulations, time-dependent correlation functions of microscopic dynamical variables and their Fourier transforms are integral to the study of collective excitations, such as lattice vibrations and spin waves [17, 2]. Results of the simulations are usually conveyed as the dynamic structure factor $S(\mathbf{q}, \omega)$ for momentum transfer $\mathbf{q}$ and frequency transfer $\omega$, a quantity that can be directly measured in inelastic neutron scattering experiments [18, 2].

Spatial Fourier transform of space-displaced, time-displaced density-density correlation function, namely the intermediate scattering function, is given by [19]

$$F_{nn}(\mathbf{q}, t) = \frac{1}{N} \langle \rho_n(\mathbf{q}, t) \rho_n(-\mathbf{q}, 0) \rangle,$$

(12)
where the angle brackets \( \langle \cdots \rangle \) denote the ensemble average, and \( \rho_n(q, t) = \sum_i \exp(-i q \cdot r_i(t)) \) is the spatial Fourier transform of microscopic atom density, \( \rho_n(r, t) = \sum_i \delta(r - r_i(t)) \).

Similarly, by defining microscopic spin density as \( \rho_s(r, t) = \sum_i e_i(t) \delta(r - r_i(t)) \), we write spin-spin intermediate scattering function as

\[
F^{\tau}_{ss}(q, t) = \frac{1}{N} \left\langle \rho^z_s(q, t) \rho^z_s(-q, 0) \right\rangle ,
\]

(13)

where \( k = x, y, \) or \( z \), and \( \rho_s(q, t) = \sum_i e_i(t) \exp(-i q \cdot r_i(t)) \). By choosing a Cartesian coordinate system in the spin space such that the \( z \) axis is parallel to the magnetization vector, we regroup

\[
F^L_{ss}(q, t) = F^z_{ss}(q, t),
\]

(14)

and a transverse component

\[
F^T_{ss}(q, t) = \frac{1}{2} (F^x_{ss}(q, t) + F^y_{ss}(q, t)).
\]

(15)

Fourier transforms of \( F_{nn}(q, t) \), \( F^L_{ss}(q, t) \) and \( F^T_{ss}(q, t) \) yield the dynamic structure factor

\[
S(q, \omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} F(q, t)e^{-i\omega t} dt.
\]

(16)

3. Results

3.1. Performance of the integration algorithm

Stability of any numerical integration scheme depends on the accuracy within which the conservation laws of the dynamics are observed over a period of time. The equations of motion for our model impose conservation of total energy, and for the special case of constant magnitudes for magnetic moments, conservation of magnetization as well. To illustrate the performance of our algorithm with regard to conservation laws, we have carried out microcanonical molecular-spin dynamics simulations on a \( 10 \times 10 \times 10 \) simulation cell with periodic boundary conditions, starting from well equilibrated initial configurations at temperature \( T = 800 \) K.

At this point, we would like to elaborate more on the procedure followed in generating initial states for the time integration. Although our Hamiltonian directly allows transfer of energy between the lattice and spin subsystems through the coordinate dependence of the exchange interaction, due to the absence of a spin-orbit coupling term it does not facilitate transfer of angular momentum between the two subsystems. That is, in the absence of any external torques on the spins, the total spin angular momentum will remain constant, irrespective of any external perturbations applied to the lattice subsystem. As a consequence, thermostat algorithms used in conventional molecular dynamics simulations would fail to thermalize the spin subsystem to the desired temperature in the same way that they would equilibrate the lattice subsystem. Therefore, in order to prepare initial configurations for any finite temperature \( T \), we adhere to the following procedure. As the first step, we equilibrate the subspace consisting of positions and spins using Metropolis Monte Carlo method [20]. Then we assign initial velocities to the atoms based on the Maxwell-Boltzmann distribution at the desired temperature. Finally, we carry out a microcanonical molecular-spin dynamics equilibration run which would ultimately bring the system to the equilibrium as a whole by resolving any inconsistencies between the position-spin subspace and the velocity distribution.

Fig. 1 shows energy [subset (a)] and magnetization [subset (b)] per atom as a function of time for different integration time steps. For the larger time steps considered (\( \tau = 5 \) fs and \( \tau = 10 \) fs), we observe systematic drifts in the energy whereas with \( \tau = 1 \) fs, we were able
Figure 1. Time dependence of total energy (a) and magnetization (b) per atom for microcanonical molecular-spin dynamics simulations performed at temperature $T = 800$ K. The curves are for different integration time steps and the same initial configuration.

maintain the total energy conserved within an accuracy of six significant digits, without any noticeable drifts. Due to the isotropic nature of the spin-dependent term of our Hamiltonian, in principle, magnetization should also be a constant of motion. However, this conservation law breaks down in our model as a result of the volume dependence of the magnitudes of moments. Large fluctuations in the net magnetization shown in Fig. 1 for $\tau = 1$ fs are merely consequences of this artifact, and should not be misinterpreted as numerical errors.

