Destruction of antiferromagnetic properties through site dilution of the two-dimensional Hubbard model

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The persistence of long-range magnetic order in the two-dimensional diluted Hubbard model is explored using Deterministic Quantum Monte Carlo simulations. For this initial investigation, lattice sizes up to 16×16, inverse temperatures up to $\beta = 16$, and dilutions up to $f = 0.35$ were studied. Only lattices at half-filling were considered. In searching for a region of dilution where antiferromagnetism is destroyed, yet is still below the percolation threshold ($f \approx 0.4$), candidates for transitions were found for $U = 3$ and $U = 4$ between $f = 0.2$ and $f = 0.3$. There appears to be a possible insulating region for $U = 3$, but more thorough investigations are needed to be conclusive.

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I. INTRODUCTION

The Hubbard model is used to investigate how the interaction between electrons in a lattice produces insulating, magnetic, and sometimes superconducting effects in condensed matter. Information derived from this theoretical model is most often applied to materials such as transition metal oxides and high temperature superconductors. Though it is a relatively simplistic model, it still displays known interesting effects, such as the Mott insulating gap that can only be explained by including electron-electron interactions.

Our investigation is concerned with diluting a square lattice of antiferromagnetic material, for which the spins tend to line up such that they alternate up and down. Dilution of a lattice involves randomly removing a fraction of sites, meaning electrons sit on these sites with zero (or nearly zero) probability. Once these sites are removed from the lattice, we run a simulation to observe the persistence of long-range magnetic order.

In previous studies, our group diluted the lattice by adding an (essentially) infinite potential to the removed sites. This makes it energetically costly for an electron to sit on one of these sites, and it would therefore have a high probability of tunneling to another site.

For this project, we are using another more efficient method—cutting out sites from the lattice completely. Instead of letting the removed sites still exist and accept electrons, all tunneling paths are removed such that removed sites are completely isolated and are not considered in computations, resulting in quicker runtimes.

II. HUBBARD MODEL

The Hubbard model starts with a lattice of atoms, or sites, for the electrons to occupy. To simplify things, the atoms are considered to have only one energy level. Thus, from the Pauli exclusion principle, there can be a maximum of two electrons per site (i.e. $\uparrow$ and $\downarrow$).

The Hamiltonian of the standard two-dimensional Hubbard model includes a kinetic term and a single potential term:

$$H = -t \sum_{\langle j,l\rangle\sigma} c^{\dagger}_{j\sigma} c_{l\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

The potential term is derived from the screened Coulomb interaction between electrons. Since this interaction decays exponentially with distance, the dominant Coulomb interaction will be between two electrons sitting on the same site. For the Hubbard model, all other Coulomb interactions are neglected. The kinetic term denotes electrons tunneling, or hopping, from one site to a neighboring site. A neighboring is any site that is exactly one unit of distance away; therefore, a site in a square lattice then has four nearest neighbors. One can also include a chemical potential term, which controls the filling of the lattice:

$$H = -t \sum_{\langle j,l\rangle\sigma} c^{\dagger}_{j\sigma} c_{l\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} + \mu \sum_{j} n_{j\uparrow} - n_{j\downarrow}$$

This can then be adjusted such that when $\mu = 0$, the lattice is always at half-filling, regardless of all other parameters:

$$H = -t \sum_{\langle j,l\rangle\sigma} c^\dagger_{j\sigma} c_{l\sigma} + U \sum_j (n_{j\uparrow} - \tfrac{1}{2})(n_{j\downarrow} - \tfrac{1}{2}) + \mu \sum_j n_{j\uparrow} - n_{j\downarrow}$$

The preceding is the form of the Hubbard Hamiltonian used in our simulations, as we only considered lattices at half-filling.

III. DILUTION

Diluting a lattice removes a fraction of the original number of sites. The dilution parameter f is simply the percentage of sites removed, such that a diluted $L \times L$ lattice will have $N = L^2(1 - f)$ sites. Consider a lattice of antiferromagnetic matter—the spins tend to alternate across the lattice in order to minimize energy. The interactions between sites grow weaker as one continually dilutes the lattice. At some fraction of dilution, the antiferromagnetic properties of the lattice will be destroyed and the spins will align randomly.

One reason for this destruction of antiferromagnetism is that the lattice has reached/surpassed the percolation threshold [1]. At the percolation threshold, the lattice has been so diluted that there is no longer one large clump of sites, and the remaining smaller clumps are all isolated from each other. Clearly, if the lattice is comprised only of small isolated clumps, there can be no long-range magnetic order. The percolation threshold has been studied extensively in percolation theory, and it is established to be about 40% dilution for a square lattice [2]. This project is probing the existence of a range of dilution below the percolation threshold where antiferromagnetism is still destroyed.

For our results to be physically meaningful, we must extrapolate to the thermodynamic limit—the limit as the number of sites N increases towards infinity (or more practically speaking, N_A). However, computer performance severely limits the possible sizes of simulated lattices. The largest lattice simulated in this portion of the project was 16×16; clearly, $N = 256 \ll N_A$. In order to get an idea of whether the long-range magnetic order will still exist at these much larger sizes, we need to take the data we can get within a reasonable timeframe and extrapolate the trend to the thermodynamic limit. If the extrapolated curve does not show long-range magnetic order at this limit, then we can argue that the antiferromagnetic order is destroyed at the current dilution.

