The role of disorder symmetry in a dirty superconductor: a Bogoliubov-deGennes (BdG) study

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We study the effect of disorder symmetry in a disordered s-wave superconductor. We begin with an attractive Hubbard model on a two-dimensional square lattice in the presence of diagonal- and off-diagonal disorder. The model is studied numerically using Bogoliubov-deGennes approach, which proceeds via the decoupling of attractive Hubbard term in the pairing channel. We find that the off-diagonal disorder is much more efficient in destroying superconducting order. A detailed analysis brings out very distinct qualitative pictures in the two cases: diagonal disorder leads to formation of small scale isolated superconducting islands separated by large region of normal metal, whereas off-diagonal disorder leads to a connected network of superconducting region. Naively, it seems that the connected network of superconducting regions should have a large average value for superconducting order parameter, but this does not hold true for large disorder, as we demonstrate explicitly. Our qualitative picture is supported by real-space data on local order parameters.

**Introduction:** The behavior of a fermion system in the presence of disorder and strong inter-particle interactions has been a challenging question in condensed matter physics for many decades.\textsuperscript{2,4,5} Anderson's seminal discovery that the wave nature of electrons in a quantum mechanical context can cause the electrons to completely localize in a disordered system gave rise to the field of Anderson localization.\textsuperscript{2} On the other hand, in the clean system, the Coulomb repulsion between the electrons themselves can also cause the electrons to localize, a phenomenon known as Mott localization.\textsuperscript{2} The most famous example of such materials being the undoped parent compounds of the high-T\textsubscript{C} Cuprate superconductors.\textsuperscript{2}

A well-studied problem in condensed matter physics has been the properties of a dirty superconductor, with early theories by Anderson\textsuperscript{6} and Abrikosov and Gorkov\textsuperscript{7} in the regime when the disorder was weak. With the advent of advanced experimental techniques of growing highly inhomogeneous films, research on the properties of a dirty superconductor in the strong disorder regime has become possible.\textsuperscript{10,11} This is also the regime where electron interactions start to play an important role, which then becomes a very challenging theoretical problem.\textsuperscript{2} Also, controlled studies of the related quantum phase transition between the superconductor and the Anderson Insulator (SIT) have been widely carried out. In the SIT, the early theoretical prediction of a universal conductivity (in units of $e^2/h$) demarcating the critical point between the two phases generated a plethora of theoretical and experimental work in this field.\textsuperscript{13–16} Recently, with the observation of Anderson localization in disordered optical lattices and the possibility of tuning the sign of the interaction between the atomic species, a new avenue has opened up to investigate the interplay of disorder and interaction among both fermionic and bosonic atoms.\textsuperscript{17–20}

In the presence of attractive interactions between fermions, disordered systems can become superconducting (for charged electrons) or superfluid (for neutral atoms). Below a critical disorder strength in $d = 2$, the two-particle states may sustain dissipationless flow even though all single-particle states are localized due to Anderson localization. The combination of attractive interactions and disorder can lead to a rich variety of phases and new physics, including the BCS-BEC crossover, various kinds of glassy phases and superfluids (superconductors).

A related very important aspect of physical systems with disorder is the symmetry of the Hamiltonian governing them. A complete classification of the symmetries of the single-particle Hamiltonians governing a disordered system was recently achieved.\textsuperscript{21–23} Depending on the presence (or absence) of time-reversal symmetry ($T$), spin-rotation ($SU(2)$) symmetry and particle-hole symmetry ($\Xi$) in the Hamiltonian, the physics of the disordered system can be markedly different, particularly with respect to Anderson localization. For example, it is now known that weak localization does not occur in the chiral symmetry class in the conventional sense, but follows a topological route which then gives way to strong localization for stronger disorder.\textsuperscript{24}

In traditional solid state systems, intrinsic disorder typically originates from random locations of dopant ions. This invariably affects both the on-site potential and the hopping parameters in the corresponding model Hamiltonian. Depending on the details of the structure and ions involved, this may affect one or the other more strongly and therefore can be modelled via either a randomness in on-site potentials (diagonal disorder) or hopping strengths (off-diagonal disorder). In addition, disordered optical lattices provide another promising direction to investigate the influence of symmetries on the localization problem.

