Statistical recovery of the classical spin Hamiltonian

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We propose a simple procedure by which the interaction parameters of the classical spin Hamiltonian can be determined from the knowledge of four-point correlation functions and specific heat. The proposal is demonstrated by using the correlation and specific heat data generated by Monte Carlo method on one- and two-dimensional Ising-like models, and on the two-dimensional Heisenberg model with Dzyaloshinskii-Moriya interaction. A recipe for applying our scheme to experimental images of magnetization such as those made by magnetic force microscopy is outlined.

Condensed matter, either in their natural form or as synthesized in laboratories, are invariably complicated and have complex interactions among its constituents. Spin-spin interaction in magnetic insulators for one thing can have ranges well beyond the first neighbor, and yet models almost uniquely focus on cases with only one or just a few interaction parameters. Even between a pair of nearest-neighbor spins, the interactions can take on symmetric or anti-symmetric forms, either preserving the spin rotation symmetry or breaking it altogether. Deducing the proper interaction parameters is also of paramount importance in the search for exotic spin liquid states. On the other hand, the spin rotation symmetry or breaking it altogether can have ranges well beyond the first neighbor, and yet models almost uniquely focus on cases with only one or just a few interaction parameters.

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Statistical properties of the model are easy to generate by means of the Monte Carlo (MC) simulation. Given some material whose interactions are assumed to fit the above $H$ with some choice of $J_r$’s, and some of its thermodynamic properties known experimentally, would it be possible to fix the parameters $J_r$ by virtue of the known experimental input? We claim the answer is in the affirmative, specifically if the four-point correlation function and the specific heat are known accurately as a function of temperature. We support our claim and illustrate the recovery procedure using the statistical data generated by the MC simulation.

A well-known theorem of equilibrium statistical mechanics is ($k_B = 1$)

$$\langle H^2 \rangle - \langle H \rangle^2 = T^2 C(T)$$

where $C(T)$ refers to the specific heat. In terms of the general Hamiltonian \textsuperscript{[1]}, one can re-cast the identity as

$$\sum_{r,r'} J_r C_{r,r'} J_{r'} = T^2 C(T),$$

$$C_{r,r'} = \langle \Sigma_r \Sigma_{r'} \rangle - \langle \Sigma_r \rangle \langle \Sigma_{r'} \rangle,$$

where $\Sigma_r = \sum_i \sigma_i \sigma_{i+r}$. The four-point correlation functions $C_{r,r'}$ form a temperature-dependent, real and symmetric matrix. One can write the identity in the matrix form

$$\mathcal{J}^T C(T) \mathcal{J} = T^2 C(T),$$

where $\mathcal{J}$ is a vector consisting of all the interaction parameters.

With the given knowledge of $C(T)$ and $C(T)$ over a sufficiently wide temperature range, it becomes a matter of determining $\mathcal{J}$ that best reproduces the thermodynamic identity. Defining the difference function $D(\mathcal{J}, T) = \mathcal{J}^T C(T) \mathcal{J} - T^2 C(T)$, the cost function to minimize is

$$I[\mathcal{J}] = \sum_T [D(\mathcal{J}, T)]^2.$$

The summation $\sum_T$ takes place over all temperatures for which correlation and specific heat data are available. Applying the gradient descent (GD)
one can update the parameters $J_r$ iteratively until convergence is reached, thus completing the “statistical recovery” of the original Hamiltonian.

In practice, some pre-conditioning of the data is required to ensure the convergence of the GD scheme. The inevitable noise from statistical fluctuations in the temperature dependence of the correlation functions $C_{r,r}'(T)$ as well as the specific heat function $C(T)$ carry over to the gradient $\partial I/\partial J_r$ in (6), creating unwanted local minima in the cost function’s landscape. On the other hand, the GD method proved to work very well if we first smooth out both functions with a Gaussian filter, and then apply the descent scheme. The correlation function $C_{1,1}(T)$ and the specific heat $C(T)$ before and after smoothing are shown in Fig. 1.