IV. SIMULATION

For the purposes of this paper, I will be very brief regarding the code used for this project, as I did not have a chance to learn about it in greater detail. As previously mentioned, the code was originally written for the onsite infinite potential dilution method. After deciding to try the new dilution technique, the front end of the code was readjusted so that I could run the simulations.

The code uses Deterministic Quantum Monte Carlo and, in addition to the two spatial dimensions of the lattice, includes an imaginary time dimension. Over an imaginary time iteration, the electrons are given random suggestions to realign their spins, which are accepted with some probability controlled by the DQMC algorithm. In order to help counteract finite size and edge effects, periodic boundary conditions are employed.

From the massive amount of data output, only a few values related to magnetization—the magnetic structure factor and the spin-spin correlation—were analyzed. The spin-spin correlation between the two farthest points on the square lattice (i.e., a corner and the center due to periodic boundary conditions)

$$C_{\frac{L}{2},\frac{L}{2}} = \langle \sigma^z_0 \sigma^z_{x=\frac{L}{2},y=\frac{L}{2}} \rangle$$

gives the square of the magnetization. The magnetic structure factor

$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_j)} \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle$$

is the fourier transform of the correlation function and has a peak at $\mathbf{q} = (\pi, \pi)$. $S(\pi, \pi)$ divided by the lattice size is roughly the magnetization squared as well, differing only by a negligible additive constant. [3]

Using the $S(\pi, \pi)$ and $C(\frac{L}{2}, \frac{L}{2})$ values taken from the simulation of our relatively small lattices, we can extrapolate the magnetization at the thermodynamic limit. As

stated earlier, if the magnetization is no longer present at the thermodynamic limit, we can argue antiferromagnetism has been destroyed at that dilution value.

V. DATA AND ANALYSIS

Running the simulation at colder temperatures increases the number of imaginary time iterations (by a factor of eight with our setup), and thus significantly extends the runtime of the simulation. Therefore, we needed to first plot $S(\pi,\pi)$ against inverse temperature β to check the lattices were at cold enough temperatures that $S(\pi,\pi)$ had leveled off, while not spending unnecessary time at even colder temperatures. For example, in our initial studies with $U=4$, there was a significant enough increase in $S(\pi,\pi)$ for the larger lattice sizes from $\beta=8$ to $\beta=12$ that we needed to look at a colder temperature, $\beta=16$ (See Fig. 1).

After extracting the saturated values of $S(\pi,\pi)$ and $C(\frac{L}{2},\frac{L}{2})$, $S(\pi,\pi)$ per site and $C(\frac{L}{2},\frac{L}{2})$ were plotted against $\frac{1}{\sqrt{N}}$, or $\frac{1}{L}$. From this plot, the trends can be extrapolated to intercepts at $\frac{1}{L}=0$. A positive intercept indicates there is still antiferromagnetic order, otherwise the long-range magnetic order has been destroyed at that dilution.

A first look at data collected on $U=4$ indicated the possible destruction of antiferromagnetism below $f=0.3$, but there were concerns that S/N was not linear in the lattice size range we were considering. If this were correct, all the intercepts would be shifted up by some factor. Comparing initial results for $U=3,4,5$, we saw that $U=3$ showed more promise of having an insulating range before the percolation limit, as the intercepts were lower than those of either $U=4$ and $U=5$ (See Fig. 2). Thereafter, the bulk of my work was focused on refining my results for $U=3$, which will be the focus for the remainder of this paper.

To corroborate our S/N intercept values, the linear

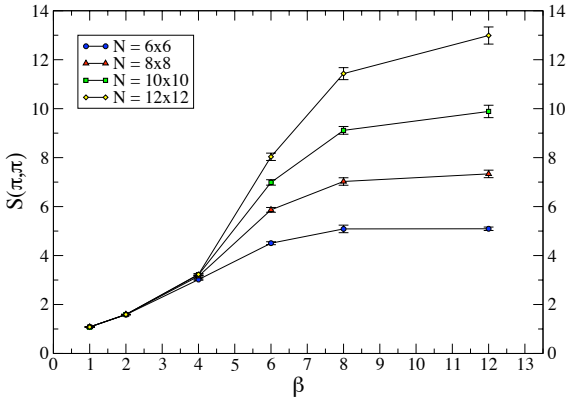
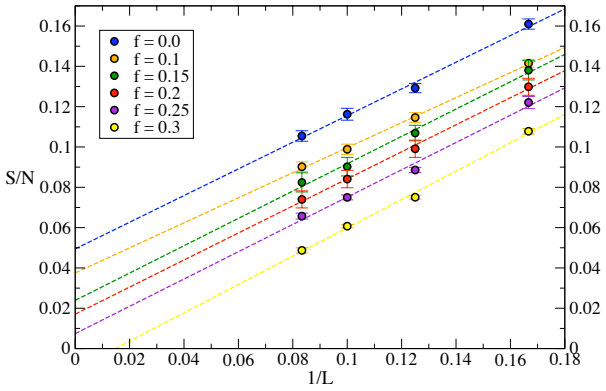
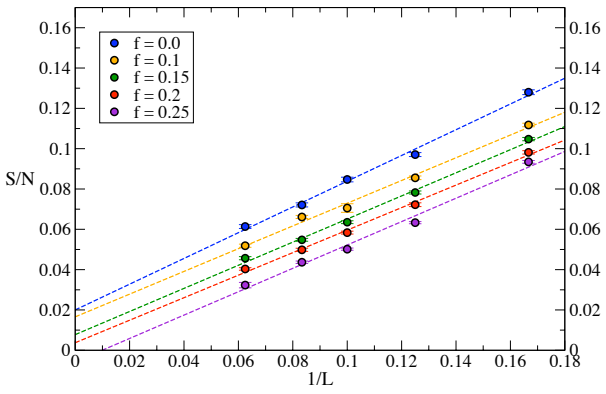