The SIT has been investigated in considerable detail
in the literature with orthogonal disorder i.e., on-site or diagonal disorder with and without the spin-rotation (SU(2)) symmetry. In this paper, we investigate the influence of off-diagonal disorder in the physics of a dirty superconductor, which belongs, in the classification of Altland and Zirnbauer, in the chiral-BdG symmetry class, and compare it to similar physics in the usually studied BdG-orthogonal symmetry class. Even though we do not explicitly investigate the physics of the critical point itself, the effect of imminent localization is always present in the physics of a dirty superconductor, and the nature and the properties of the inhomogeneities in the superconducting state itself is a very important indicator of the subsequent physics of localization. Elucidating how the superconducting state responds to the nature of the disorder potential will be the main goal of this paper.

Model and Method: The starting point of our investigation is the attractive Anderson-Hubbard model on a square lattice, given by the Hamiltonian

\[ H = H_{\text{sp}} + H_{\text{int}}, \]

where \( H_{\text{sp}} \) is the single-particle part and \( H_{\text{int}} \) is the interaction part. \( H_{\text{sp}} \) is given by

\[ H_{\text{sp}} = - \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} - \mu \sum_{i \sigma} c_{i \sigma}^\dagger c_{i \sigma} + \sum_{i \sigma} \varepsilon_i c_{i \sigma}^\dagger c_{i \sigma}. \]

Here \( c_{i \sigma} (c_{i \sigma}^\dagger) \) annihilates (creates) an electron at site \( \tilde{R}_i \) with spin-projection \( \sigma \), \( \langle ij \rangle \) implies that \( \tilde{R}_i \) and \( \tilde{R}_j \) are nearest neighbors, \( \mu \) is the chemical potential and \( t_{ij} \) is the hopping matrix element between sites \( \tilde{R}_i \) and \( \tilde{R}_j \). We write \( t_{ij} (= t_{ji}) \) as

\[ t_{ij} = t + \delta_{ij}, \]

where \( \delta_{ij} \) is drawn randomly from a box probability distribution \( P(\delta_{ij}) = \frac{1}{V} \Theta (\frac{V}{2} - |\delta_{ij}|), \Theta (x) \) being the Heaviside \( \Theta \)-function. Similarly, the on-site diagonal disorder term is denoted by the random site-energy \( \varepsilon_i \), which is drawn from a box-distribution given by \( P(\varepsilon_i) = \frac{1}{\varepsilon} \Theta (\frac{\varepsilon}{2} - |\varepsilon_i|) \). The attractive Hubbard interaction term \( H_{\text{int}} \) is given by

\[ H_{\text{int}} = - |U| \sum_i n_{i \uparrow} n_{i \downarrow}, \]

where \( n_{i \sigma} = c_{i \sigma}^\dagger c_{i \sigma} \) is the number operator at site \( \tilde{R}_i \) and spin-projection \( \sigma \). We set \( t = 1 \) as the basic scale for energy, therefore all energy parameters are in units of \( t \). This leaves four independent energy-scales in the model: the interaction strength \( |U| \), the off-diagonal disorder bandwidth \( V_L \), the diagonal disorder bandwidth \( V \) and the temperature \( T \). If \( V_L = 0 \), the model reduces to the class of disorder Hamiltonians with orthogonal symmetry. If \( V = 0 \), it reduces to the class of disorder Hamiltonians with chiral symmetry.

At half-filling, the clean (i.e., no disorder) attractive Hubbard model (in \( d = 2 \)) has a phase diagram in which the charge density wave (CDW) state and the superconducting state (SC) are exactly degenerate in energy and co-exist at \( T = 0 \). As one dopes the system away from half-filling, the CDW state gradually disappears, and the system makes a Berezinskii-Kosterlitz-Thouless (BKT) transition to a conventional s-wave SC ground state.

A discussion of the effect of non-magnetic disorder on superconductivity (in particular, \( T_C \)) begins with Andeison’s theorem, which states that, at least for weak impurity scattering, \( T_C \) is not affected by disorder. In the context of mean-field BdG formalism with diagonal disorder, Ghosal et al. found that it is impossible to destroy superconductivity through amplitude fluctuations by increasing disorder (an extreme case of Anderson’s theorem), and in fact, there is a disorder strength for which the spectral gap (the superconducting gap) shows a non-zero minimum, beyond which the gap actually increases with disorder strength, even though the spatially averaged SC order parameter monotonically vanishes. Conventional wisdom suggests that the impurity states will gradually fill in the superconducting gap and destroy SC. However, as we shall see, this intuitive picture is not always true, and in fact, depends on the type of disorder.

