Monte Carlo Simulation of Spin-fermion Model

Based on

Phase Separation in Electronic Models for Manganites

S. Yunoki, J. Hu, A. L. Malvezzi,

A. Moreo, N. Furukawa, and E. Dagotto.

Phys. Rev. Lett., 80:845–848, Jan 1998.

Amit Bikram Sanyal

May 3, 2020

Modelling a crystal: Hubbard Model

- Let us consider a model of a rectangular lattice where the electrons can hop to nearest neighboring sites, and interact on the same site. This can be represented by

$$\hat{H} = -t \left(\sum_{\sigma=\uparrow,\downarrow} \sum_{\langle i,j \rangle} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + U \sum_{i=1}^{N} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \tag{1}$$

- This is known as the Hubbard Model.
- It is intrinsically a many-body system due to the 4-fermionic interaction term $\hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$.
- As a result, the Hilbert space grows as $\mathcal{O}(N!)$: this is an obvious problem for computation.

Simplifying to a smaller Hilbert space

- There are several, almost equivalent ways of tacking this problem.
- One of these methods is the Mean-field solution, where we assume that a single electron is moving in a a effective field created by the rest of the electrons.
- We can show that interaction can be approximately decomposed into *auxiliary fields*, which act as an effective classical spin sitting at each location that interacts with the itinerant electron.

The Spin-fermion Model

- The Spin-fermion (SF) model was initially a phenomenological model.
- We pretend that each site is actually occupied by a classical spin that can take any orientation, and at each site, a single fermionic interaction term appears that can simulate the effects of the electron-electron interaction.
- For an $L_x \times L_y$ lattice, this only creates a much smaller Hilbert space of dimension $2L_xL_y$, as opposed to $\mathcal{O}((L_xL_y)!)$ in the many-body case. The factor of 2 appears because of the two spin sectors of the problem.
- Although phenomenological in nature, it was shown to be highly effective in capturing the effects of interaction in the system.

The Spin-fermion Model

- Later on, it was discovered that there are actual materials in nature with multi-orbital crystals, such as cuprates and manganites, which realistically have a structure similar to the SF model![1].
- This further cemented the importance of this model as an investigative tool.

The Spin-fermion Model

- The single-orbital SF Hamiltonian is given as

$$\begin{aligned}\hat{H} &= -t\sum_{\langle i,j\rangle,\sigma}\left(\hat{a}^{\dagger}_{i,\sigma}\hat{a}_{j,\sigma}+h.c.\right)-J_H\sum_i \vec{s_i}\cdot\vec{S}_i+J_{AF}\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j \\ &= -t\sum_{\langle i,j\rangle,\sigma}\left(\hat{a}^{\dagger}_{i,\sigma}\hat{a}_{j,\sigma}+h.c.\right)-\frac{J_H}{2}\sum_{i,\alpha,\beta}\hat{a}^{\dagger}_{i,\alpha}\vec{\sigma}_{\alpha,\beta}\hat{a}_{i,\beta}\cdot\vec{S}_i \\ &\quad + J_{AF}\sum_{\langle i,j\rangle}\vec{S}_i\cdot\vec{S}_j \qquad (2)\end{aligned}$$

- For our problem, we will set $J_{AF}=0$.
- $\left|\vec{S}_i\right|=1 \implies \vec{S}_i=[\sin(\theta_i)\cos(\phi_i),\sin(\theta_i)\sin(\phi_i),\cos(\theta_i)]$

Writing the Hamiltonian matrix

- The Hamiltonian matrix can now be evaluated in the single particle basis, which gives the following non-zero elements of the tight-binding Hamiltonian as well as the Hund-interaction Hamiltonian.
- For the Hund interaction Hamiltonian, we get the following non-zero terms:

$$H_{i,i} = \frac{J_H}{2}\cos(\theta_i) \tag{3a}$$

$$H_{i+L_xL_y,i+L_xL_y} = -\frac{J_H}{2}\cos(\theta_i) \tag{3b}$$

$$H_{i,i+L_xL_y} = \frac{J_H}{2}\sin(\theta_i)\exp(-\mathrm{i}\phi) \tag{3c}$$

- $H = H_{TB} + H_{Hund}$
- The eigenvalues therefore only depend on the set of $\{\theta_i, \phi_i\}$ at a given temperature and filling.

Finding the ground state via Metropolis algorithm

- For sake of simplicity, we fix the classical spins on plane, implying all $\phi_i = 0$.
- The algorithm is now as follows:
  1. Start with a random set of θ_i
  2. Start at site one, and calculate the energy of the system.
  3. Change the value of θ_i at that site, and diagonalize the Hamiltonian again to recalculate the energy of that configuration.
  4. Calculate the probability of transition from the old state to the new one.
  5. Roll a random number to probabilistically accept or reject this transition.
  6. Move on to subsequent sites till last site.
  7. Repeat entire process several times till energy values have settled.

Calculation of probability

- We define a function

$$\begin{aligned} P &= \mathrm{tr}(Z) \\ &= \prod_{\lambda} \left[1 + \exp(-\beta\left(\epsilon_\lambda - \mu\right))\right] \end{aligned} \tag{4}$$

- We calculate P' after perturbing the angle at a given site. This changes P as changing the angle changes the Hamiltonian and hence, the spectrum.
- Probability of this change being accepted is $\frac{P}{P'}$.

