Heisenberg model

The Heisenberg model generalises the Ising model, where, instead of binary values, the spins are 3-component vector valued and take values on the surface of the unit sphere, i.e. $\vec{S}_i \in \mathbb{S}^2 \subset \mathbb{R}^3$. With $J > 0$, the Hamiltonian penalises misalignment of nearest-neighbour spins:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j. \tag{1}$$

Since we have no magnetic field, we set $J = 1$ for the remainder of this sheet.

While for the XY model ($\vec{S}_i \in \mathbb{S}^1 \subset \mathbb{R}^2$) it is advantageous to use polar coordinates, it not clear if in the 3-component spin case the added complexity and the additional floating point operations justifies the memory savings.

Task 1: Implement a Metropolis simulation of the 3D Heisenberg model. Except for a few changes in the update probability computation and the representation of your cluster, you should not need to drastically modify your code for the Ising model. Remember to normalize your vectors if you use a Cartesian representation.

Task 2: The cluster algorithms (Swendsen-Wang or Wolff) can be extended to systems with any number of spin components by considering reflections around a random plane at each MC step.

1. Select a random reflection plane by drawing a random normal unit vector $\hat{n}$.
2. Grow a cluster with bond probability
$$p_{i,j} = 1 - \exp\left\{\min\left[0, 2\beta\left(\vec{S}_i \cdot \hat{n}\right)\left(\vec{S}_j \cdot \hat{n}\right)\right]\right\}, \tag{2}$$
where $\beta = 1/k_\mathrm{B}T$.
3. In the case of acceptance, flip the spins as $\vec{S}_i \leftarrow \vec{S}_i - 2\hat{n}(\vec{S}_i \cdot \hat{n})$.

Plot your results for the order parameter of this system, which is the spontaneous magnetisation density:

$$\langle|\vec{m}|\rangle = \langle m \rangle = \left\langle \frac{1}{L^3} \left| \sum_{i=1}^{L^3} \vec{S}_i \right| \right\rangle. \tag{3}$$

Also plot the energy density $\langle \mathcal{H} \rangle / L^3$ and the response functions: magnetic susceptibility χ and specific heat c_V as a function of T for different L. Compare the size of magnetisation fluctuations to the Ising model by inspecting χ and physically interpret your observation.

Task 3: Estimate the critical temperature T_c using the Binder cumulant for order parameter m

$$U_4(T, L) = 1 - \frac{\langle m^4(T) \rangle}{3\langle m^2(T) \rangle^2}. \tag{4}$$

Hint: Recall that $U_4(T_c, L) = U_4(T_c)$. You can use small system sizes.

Task 4 (optional): Compute the autocorrelation time τ for different L, either for E or m, at T_c and find the dynamical critical exponent z_c, which describes the algebraic finite-size scaling $\tau \sim L^{z_c}$, by finding the best fit to your data.