We revisit this scenario where the disorder resides on the bonds (off-diagonal/bond/hopping disorder) rather than on the sites (diagonal/site/potential disorder). The BdG equations are derived as usual, by decoupling the attractive Hubbard interaction in the pairing channel. This leads to the effective BdG Hamiltonian:

\[ H_{\text{eff}} = - \sum_{\langle ij \rangle, \sigma} t_{ij} c_{i \sigma}^\dagger c_{j \sigma} - \sum_{i \sigma} \tilde{\mu}_{i \sigma} n_{i \sigma} + \sum_{i \sigma} \varepsilon_i n_{i \sigma} + \sum_i \left[ \Delta_i c_{i \uparrow}^\dagger c_{i \downarrow} + \Delta_i^* c_{i \downarrow} c_{i \uparrow} \right], \]

where \( \tilde{\mu}_{i \sigma} = \mu + |U| (n_{i \uparrow - n_{i \downarrow}}) \). \( H_{\text{eff}} \) is diagonalized via the Bogoliubov transformation:

\[ c_{i \uparrow} = \sum_n \left[ \gamma_{n \uparrow} u_{in} - \gamma_{n \uparrow}^* v_{in} \right], \]

\[ c_{i \downarrow} = \sum_n \left[ \gamma_{n \downarrow} u_{in} + \gamma_{n \downarrow}^* v_{in} \right], \]

where \( \gamma_{n \sigma} (\gamma_{n \sigma}^\dagger) \) are annihilation(creation) operators for the Bogoliubov quasiparticles in the single-particle state \( (n, \sigma) \) and satisfy canonical anticommutation relations for fermions. The local superconducting order parameter \( \Delta_i \) and particle densities are obtained self-consistently via

\[ \Delta_i = - |U| \langle c_{i \uparrow} c_{i \downarrow} \rangle = - |U| \sum_n f \left( E_n \right) u_{in} v_{in}^*, \]

\[ \langle n_{i \uparrow} \rangle = \sum_n f \left( E_n \right) |u_{in}|^2, \]

\[ \langle n_{i \downarrow} \rangle = \sum_n f \left( -E_n \right) |v_{in}|^2, \]

where \( E_n \) is measured from the global chemical potential, \( \mu \) and \( f \left( E_n \right) \) is the corresponding Fermi function.
The original Hamiltonian in Eqn. 1 and the effective BdG Hamiltonian in Eqn. 5 are manifestly invariant under $T$ and $SU(2)$. If $V = 0$ (but $V_i \neq 0$), the energy eigenvalues also appear in ± pairs about the chemical potential, thus exhibiting chiral symmetry. In the superconducting state, the disordered BdG Hamiltonian thus belongs to the BdG chiral class.

All calculations are performed in the grand canonical ensemble scheme by keeping the chemical potential $\mu$ constant and allowing the average electronic density $n$ to vary freely. This approach is conceptually accurate since no adjustments are required in order to achieve a target average density at the end of the calculation. The disadvantage is that we need to perform calculations for a range of $\mu$ values in order to achieve the desired $n$. However, this approach naturally provides us results for density dependence as well. The consistency loop is started by picking a random set for the local order parameters $\Delta_i$. Subsequently, numerical diagonalization is carried out and the eigenvectors and eigenvalues are used to compute the new set of $\Delta_i$, and so on until the order parameters and local densities converge to a desired accuracy. In this work we use a convergence accuracy of $10^{-4}$ for both the $\Delta_i$ and the charge density, i.e., we stop the self-consistency loop when the value in $(k+1)^{th}$ step differs from the one in $k^{th}$ step by less than $10^{-4}$.

**Results:**

We begin our discussion by showing the behavior of the spatially averaged superconducting order parameter $\Delta_{op}$ with disorder strength, $V$, in Fig. 1(a) and (b). Here, $\Delta_{op}$ is defined as

$$\Delta_{op} = \frac{1}{N_x} \sum_i \Delta_i, \quad (8)$$

where $N_x$ denotes the number of lattice sites and the overbar denotes an average over different realizations of quenched disorder.

In Fig. 1 panel (a) shows the behavior of a system with diagonal (site-) disorder and panel (b) shows the behaviour of a system with off-diagonal (bond-) disorder. In both cases, we present results for systems where the linear lattice size takes values ranging from $L = 24$ to $L = 64$. It is clear from Fig. 1 that $\Delta_{op}$ has very little system-size dependence and has, in fact, converged very well already for the system sizes $L = 24$ and $L = 32$. We have ascertained that, in this and all our subsequent results, all quantities have converged by increasing the system size.

