Destruction of Superconductivity by Disorder: A Study of Spin-Dependent Hopping Disorder in the Attractive Hubbard Model

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The Hubbard Model in two dimensions was studied on a square lattice using Bogoliubov de-Gennes mean field theory. Spin-dependent disorder was applied to the hopping term in the Hubbard Hamiltonian. The order parameter was found to drop sharply to zero with increasing disorder, signaling the destruction of superconductivity.

I. Introduction

Disordered superconductors are of great of theoretical and experimental interest. Anderson's Theorem (1959) states that thermodynamic properties of disordered superconductors are unaffected by the degree of disorder. However, a bound of "weak disorder" was later put on this theorem through theoretical and experimental investigations that suggested that disorder does affect superconductivity. Previously, spin-independent disorder has been studied in the Hubbard model. Due to the emergence of optical lattice technology, the case of spin-dependent disorder has become an interesting and relevant problem.

II. Model and Simulation Measurements

Superconductivity arises when pairs of fermions attract to form entities called "Cooper pairs." A major question involves researching the exact cause of this attractive interaction between fermions for various types of superconductors. This paper does not focus on this question but rather, assumes the interaction to be attractive and studies the results of such a model. In the Hubbard hamiltonian, equation 1, each electron hopping between near-neighbor sites contributes an energy of *t*. Each doubly occupied site contributes and interaction energy of *U*. Additionally, U is negative because the attractive interaction contributes a negative (lowering) energy to the system. Finally, the third term is the chemical potential and this controls the average filling $(n_{1,average})$ of the sites.

$$H = -t \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) + U \sum_{j} n_{j\uparrow}n_{j\downarrow} - \mu \sum_{j} (n_{j\uparrow} + n_{j\downarrow})$$
(1)

The Hubbard Hamiltonian is quartic in the creation and annihilation operators. As a result, the Hamiltonian can not, in general, be solved analytically. Therefore, Bogoliubiv de-Gennes mean field theory (BdG MFT) was used to solve the Hamiltonian. BdG MFT is an approximation

technique where the troublesome quartic term is replaced by a sum of quadratic terms. The BdG Hubbard Hamiltonian with spin-dependent hopping disorder, $V_{ij,\sigma}$, is shown in equation 2.

$$H = \sum_{\langle i,j \rangle,\sigma} (V_{ij,\sigma} - t)(c_{i\sigma}^{\dagger}c_{j\sigma} + h.c.) - \sum_{i\sigma} \tilde{\mu}_{i\sigma}n_{i\sigma} + \sum_{i} [\Delta(\mathbf{r}_{i})c_{i\uparrow}^{\dagger}c_{i\downarrow}^{\dagger} + \Delta^{*}(\mathbf{r}_{i})c_{i\downarrow}c_{i\uparrow}]$$
(2)

where:

$$\tilde{\mu}_{i\sigma} = \mu_{\sigma} + |U| < n_{i-\sigma} > \tag{3}$$

$$\Delta(\mathbf{r}_i) = -|U| < c_{i,\downarrow}c_{i,\uparrow} > \tag{4}$$

$$\Delta^{*}(\mathbf{r}_{i}) = -|U| < c^{\dagger}_{i,\uparrow}c^{\dagger}_{i,\downarrow} > \qquad (5)$$

The Hamiltonian was solved for its eigenvalues (E_n) and eigenvectors ($x_{i,n}$) using a LAPACK matrix diagonalizer. These quantities were then used in a set of self consistency equations derived from BdG mean field theory. In these equations, $\beta = 1/k_BT$, where T is the temperature and k_B is the Boltzmann constant. One way the following self-consistency equations can be derived is by minimizing the free energy of the Hamiltonian. Additionally, note that a particle hole transformation was performed on the spin-up fermions, producing a negative sign in front of the energies E_n in the Fermi-Dirac function in the self consistency equations 6 and 8.

$$\langle n_{i\uparrow} \rangle = \langle c_{i\uparrow} c_{i\uparrow}^{\dagger} \rangle = \sum_{n} |x_{i,n}|^2 \frac{1}{e^{-\beta E_n} + 1}$$

$$\tag{6}$$

$$\langle n_{i\downarrow} \rangle = \langle c_{i\downarrow}^{\dagger} c_{i\downarrow} \rangle = \sum_{n} |x_{N+i,n}|^2 \frac{1}{e^{+\beta E_n} + 1}$$

$$\tag{7}$$

$$\Delta(\mathbf{r}_i) = -|U| < c_{i\downarrow}c_{i\uparrow} > = -|U| < c_{i\downarrow}c_{i\uparrow}^{\dagger} > = -|U| \sum_n x_{N+i,n} x_{i,n}^* \frac{1}{e^{-\beta E_n} + 1}$$
(8)

