Dynamical mean field theory of the repulsive BCS + $U$ model

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Abstract. The Gutzwiller-projected BCS Hamiltonian is a useful model for high-temperature superconductivity due to its equivalence to the Heisenberg model at half filling and a close connection to the $t$–$J$ model at moderate doping. In this work, a dynamical mean field theory (DMFT) is developed for the BCS Hamiltonian with d-wave pairing subject to on-site repulsive interaction, $U$, which we call the BCS + $U$ model. The large-$U$ limit corresponds to the Gutzwiller-projected BCS Hamiltonian. It is shown that the equivalence between the Heisenberg and the Gutzwiller-projected BCS model is a manifestation of a broader duality in the BCS + $U$ model: for any finite $U$, the local dynamics of the BCS + $U$ model is dual at half filling with respect to the exchange between the hopping parameter, $t$, and the pairing amplitude, $\Delta$. It is explicitly demonstrated in our DMFT analysis that the real superconducting gap, determined from the sharp coherence peaks in the local density of states, shows strong renormalization from its bare value as a function of $U$. 
1. Introduction

While the pairing mechanism is arguably still the most fundamental issue in high-temperature superconductivity, many physical properties of the superconducting phase itself can be rather well understood in terms of the conventional BCS theory with modification of d-wave pairing. There is, however, a wealth of peculiar behavior observed in the vicinity of the superconducting phase of cuprates (particularly pronounced in the underdoped regime) that seems to lie beyond the reach of conventional BCS theory.

Despite the diversity of involved experimental setups, the origin of various unconventional behavior can be attributed to the existence of an energy gap called the pseudogap [1, 2]. While there exist various interpretations for the pseudogap, a reasonable point of view is that this is an energy gap required for the formation of spin-singlet pairs [1, 3, 4]. In this view, it is expected that spin susceptibility should be reduced from that of the paramagnetic phase even in the normal phase, provided that the onset temperature for the spin-singlet formation is above $T_c$. This expectation is in fact fully consistent with the Knight shift measurements [5]. Also, the decrease in the specific heat [6] can be understood in terms of the spin entropy loss. Furthermore, the high-temperature pullback of the leading edge observed in angle-resolved photoemission spectroscopy [7] can be interpreted as a consequence of the energy cost in breaking pairs. The gap formation in the frequency-dependent $c$-axis conductivity [8] can also be explained similarly since inter-copper-layer transport inevitably involves pair breaking.

Now, an important question is how this pseudogap is related to the real superconducting gap. In this context, it is crucial to note that the pseudogap effects become prominent particularly in underdoped regimes where superconducting order is subject to strong phase fluctuations. The importance of superconducting phase fluctuations at low doping was first noted by Randeria et al [9] and later by Emery and Kivelson [10], who conjectured that the pseudogap phenomena could be explained by the presence of a well-defined pairing amplitude juxtaposed with large fluctuations in phase. The basic idea is as follows [3]. When combined with low hole concentration, the strong on-site repulsive interaction forces the ground state to have almost exclusively one electron per site, suppressing the electron-number fluctuation. Since electron number (strictly speaking, Cooper pair number) is conjugate with phase, small fluctuations in
electron number give rise to wild fluctuations in phase. In this view, the real superconducting gap can be identified with the fully renormalized pairing amplitude while the pseudogap, which is associated with the spin-singlet formation, has to do with its bare value.

It is currently believed that, if so obtained, the ultimate theory of high-temperature superconductivity should provide not only an explanation for pairing, but also an incorporation of pseudogap phenomena as a natural part. Setting aside the issue of constructing a complete phenomenology of high-temperature superconductivity, the fundamental reason for this is that the strong Coulomb correlation, as explained above, plays a key role in various unconventional behavior of cuprate superconductors, particularly in pseudogap phenomena. This strong correlation is, on the other hand, also believed to be responsible for the pairing mechanism in cuprates, resolving the mystery of how pairing can arise in a purely repulsive system \[3, 4\]. It is thus crucial to construct a theoretical framework that can address these issues in a computationally reliable manner. This is the main goal of this work.

The Gutzwiller-projected BCS Hamiltonian is a useful model to pursue this goal. This is partly due to the fact that, at half filling, this model generates an energy eigenstate spectrum exactly identical to that of the Heisenberg model \[11\]. Moreover, even for a moderate doping level \((x \sim 0.1)\), the overlap between the ground state of the Gutzwiller-projected BCS Hamiltonian and that of the \(t–J\) model remains rather high, \(\sim 90\%\), in an appropriate parameter range of \(J/t = 0.5 – 1\) \[11\]. Perhaps more important from a fundamental viewpoint is that the high overlap is adiabatically connected to the unity overlap in the strong-coupling regime of \(J/t \to \infty\). Therefore, the high overlap is not just a fortuitous coincidence, but rather an inevitable consequence of the fundamental connection between the \(t–J\) model and the Gutzwiller-projected BCS model in the strong-coupling regime.