In Fig. 1(a) and (b), there is already a clear qualitative difference in the behaviour of the superconducting order parameter for the two kinds of disorder as disorder strength is gradually increased. For the diagonal disorder case (Fig. 1(a)), the order parameter is seen to gradually converge to a non-zero value as disorder strength $V/t$ is increased. Indeed, even when the disorder strength is as large as the kinetic bandwidth $W_{kin} = 8t$, significant non-zero superconducting order parameter is found, when averaged over the entire system. This was understood in terms of a phase separation of the system between superconducting islands (with large values of $\Delta_i$) separated by insulating normal regions with very small $\Delta_i$.

On the other hand, the figure is very different for off-diagonal disorder. As disorder strength is increased in Fig. 1(b), the order parameter supresses rapidly. In order to clarify the difference, we plot the comparison on a logarithmic scale in an inset in Fig. 1(b). It is clear from the inset that at large disorder strengths $\Delta_{op}$ is almost an order of magnitude smaller for the bond-disorder. In other words, at the level of mean superconducting order parameter, bond-disorder destroys superconductivity very quickly.

The difference in behaviour of the dirty superconductor for the two kinds of disorder becomes even more clear if we consider how the superconducting spectral gap responds to a change in the disorder strength. In Fig. 1(c) and (d), we plot the spectral gap $E_{gap}$ defined as

$$E_{gap} = E_{exc} - E_g. \quad (9)$$

Here $E_{exc}$ is the energy of the first excited state and $E_g$ is the ground state energy. The overbar, once again, denotes averaging over various realizations of quenched disorder. Our results for the diagonal disorder (panel (c) in Fig. 1) compare very well with those presented in Ghosal et al. This makes us confident that the behaviour of the superconducting gap is a physical property of the system, not a numerical artefact. Similar to Fig. 1(a) and (b), we plot the spectral gap for increasing lattice sizes. For off-diagonal disorder, Fig. 1(d), the spectral gap converges very well for all lattice sizes. Some minor
size-dependence is seen for smaller lattices in the case of diagonal disorder, Fig. 1(c), even though the results are manifestly independent of the lattice size.

For diagonal disorder, we confirm a counter-intuitive behavior first observed by Ghosal et al.\textsuperscript{25,26}: the spectral gap initially decreases with an increase in $V$, but after a minimum around $V \sim 4t$, it monotonically increases with $V$. Ghosal et al. ascribed it to the fact that at very high diagonal disorder, the non-interacting eigenstates are essentially spatially local, and only those local eigenstates near the chemical potential participate in pairing. The gap equation in this local approximation implies that the gap depends inversely on the square of the localization length ($\zeta_{loc}$), which decreases with increasing disorder. This causes the increase in the spectral gap with increasing disorder.

However, for off-diagonal disorder, Fig. 1(d), the behavior of the spectral gap is strikingly different. With increasing $V_t$, $E_{\text{gap}}$ monotonically decreases. For the largest system sizes with converged values for $E_{\text{gap}}$, it is seen to converge to a very small value - again reaffirming the fact that off-diagonal disorder is more effective compared to diagonal disorder in destroying superconductivity.

In Fig. 2 panels (a)-(d), we introduce the dependence of the superconducting state properties, $\Delta_{\text{op}}$ and $E_{\text{gap}}$ on the average electron density, $n$. In Fig. 2(a), $\Delta_{\text{op}}$ is plotted against the electron density for $U = 2t$ and for various values of $V/t$ (full symbols with full lines) and $V_t/t$ (open symbols with dashed lines). We use the same set of values for both $V$ and $V_t$ (from $V = 0.2$ to $V = 4.0$), so that comparisons become meaningful. For $U/t = 2$, Fig. 2(a), the magnitude of $\Delta_{\text{op}}$ decreases monotonically with $V/t$. At weak disorder, $\Delta_{\text{op}}$ is weakly density-dependent for both types of disorders. As the disorder bandwidth increases, the $\Delta_{\text{op}}$ for the diagonal disorder becomes essentially independent of $n$, whereas, the $\Delta_{\text{op}}$ for off-diagonal disorder continues to have a significant density dependence. Interestingly, there seems to be a crossover density $n_{\text{cr}}$ above which bond-disorder has stronger superconductivity than site-disorder (in terms of having a larger $\Delta_{\text{op}}$). For example, at half-filling, $\Delta_{\text{op}}$ is consistently larger for $V_t$ than for the same $V$, for all disorder strengths investigated. Fig. 2(b) shows that the same conclusion is true for $U/t = 3.0$, except that $n_{\text{cr}}$ is pushed towards lower densities. However, Fig. 2(a) and (b) show that for even larger disorder strengths (for example, at $V = V_t = 6t$, $n \sim 0.88$ and $U/t = 3.0$), this trend will again be reversed and the order parameter, although small, will be larger for site-disorder than for bond-disorder.

