Supplemental Material: Fast, hierarchical, and adaptive algorithm for Metropolis Monte Carlo simulations of long-range interacting systems

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In this supplement we show for general O(n) models in a more formalistic way how the bounds for the change of energy from the main text and an alternative employing the longitudinal and transversal projections can be derived.

Using the Heaviside function θ, a weighted sum of variables $s_j^* \in [-1, 1]$ with weights J_{ij} can be divided into two sums

$$\sum_{j\in B} J_{ij} s_j^* = \sum_{j\in B} J_{ij} s_j^* \theta(s_j^*) + \sum_{j\in B} J_{ij} s_j^* \theta(-s_j^*) \tag{S1}$$

such that each sum contains terms with identical signs. With $0 \leq J^{\min} \leq J_{ij} \leq J^{\max}$ follows

$$\begin{aligned}\sum_{j\in B} J_{ij} s_j^* \theta(s_j^*) &\in \left[\sum_{j\in B} J^{\min} s_j^* \theta(s_j^*),\, \sum_{j\in B} J^{\max} s_j^* \theta(s_j^*)\right] \\ &= [J^{\min} M^+, J^{\max} M^+],\end{aligned} \tag{S2}$$

and for the sum of negative terms

$$\begin{aligned}\sum_{j\in B} J_{ij} s_j^* \theta(-s_j^*) &\in \left[\sum_{j\in B} J^{\max} s_j^* \theta(-s_j^*),\, \sum_{j\in B} J^{\min} s_j^* \theta(-s_j^*)\right] \\ &= [-J^{\max} M^-,\, -J^{\min} M^-],\end{aligned} \tag{S3}$$

with $M^+ \coloneqq \sum_{j\in B} s_j^* \theta(s_j^*)$ and $M^- \coloneqq -\sum_{j\in B} s_j^* \theta(-s_j^*)$. Consequently

$$\sum_{j\in B} J_{ij} s_j^* \in [J^{\min} M^+ - J^{\max} M^-,\, J^{\max} M^+ - J^{\min} M^-]. \tag{S4}$$

Here, the dependency on the spin-box vector $\mathbf{R}$ is suppressed. Identifying s_j^* with Ising spins s_j or with projections $s_{j,\alpha}$ of O(n) spins onto Cartesian directions and multiplying with $-\Delta s_i$ or $-\Delta s_{i,\alpha}$, respectively, recovers the **Bounds 2** discussed in the main article.

For the O(n) model with $n \geq 2$, alternative coordinates with components parallel and perpendicular to the magnetization $\mathbf{M}_B = \sum_{j\in B} \mathbf{s}_j$ may be considered. The change in energy can be expressed as

$$\Delta E_B = -\Delta \mathbf{s}_i \sum_{j\in B} J_{ij} \mathbf{s}_j \tag{S5}$$

$$= -\Delta \mathbf{s}_i \sum_{j\in B} J_{ij} (s_j^{\parallel} \mathbf{e}_{\parallel} + s_j^{\perp} \mathbf{e}_{\perp} + s_j^{III} \mathbf{e}_3 + s_j^{IV} \mathbf{e}_4 + \dots), \tag{S6}$$

where $s_j^{\parallel} = \mathbf{s}_j \mathbf{e}_{\parallel}$ and $s_j^{\perp} = \mathbf{s}_j \mathbf{e}_{\perp}$ are projections onto directions within the $\mathbf{M}_B - \Delta \mathbf{s}_i$-plane that are parallel and perpendicular to $\mathbf{M}_B$:

$$\mathbf{e}_{\parallel} = \mathbf{M}_B / |\mathbf{M}_B|, \tag{S7}$$

$$\mathbf{e}_{\perp} = \frac{\Delta \mathbf{s}_i - (\Delta \mathbf{s}_i \mathbf{e}_{\parallel}) \mathbf{e}_{\parallel}}{|\Delta \mathbf{s}_i - (\Delta \mathbf{s}_i \mathbf{e}_{\parallel}) \mathbf{e}_{\parallel}|}. \tag{S8}$$

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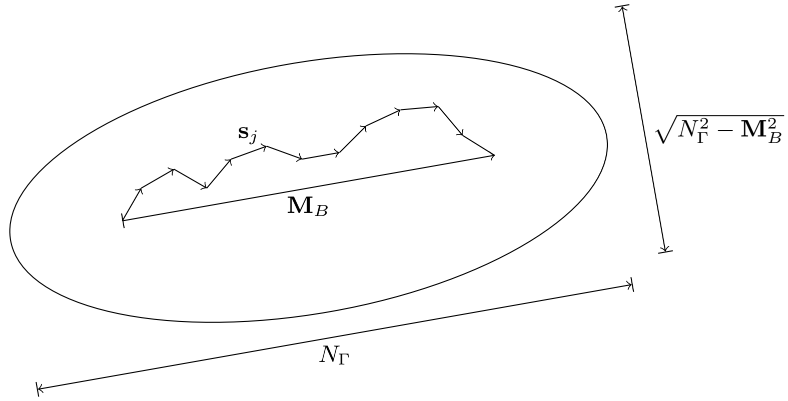

FIG. 1. The spins of box B form a polygonal chain of N_Γ segments that is confined by an ellipse. The depiction shows the case of $n = 2$ (XY model) where the arrows are the actual spins. For $n > 2$ the arrows would be their projections onto the $\mathbf{M}_B - \Delta\mathbf{s}_i$-plane and generally would not be of equal length.