These new values for $\langle n_i \uparrow \rangle$, $\langle n_i \downarrow \rangle$, and $\Delta(r_i)$ then replace the original values in the Hamiltonian and the Hamiltonian is again solved for its eigenvalues and eigenvectors. This iteration continues until the change in $\langle n_i \uparrow \rangle$, $\langle n_i \downarrow \rangle$, and $\Delta(r_i)$ for every site is smaller than a specified magnitude which was chosen to be 10⁻⁵. Additionally, the average filling of the sites is adjusted after each iteration by way of changing the chemical potentials. A target average filling is specified in the beginning of the code and equations 9 and 10 are used to calculate the new chemical potentials from the old chemical potentials. The average filling is calculated after each iteration and alpha is a tuning constant which was chosen to be 0.5 in our calculation.

$$\mu_{\uparrow} = \mu_{\uparrow} + \alpha (n_{\uparrow,target} - n_{\uparrow,average}) \tag{9}$$

$$\mu_{\downarrow} = \mu_{\downarrow} + \alpha (n_{\downarrow,target} - n_{\downarrow,average}) \tag{10}$$

Once the self-consistency iteration is carried out to completion, two properties of the system are measured. First, the order parameter of superconductivity, which is the average delta over all sites, was calculated. Secondly, the energy gap, which is the smallest positive eigenvalue of the final Hamiltonian, was measured.

III. Results and Analysis

The first results were used to test the accuracy of the code. According to Bardeen, Cooper, and Schrieffer's theory of superconductivity there is a universal ratio that is valid for all superconductors, stated in equation 11.

$$\frac{\Delta(0)}{k_B T_c} = 1.76\tag{11}$$

The numerator of this ratio is the order parameter at temperature 0 and the denominator is the Boltzmann constant times the critical temperature of superconductivity. In order to calculate this ratio, the order parameter was measured as a function of temperature. Additionally, U= -4 and the target average filling was $n_{\uparrow,average target} = 0.4$ and $n_{\downarrow,average target} = 0.4$. Graph 1 was produced.



Graph 1:

The results of this calculation were $\Delta(0) \approx 1.332$ and $T_c \approx .72$. Additionally, the Boltzmann constant was set to be 1 in the calculation. Therefore, $\Delta(0)/K_b T_c = 1.85$. The discrepancy from the exact ratio is attributable to a finite lattice size calculation. In this case, a 15x15 site lattice was used.

Finally, the case of spin-dependent hopping was studied. The strength of disorder, $V_{ij,\sigma}$, in the Hamiltonian (2) was varied from 0.0 to 0.6 with t =1. In other words, random values between t +V and t-V were generated for the hopping energy between each pair of sites and for each spin. Each of these calculations was done at T = 0.01 and the target average filling was $n_{\uparrow,average target} = 0.4$ and $n_{\downarrow,average target} = 0.4$. For each calculation the order parameter and the energy gap were measured and the results are shown in graph 2.



Graph 2:

As evidenced by the graph, the order parameter drops to zero as disorder increases. Thus, superconductivity is shown to be destroyed by a certain strength of disordered hopping. Additionally, the energy gap is shown to drop to zero linearly and reach zero at a weaker disorder than the order parameter. This implies the possible existence of a gapless superconducting state.

The significance of these results becomes apparent when compared to the results for the spinindependent disorder case studied by Amit Ghosal, Mohit Randeria, and Nandini Trivedi in 2001. The spin-independent version of graph 2 is shown in graph 3.

Graph 3:



As evidenced by graph 3, the order parameter and energy gap do not exhibit the same sharp transition to zero as was found in the spin-dependent disorder case.

IV. Conclusions

It has been shown that superconductivity can be destroyed through the presence of spindependent hopping disorder. Further analysis will involve using a larger, 24x24 site lattice and performing disorder averaging over multiple disorder realizations. Also, additional thermodynamic properties will be measured including the chemical potentials and, for one disorder realization, the pairing amplitude $\Delta(r_i)$, fillings, and disordered hoppings, all as a function of site.

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