In this paper, we focus on a related, but somewhat more general model called the BCS + \(U\) model, which is actually nothing but the BCS model with a built-in d-wave pairing amplitude competing against on-site repulsive interaction, \(U\). The large-\(U\) limit corresponds to the full Gutzwiller projection. Note that the Gutzwiller projection completely eliminates any configurations containing two electrons occupying the same site while finite \(U\) simply imposes a finite energy cost. Consequently, a richer parameter phase space can be explored by using the BCS + \(U\) model, which in turn can shed light on the physics of the Gutzwiller-projected BCS model as well. A particularly useful property of the BCS + \(U\) model in this regard is a duality in the local dynamics at half filling with respect to the exchange between the hopping parameter, \(t\), and the pairing amplitude, \(\Delta\), which will be discussed later in more detail.

Technically, we analyze the BCS + \(U\) model by using the dynamical mean field theory (DMFT). In essence, the DMFT is a quantum generalization of the classical mean field theory, with the key difference that it averages out only spatial variations while fully taking into account quantum-mechanical, temporal fluctuations \[12\]. We make use of the DMFT formalism since we believe that the frequency dependence of the self-energy plays the most dominant role in driving the superconductor-to-insulator transition in the BCS + \(U\) model as a function of \(U\). Reasons for choosing the DMFT formalism are further elaborated in succeeding sections.

As a result of the DMFT analysis, it is shown that the ‘real’ superconducting gap, determined from the sharp coherence peaks in the local density of states (LDOS), shows strong renormalization from its bare value as a function of \(U\). In fact, this gap completely vanishes at half filling when \(U\) reaches a critical value, \(U_c\). In the following sections, it is argued that the disappearance of the ‘real’ superconducting gap is mainly caused by the collapse of the quasiparticle spectral weight, i.e. the \(Z\) factor.
The rest of the paper is organized as follows. We begin section 2 by providing a precise mathematical expression for the BCS + $U$ Hamiltonian. Physical motivations for studying this Hamiltonian are described in this section. In section 3, a DMFT formalism is formulated for the analysis of the BCS + $U$ Hamiltonian. Our DMFT formalism maps the lattice BCS + $U$ model to an effective model for an impurity submerged in a d-wave superconducting medium. Main results are reported in section 4. It is first proven in section 4.1 that, for any finite $U$, the local dynamics of the BCS + $U$ model is dual at half filling with respect to the exchange between the hopping parameter, $t$, and the pairing amplitude, $\Delta$. In section 4.2, it is explicitly shown that there is in fact an essential identity between the local physics of the Hubbard and the strong-pairing BCS + $U$ model at half filling, which is fundamentally connected to the precise equivalence between the Heisenberg model and the strong-pairing Gutzwiller-projected BCS model in the large-$U$ limit [11]. It is interesting to note that this equivalence is actually a manifestation of a broader duality in the BCS + $U$ model. Also, at half filling, there is a $U$-driven phase transition from a superconducting to an insulating state, which is analyzed in section 4.3 in detail. The doping dependence of the LDOS is studied in section 4.4, which shows a reemergence of superconductivity with doping. Finally, the paper is concluded in section 5, where our theory is placed in perspective.

2. Motivation for the BCS + $U$ model

This work is based on the analysis of the BCS + $U$ Hamiltonian where the repulsive interaction, $U$, imposes a partial Gutzwiller projection. Mathematically, the BCS + $U$ model is given as follows:

$$H_{\text{BCS+}U} = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - \mu \sum_i c_{i\sigma}^\dagger c_{i\sigma}$$

$$+ \sum_{\langle i,j \rangle} \Delta_{ij} \left( c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger - c_{i\downarrow}^\dagger c_{j\uparrow}^\dagger + \text{H.c.} \right)$$

$$+ U \sum_i n_{i\uparrow} n_{i\downarrow},$$

where the spin index, $\sigma$, denotes either $\uparrow$ or $\downarrow$. As usual, $\langle i, j \rangle$ indicates that $i$ and $j$ are nearest neighbors. Here, $t$ is the hopping amplitude and $\mu$ is the chemical potential. Since we are interested in d-wave pairing, the (bare) pairing amplitude, $\Delta_{ij}$, is chosen to be $\Delta$ for $j = i + \hat{x}$ and $-\Delta$ for $j = i + \hat{y}$. The large-$U$ limit corresponds to the (fully) Gutzwiller-projected BCS Hamiltonian.