The remaining basis vectors $\mathbf{e}_3, \mathbf{e}_4, \ldots$ are perpendicular to $\Delta\mathbf{s}_i$ and the respective spin components do not contribute to ΔE_B. Since throughout a typical simulation $\mathbf{e}_\parallel$ and $\mathbf{e}_\perp$ are not constant, it is impractical to permanently measure $M_\parallel^\pm = \pm\sum_{j\in B} s_j^\parallel \theta(\pm s_j^\parallel)$ or $M_\perp^\pm = \pm\sum_{j\in B} s_j^\perp \theta(\pm s_j^\perp)$ which instead have to be estimated as well. On the other hand the box magnetization $\mathbf{M}_B$ is available at any point in time, by always updating it after every successful spin rotation. We consider the set of all spins in B as a polygonal chain of length $N_\Gamma = \sum_{j\in B} 1$ starting from the origin and ending at $\mathbf{M}_B$ as shown in Fig. 1. It is confined by an ellipsoid with an extension of N_Γ in the direction parallel and $\sqrt{N_\Gamma^2 - \mathbf{M}_B^2}$ in the directions perpendicular to $\mathbf{M}_B$ which implies

$$|\mathbf{M}_B| \leq M_\parallel^+ \leq (N_\Gamma + |\mathbf{M}_B|)/2, \tag{S9}$$

$$0 \leq M_\parallel^- \leq (N_\Gamma - |\mathbf{M}_B|)/2, \tag{S10}$$

as as well as

$$0 \leq M_\perp^+ \leq \sqrt{(N_\Gamma^2 - \mathbf{M}_B^2)}/2, \tag{S11}$$

$$0 \leq M_\perp^- \leq \sqrt{(N_\Gamma^2 - \mathbf{M}_B^2)}/2. \tag{S12}$$

From Eq. (S4) with $M_\parallel^+ = |\mathbf{M}_B| + M_\parallel^-$ the analog of **Bounds 2** follows:

$$\sum_{j\in B} J_{ij} s_j^\parallel \in \left[J^{\min}|\mathbf{M}_B| - (J^{\max} - J^{\min})\frac{N_\Gamma - |\mathbf{M}_B|}{2},\ J^{\max}|\mathbf{M}_B| + (J^{\max} - J^{\min})\frac{N_\Gamma - |\mathbf{M}_B|}{2}\right] \tag{S13}$$

$$= \left[\frac{J^{\max} + J^{\min}}{2}|\mathbf{M}_B| - \frac{J^{\max} - J^{\min}}{2}N_\Gamma,\ \frac{J^{\max} + J^{\min}}{2}|\mathbf{M}_B| + \frac{J^{\max} - J^{\min}}{2}N_\Gamma\right], \tag{S14}$$

and using $M_\perp^- = M_\perp^+$

$$\sum_{j\in B} J_{ij} s_j^\perp \in \left[-\frac{J^{\max} - J^{\min}}{2}\sqrt{N_\Gamma^2 - \mathbf{M}_B^2},\ \frac{J^{\max} - J^{\min}}{2}\sqrt{N_\Gamma^2 - \mathbf{M}_B^2}\right]. \tag{S15}$$

For the direction parallel to $\mathbf{M}_B$, **Bounds 3** are a viable alternative. Instead of (S1) we write

$$\sum_{j\in B} J_{ij} s_j^\parallel = \sum_{j\in B} J_{ij}(\pm 1 \mp 1 + s_j^\parallel) \tag{S16}$$

$$= \pm\sum_{j\in B} J_{ij} \mp \sum_{j\in B} J_{ij}(1 \mp s_j^\parallel) \tag{S17}$$

$$= \pm J_\Gamma^{\text{int}} \mp \sum_{j\in B} J_{ij}(1 \mp s_j^\parallel). \tag{S18}$$

Since $|s_j^{\|}| \leq 1$ it is

$$\sum_{j\in B} J_{ij}(1 \mp s_j^{\|}) \in \left[\sum_{j\in B} J_\Gamma^{\min}(1 \mp s_j^{\|}),\, \sum_{j\in B} J_\Gamma^{\max}(1 \mp s_j^{\|})\right] \tag{S19}$$

or using $\sum_{j\in B} 1 = N_\Gamma$ and $\sum_{j\in B} s_j^{\|} = |\mathbf{M}_B|$

$$\sum_{j\in B} J_{ij}(1 \mp s_j^{\|}) \in \left[J_\Gamma^{\min}(N_\Gamma \mp |\mathbf{M}_B|),\, J_\Gamma^{\max}(N_\Gamma \mp |\mathbf{M}_B|)\right]. \tag{S20}$$

From the two options we select the more narrow bounds and obtain for the direction parallel to $\mathbf{M}_B$

$$\sum_{j\in B} J_{ij} s_j^{\|} \in [\mathcal{S}_{\min}^{\|}, \mathcal{S}_{\max}^{\|}], \tag{S21}$$

with

$$\mathcal{S}_{\min}^{\|} = \max\left(J_\Gamma^{\text{int}} - J_\Gamma^{\max} K_B^-, -J_\Gamma^{\text{int}} + J_\Gamma^{\min} K_B^+\right), \tag{S22}$$

$$\mathcal{S}_{\max}^{\|} = \min\left(J_\Gamma^{\text{int}} - J_\Gamma^{\min} K_B^-, -J_\Gamma^{\text{int}} + J_\Gamma^{\max} K_B^+\right), \tag{S23}$$

and $K_B^{\pm} = N_\Gamma \pm |\mathbf{M}_B|$.