3.2. Effect of lattice vibrations on spin waves

To characterize collective excitations in our model, we have calculated density-density and spin-spin dynamic structure factors for $(q, 0, 0)$ direction at equilibrium temperatures $T = 293$ K and $T = 800$ K. For finite linear lattice dimension $L$, only $q = 2\pi n q / (La)$ with $n q = \pm 1, \pm 2, \ldots, \pm L$ are allowed, where $a$ is the lattice constant. Equations of motion were integrated up to $t_{\text{max}} = 1.0 \, \text{ns}$ using a time step of $\tau = 1$ fs. The ensemble averages in Eq. (12) and (13) were computed using the results from 200 independent simulations, each initiated from an equilibrium configuration drawn from the canonical ensemble, using the procedure explained in section 3.1.

In Fig. 2, we have shown the transverse component of the spin-spin dynamic structure factor at temperature $T = 293$ K for $|q| = 0.66 \, \text{Å}^{-1}$ [subset (a)] and $|q| = 1.1 \, \text{Å}^{-1}$ [subset (b)]. Here, the full circles represent data obtained from molecular-spin dynamics simulations, whereas the open squares are from SD simulations performed with atoms frozen at perfect lattice positions. In order to make a fair comparison, exchange interaction parameters for the rigid lattice SD simulations were determined from the same pairwise function as used in molecular-spin dynamics simulations. In the presence of lattice vibrations, we observe that the peak positions of the transverse spin-spin dynamic structure factor systematically shift to lower frequencies. In addition, especially for larger $q$ values, we find significant decrease in the peak amplitudes as well as increase in the half-widths, a behavior which clearly suggests damping of the spin waves. These effects of softening and damping of spin wave modes are in good qualitative agreement with the theoretical predictions by Woods et al. [21].

Fig. 3 shows the longitudinal component of the spin-spin dynamic structure factor for $|q| = 0.22 \, \text{Å}^{-1}$ at $T = 800$ K, for molecular-spin dynamics simulations [subset (a)] and rigid lattice SD simulations [subset (b)]. We conjecture that the multiple peak structure observed in the longitudinal component is a result of the two-spin-wave annihilation or creation, an effect which becomes more pronounced for small lattice sizes [22]. Curves in subset (a) and
Figure 2. Transverse component of spin-spin dynamic structure factor $S_{ss}^T(q, \omega)$ at temperature $T = 293$ K for (a) $|q| = 0.66 \, \text{Å}^{-1}$ and (b) $|q| = 1.1 \, \text{Å}^{-1}$, along the $(q, 0, 0)$ direction for a $10 \times 10 \times 10$ simulation cell. Full circles (●) represent data obtained from molecular-spin dynamics (MD-SD) simulations while open squares (□) are from pure spin dynamics (SD) simulations performed on a rigid lattice.

Figure 3. Longitudinal component of spin-spin dynamic structure factor $S_{ss}^L(q, \omega)$ at $T = 800$ K for $|q| = 0.22 \, \text{Å}^{-1}$, along the $(q, 0, 0)$ direction for a $10 \times 10 \times 10$ simulation cell. (a) Molecular-spin dynamics simulations (b) Pure spin dynamics simulations on a rigid lattice. The additional sharp peak at $\omega \approx 7.5 \, \text{meV}$ coincides with the peak position of the density-density structure factor for the same $|q|$. (b) are nearly identical, except for the sharp peak at $\omega \approx 7.5 \, \text{meV}$ which only appears in subset (a), for the case of molecular-spin dynamics simulations. The position of this peak coincides with the peak position of the density-density dynamic structure factor (Fig. 4) for the same $|q|$ value, which suggest the existence of a propagating spin wave excitation coupled with the longitudinal phonon mode of the same frequency. We have observed similar coupled phonon-magnon excitations for all $|q|$ values accessible through our simulations. Presence of longitudinal spin wave excitations at sound frequency is a new form of dynamical behavior in magnetic materials yet to be observed experimentally.
4. Summary
In conclusion, we have used a compressible magnetic model to investigate the collective excitations in BCC iron. With the second order Suzuki-Trotter decomposition method we use for time integration, we were able to achieve stable numerical solutions over reasonably long time periods, with respect to the accuracy in energy conservation. In order to investigate the effect of lattice vibrations on spin wave excitations, we have computed spin-spin and density-density dynamic structure factors, and compared them to the results obtained from spin dynamics simulations performed on rigid lattices. In the presence of lattice vibrations, we observe softening and damping of spin wave modes. The additional peaks we observe in the longitudinal spin-spin dynamic structure factor coincide with the peak positions of the density-density dynamic structure factor, which indicates the possibility of longitudinal spin wave excitations at sound frequency.

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Figure 4. Density-density dynamic structure factor $S_{nn}(q, \omega)$ at $T = 800$ K for $|q| = 0.22 \text{ Å}^{-1}$, along the $(q,0,0)$ direction for a $10 \times 10 \times 10$ simulation cell.
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