In Fig. 2 panels (c) and (d), we plot the superconducting energy gap for two values of $U$, $U = 2.0t$ and $U = 3.0t$. The non-monotonicity in the energy gap for site-disorder is seen to occur for all densities and for both the values of the interaction strength, indicating that this is a ubiquitous phenomenon for a dirty superconductor with on-site disorder. On the other hand, it is absent for off-diagonal disorder for any parameter regime. The differences in the density dependence for the two disorder types also show up in the superconducting energy gap. The plots for diagonal disorder are essentially flat for $V = 2t$ (filled down triangles) for both values of $U/t$. The corresponding plots for the off-diagonal disorder show a relatively strong density dependence.
In order to emphasize the qualitative differences between the density dependence for the two disorder types, we plot $\Delta_{op}$ for four representative values of the average electron density in Fig. 3 panels (a) - (d). Close to half-filling ($n = 1$), the bond-disorder has larger average order parameter, while the site-disorder dominates for all disorder strengths as we move away from half-filling. The difference in the density dependence points to a qualitative difference between the manner in which the two disorder types affect the superconducting state.

In order to investigate further the differences between the effects of the two disorder types, we present the real-space data in Fig. 4 and Fig. 5. We plot the real space distribution of the local order parameter for both diagonal and off-diagonal disorder (Fig. 4 and Fig. 5) and at the interaction strength $U = 3.0t$ and the average electron density $n \sim 0.88$. Looking at the real space distribution of local quantities provide important clues about the underlying physics. In Fig. 4 for diagonal disorder, we clearly see the formation of disconnected superconducting islands which has large values of the superconducting order parameter $\Delta_{op}$, separated by large normal regions with no superconducting order. As the disorder strength is increased, the separation of the homogeneous superconducting system into superconducting and normal regions become more and more pronounced. For very large diagonal disorder, it is expected then that the system will break up into nearly microscopic regions of superconducting islands, interspersed by normal regions in between.

In Fig. 5 for off-diagonal disorder, we see a different behavior of the real-space distribution of $\Delta_{op}$ (note that we show the same disorder bandwidths for both diagonal and off-diagonal disorder, so that comparisons are meaningful). For off-diagonal disorder, even for high disorder strengths, the distribution of the superconducting order parameter is much more homogeneous, not only in space but also in magnitude. There are very few lattice sites (or regions) with very high values of $\Delta_i$. Thus, for the off-diagonal disorder, superconductivity is spread more homogeneously but weakly over the entire system as opposed to diagonal disorder. We see a similar behavior for all the individual disorder configurations we have investigated.

Discussion: In the absence of a full analytical solution to the problem of a superconductor in the presence of strong disorder, any explanation of the different behavior of the dirty superconductor with diagonal and off-diagonal disorder can be at best heuristic. Typically, in a disordered system with on-site disorder, sites with the similar disorder potential reside far away from each other. In other words, the local potential on two neighboring sites are typically very different. This impedes the hopping of the electron over any macroscopic distance, leading to local pair formation. As disorder bandwidth increases, the system thus finds it advantageous to separate into smaller and smaller microphases of superconductor and normal regions (whether the normal regions are metallic or insulating will be discussed elsewhere).
However, the same is not true for off-diagonal disorder. A site which has a bond that impedes hopping because of very small hopping amplitude, will typically also have another bond which leads to a significant gain in kinetic energy, i.e., promotes hopping. Therefore, a connected network-like region appears with an almost homogeneous order parameter (see Fig. 6(d)). Thus the pairing amplitude is uniformly spread over the system even when the randomness in the hopping matrix element is significant. To summarize the differences, for onsite disorder the order parameter gets contributions from a few islands with large magnitudes of the order parameter, while for bond disorder, the order parameter gets contributions from all over the system, though, with increasing disorder strength, the contribution becomes uniformly weak. This qualitative picture is very well supported by the distributions of the local order parameter values shown in Fig. 6.

In fact, the qualitative difference in the effective pictures also explains the difference in the density dependence that we reported in Fig. 2 and Fig. 3. In case of diagonal disorder, since the microscopic regions with large value of $\Delta_i$ moves with increasing disorder bandwidth.

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