FIG. 1: $U=4, f=0.1$. Initial runs indicated that $\beta=12$ was not cold enough for $S(\pi,\pi)$ to saturate at larger N. After determining $\beta=20$ required too much time, and did not indicate a significant enough change in $S(\pi,\pi)$, $\beta=16$ was deemed sufficient for this initial investigation.



(a)$U=4$, f_{crit} possibly between $f=0.25$ and $f=0.3$.



(b)$U=3$, f_{crit} possibly between $f=0.2$ and $f=0.25$.

FIG. 2: Linear extrapolations indicate possible destruction of long-range magnetic order. Similar plots were made for $C(\frac{L}{2},\frac{L}{2})$.

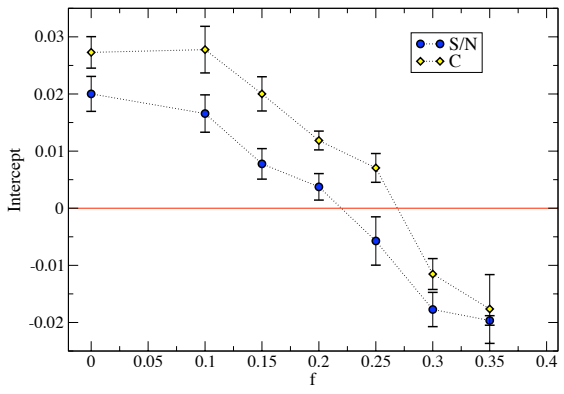


FIG. 3: $U = 3$. Intercepts for S/N and C.

fits for S/N were compared to linear fits of the spin-spin correlation $C(\frac{L}{2}, \frac{L}{2})$. Both should give the same value at the thermodynamic limit, therefore they should have the same extrapolated intercepts. However, there is a consistent disagreement in the intercepts (Fig. 3).

Our current conjecture is that the curves for S/N are in fact nonlinear in this range of lattice sizes, and that the extrapolated curves could actually approach intercepts that agree more with the C linear fits. In Fig. 4, one can see this situation is quite possible.

VI. RESULTS AND FUTURE WORK

So far, we have not been able to confirm nor rule out the existence of a range of dilution below percolation where antiferromagnetism is destroyed. The next step will probably be do the same batch of parameters with more iterations, and see if this smooths out the S/N and C curves significantly. Since the spin-spin correlation is more linear in this range, we could use C as a gauge for long-range magnetic order if it is confirmed that the S/N and C curves are in fact extrapolating to the same intercept.

Going to larger lattice sizes will help pinpoint those extrapolated intercepts, but also requires a great amount of processor time, as larger lattice sizes require colder temperatures as well. As such, we want to be sure we have accurate data at the smaller lattice sizes before moving on to more computational expensive runs.

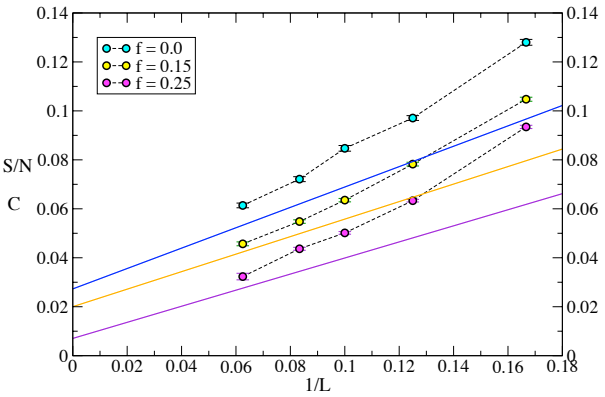


FIG. 4: $U = 3$. Data for S/N and linear fit for C. It is possible S/N is nonlinear in this range and actually approaches the same intercept.

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[1] A. W. Sandvik, Phys. Rev. B **66**, 024418 (2002).

[2] D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor & Francis, 1992), 2nd ed.

[3] J. E. Hirsch and S. Tang, Phys. Rev. Lett. **62**, 591 (1989).