Another recipe we found crucial in the successful implementation of the GD method is rooted on the physically motivated interaction hierarchy $|J_r| > |J_{r'}|$ when $r$ is less than $r'$. Instead of updating all the parameters at once, we first update $J_1$ using the gradient $\partial I/\partial J_1$, keeping all other $J_r$’s fixed. After, say, 1000 iterations for $J_1$, we start updating $J_2$ according to $\partial I/\partial J_2$ while keeping all $J_{r\neq2}$ fixed. Once the update reaches the final $J_r$, we come back to $J_1$ and start over the iteration. A small enough cost function is achieved after repeating this procedure $\sim 10^4$ times.

The validity of our scheme was tested for one-dimensional ferromagnetic model (1) of length $L = 100$ with $(J_1, J_2, J_3) = (1, 0.5, 0.33)$. MC annealing was used to generate the correlation matrix $C_{r,r'}(T)$ and the specific heat $C(T)$ over $0 < T < 2$, and the GD scheme was applied in the prescribed manner. Five hundred temperature steps were taken. After the GD iteration is complete, we find the recovery parameters $(J_1, J_2, J_3) = (1.017, 0.506, 0.329)$ in close proximity to the original values, irrespective of the initial parameters chosen for the iteration.

Deducing parameters of the Heisenberg-type spin Hamiltonian through our recovery procedure is a greater challenge. We consider as an example the Heisenberg-Dzyaloshinskii-Moriya-Zeeman (HDMZ) Hamiltonian given by

$$H_{\text{HDMZ}} = -J \sum_i \mathbf{S}_i \cdot \left( \mathbf{S}_{i+\hat{x}} + \mathbf{S}_{i+\hat{y}} \right) + D \sum_i \mathbf{S}_i \cdot \left( \mathbf{S}_{i+\hat{x}} \times \hat{y} - \mathbf{S}_{i+\hat{y}} \times \hat{x} \right) - B \cdot \sum_i \mathbf{S}_i.$$  

(7)

Its properties and phase diagram are well-known [2]. Although this model has been primarily used to understand the properties of skyrmions [23], we adopt this model here for the sake of illustrating the statistical recovery procedure.

Suppose now that we did not know the exact structure of the microscopic Hamiltonian, and instead had to assume the more general spin-spin interaction

$$H = \sum_i \left( \sum_{\alpha=x,y} \sum_{\beta=x,y,z} J_{\alpha\beta} \alpha^{\alpha} S_{i+\hat{\alpha}} \beta^{\beta} - BS_i^z \right).$$  

(8)

In the most general circumstance we have a total of 18 fitting parameters $J_{\alpha\beta}$. The energy variance for $B = 0$ follows from

![Figure 1](image1.png)

**FIG. 1.** (a) Correlation function $C_{1,1}(T)$ of the one-dimensional Ising-like model (1) with $(J_1, J_2, J_3) = (1, 0.5, 0.33)$, before and after smoothing. (b) $T^2C(T)$ before and after smoothing. The $J^T C(T) J$ curve shown here using the recovered parameters $(J_1, J_2, J_3) = (1.017, 0.506, 0.329)$ is indistinguishable from the smoothened $T^2C(T)$ curve.

![Figure 2](image2.png)

**FIG. 2.** Plots of $T^2C(T)$ and $J^T C(T) J$ for two-dimensional Ising-type model with interactions $(J_1, J_2, J_3) = (1.0, 0.7, 0.5)$ on $20 \times 20$ lattice. Two curves are indistinguishable. The scheme is subsequently applied to two-dimensional ferromagnetic Ising-type model with first- to third-neighbor interactions, $(J_1, J_2, J_3) = (1, 0.7, 0.5)$, on the $L \times L$ square lattice. Figure 2 shows $T^2C(T)$ both from original MC annealing and from the statistical recovery procedure on $20 \times 20$ lattice. One sees only one curve because of the heavy overlap of the original and recovered plots. The interaction parameters obtained through the statistical recovery were $(J_1, J_2, J_3) = (0.992, 0.691, 0.507)$ after 6000 sweeps through the parameters.
The specific heat function over $0 < T < T_f$ was used with very similar results. Both 3 and 7 parameter fits were used with very similar results.