Results

A phase diagram is taken from [2]:

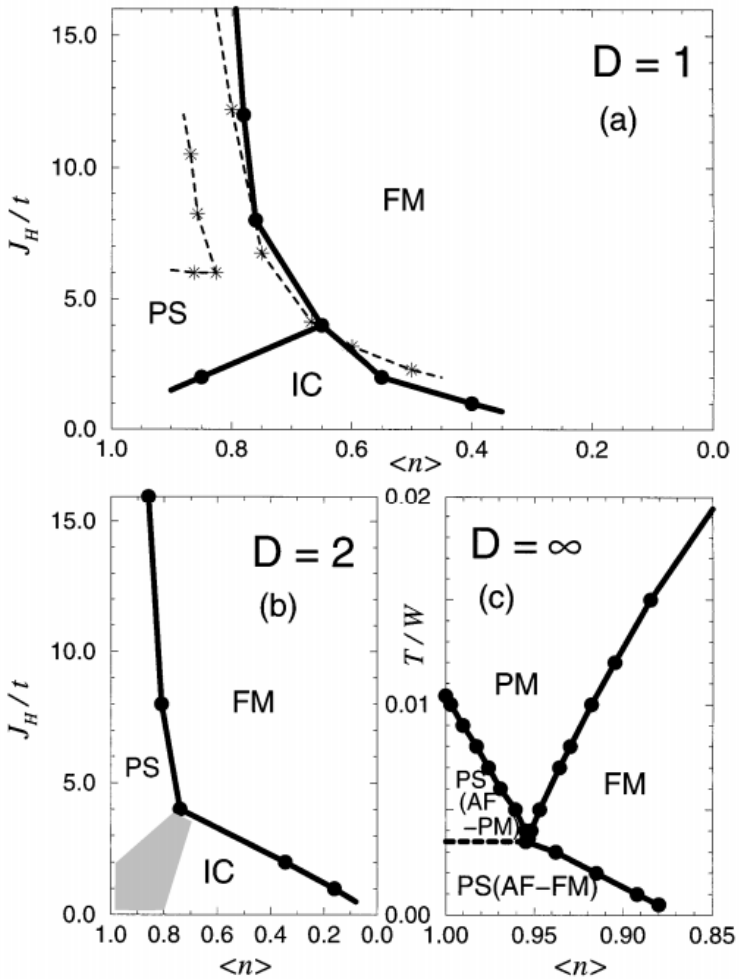

Figure: Phase diagram between J_H and μ

Results

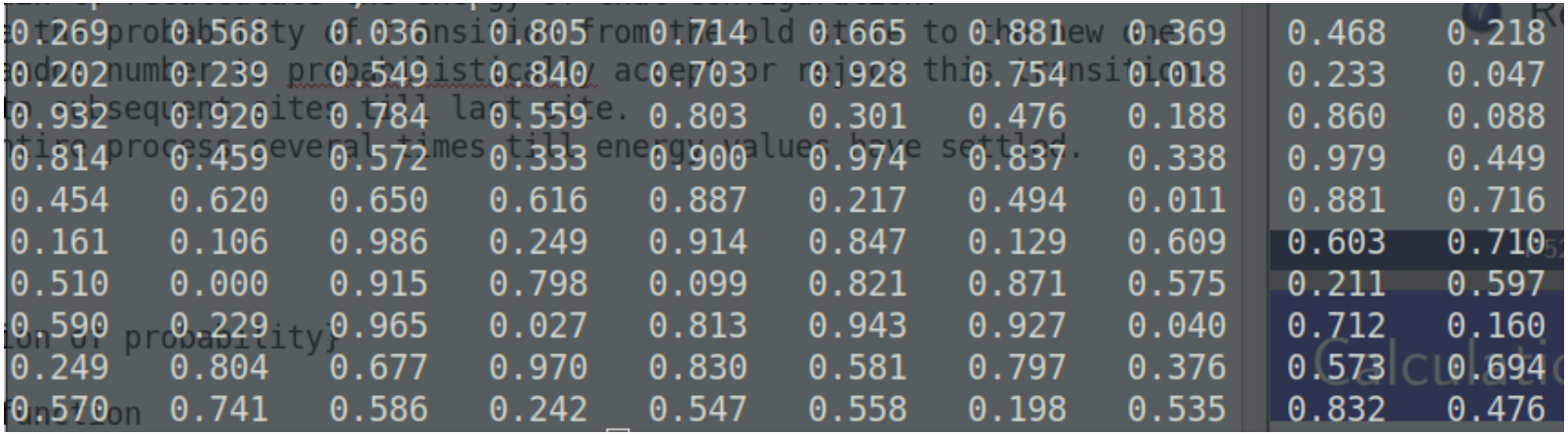

Figure: Result from my simulation, at half-filling, very low temperature, at $J_H = 1.0$.

References

Dagotto, E.
Nanoscale phase separation and colossal magnetoresistance: the physics of manganites and related compounds.
Springer, 2011.

Yunoki, S., Hu, J., Malvezzi, A. L., Moreo, A., Furukawa, N., and Dagotto, E.
Phase separation in electronic models for manganites.
Phys. Rev. Lett. 80 (Jan 1998), 845–848.