The surface data. Let’s say we are given the 512 × 512 pixel image of an MFM measurement on some surface where each pixel represents the local magnetization normal to the plane. The image can be cut into 16 × 16 pieces of equal sizes, each piece containing 32 × 32 pixels. These 256 pieces cut out from one large 512 × 512 batch constitute the ensemble of states corresponding to the same external conditions such as temperature and magnetic field. Taking M = 256 as the number of states, the ensemble average procedure goes as

$$\langle \sum_{i,j} \sigma_i \sigma_{i+r} \sigma_{j} \sigma_{j+r'} \rangle = \sum_{i,j} \sigma_i \sum_{j} \sigma_j \langle \sum_{j} \sigma_j \sigma_{j+r'} \rangle$$

$$= M^{-1} \sum_{c=1}^{M} \sum_{i,j} \sigma_i^{(c)} \sigma_{i+r}^{(c)} \sigma_j^{(c)} \sigma_{j+r'}^{(c)}$$

$$- M^{-2} \sum_{c,i} \sum_{j} \sigma_i^{(c)} \sigma_{i+r}^{(c)} \sum_{c,j} \sigma_j^{(c)} \sigma_{j+r'}^{(c)}.$$ (10)

The summation $\sum_i$ and $\sum_j$ as well as the positions $r$ and $r'$ are confined within the 32 × 32 pixel area. This is not a severe restriction in practice since the interaction parameters $J_r$ are expected to die off quickly with separation $r$.

Often the resolution of the images is not truly atomic scale, as with the MFM measurement. Each pixel in the MFM image represents an average of the local magnetization within the resolution window, much like the coarse-graining process in the real-space renormalization group theory. In that case the interaction Hamiltonian deduced by our procedure would be the coarse-grained version of the true microscopic Hamiltonian. Even a microscopic Hamiltonian involving only the nearest-neighbor interaction is known to generate longer-ranged interactions upon coarse-graining, and our demonstration of the fitting procedure in terms of several interaction parameters is of practical relevance.

An analogous proposal was made in Ref. 10 for the quantum case, which argued that a single wave function and the four-point correlations obtained with respect to it is sufficient to recover the parameters of the original local magnetization. Examples are spin-polarized scanning tunneling microscopy (SPSTM) magnetic force microscopy (MFM), and Lorentz transmission electron microscopy (LTEM), all of which are being actively used in the investigation of low-dimensional magnets. Measuring the specific heat of a truly two-dimensional material poses an obvious challenge, but there is progress in recent years to measure the thermodynamic quantity of single and multi-layer graphene. In layered materials with very weak inter-layer interaction, the measured bulk specific heat can be translated into the per-layer quantity, while surface probes reveal the four-point correlations of the magnetic moment within the plane.

We outline a prescription, partly described in an earlier publication, to extract four-point correlations from the surface data. Let’s say we are given the 512 × 512 pixel image of an MFM measurement on some surface where each pixel represents the local magnetization normal to the plane. The image can be cut into 16 × 16 pieces of equal sizes, each piece containing 32 × 32 pixels. These 256 pieces cut out from one large 512 × 512 batch constitute the ensemble of states corresponding to the same external conditions such as temperature and magnetic field. Taking $M = 256$ as the number of states, the ensemble average procedure goes as
microscopic Hamiltonian. In detail, the procedure proposed in Ref. [10] is quite different from ours, and assumes the full knowledge of either the wave function or its four-point correlation functions, both of which are extremely challenging to obtain experimentally. Our proposal is based on simple application of classical statistical mechanics, and assumes knowledge of the ensemble average rather than the quantum expectation value. An enormous range of Ising-like magnets have been identified and thoroughly studied in the past[11], and we believe direct application of our scheme to such magnets should be feasible. Fits to the specific heat and the magnetic susceptibility as a means to deduce interaction parameters of the Ising-like magnet have persisted over the years[11]. Inelastic neutron scattering also offers a strong venue for determining the interaction parameters in insulating magnets. One advantage of our method over existing ones comes from the implementation of the GD scheme, which automatically finds the appropriate set of parameters once the four-point correlation and the specific heat are known with sufficient accuracy. No fine-tuning of the parameters by hand is required, nor is it possible.

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