There are three main motivations for analyzing the BCS + $U$ model. The first one is the close connection between the $t$–$J$ and the Gutzwiller-projected BCS model. As mentioned before, at half filling, the energy eigenstate spectrum of the Gutzwiller-projected BCS Hamiltonian is entirely equivalent to that of the Heisenberg model. Moreover, even away from half filling, the overlap between the ground states of the $t$–$J$ model and the Gutzwiller-projected BCS model remains high for a range of moderate doping. Provided that the $t$–$J$ model is a reasonable model to analyze for high temperature superconductivity, the Gutzwiller-projected BCS model can prove quite useful. This leads to the second motivation.

The second motivation is due to the fact that the Gutzwiller-projected BCS model is more amenable to various theoretical tools. One such tool is the variational wave function.
technique where the Gutzwiller projection is applied to the BCS ground state wave function. The Gutzwiller-projected BCS wave function is also commonly known as the resonating valence bond state [13]. In this paper, however, we focus on a different theoretical tool known as the DMFT.

The third and last motivation is the systematic tunability of the relative strength between the pairing amplitude, $\Delta$, and the repulsive interaction, $U$, in the BCS + $U$ model. In the $t$–$J$ model, pairing correlation is an emergent property and therefore it is not a priori possible to determine how large the pairing amplitude is going to be. In fact, it is not even clear if the pairing amplitude exists at all. Even if the pairing amplitude exists and there is a way to determine its value, it is still true that the strength of the pairing amplitude is a fixed value, at least for a given hole concentration. Therefore, considering that high-temperature superconductivity in cuprates actually coexists with strong on-site repulsion, it would be quite interesting to investigate the interplay between pairing correlation and repulsive interaction by systematically tuning the relative strength between the two.

3. Formulation of the DMFT

For a concrete analysis, we develop a DMFT for the repulsive BCS + $U$ model. The DMFT is regarded as one of the most powerful theoretical tools for attacking various strongly correlated electron problems. Despite its power, however, the DMFT theory has an inherent weakness: it can only be applied to problems where spatial fluctuations are mild enough that they do not significantly modify bare dispersion.

Actually, there have been previous attempts to use the DMFT to investigate the existence of superconductivity in the Hubbard model. The basic idea is to incorporate the superconducting order parameter via the Nambu spinor formalism [12]. A more recent development is to combine the Nambu spinor formalism with the cellular dynamical mean field theory (CDMFT), which enlarges the DMFT impurity from a single site to a cluster [14, 16, 32]. An important advantage of this approach is the flexibility to allow non-local pairing such as d-wave pairing now that electrons can be paired with those in the other sites within the cluster. In this approach, while restricted by the size and shape of the impurity cluster, spatial fluctuations can be taken into account to some degree. Technically speaking, this means that the self-energy correction can develop some dependence on momenta.

Our approach is different since we begin by taking the Gutzwiller-projected BCS Hamiltonian as an effective Hamiltonian, which is derived from a more ‘fundamental’ model such as the $t$–$J$ model. Knowing that the full Gutzwiller projection is obtained in the large-$U$ limit, we then analyze the BCS + $U$ Hamiltonian as a function of $U$ via the single-site DMFT formalism. The non-local nature of d-wave pairing is embedded in the bare dispersion of the pairing amplitude.

It is now argued that a previously reported large-scale exact diagonalization result [17] provides support for the validity of the single-site DMFT formalism used in our study. Some time ago Poilblanc and Scalapino [17] performed exact diagonalization of the $t$–$J$ model on a 32-site square lattice with two doped holes. In this study, both $G_k(\omega + i\delta)$ and $F_k(\omega + i\delta)$ were explicitly computed by using the extended continued-fraction method originally devised by Ohta et al [18]. One of the most important technical breakthroughs reported by Poilblanc and Scalapino was the fact that the frequency-dependent gap function, $\Delta_k(\omega)$, could be directly
computed without any fitting procedure. The key is to assume generic mathematical forms for both $G_k(\omega + i\delta)$ and $F_k(\omega + i\delta)$ and to utilize their interdependence on $\Delta_k(\omega)$.

The main conclusion of this study is two-fold. Firstly, $\Delta_k(\omega)$ exhibits perfect $d$-wave symmetry. Secondly, $\Delta_k(\omega)$ is real and essentially a constant over a fairly wide frequency/energy region that turns out to be larger than the gap itself. This means that, over a reasonably wide frequency range, the pairing amplitude is essentially described by a constant times $d$-wave momentum dependence. In this situation, the single-site DMFT formalism can be appropriate since the anomalous self-energy correction is at most a constant that can be absorbed into the ‘bare’ pairing amplitude. Therefore, so long as the ‘bare’ pairing amplitude is properly chosen, no additional anomalous self-energy correction needs to be considered.

### 3.1. Effective impurity-bath Hamiltonian in superconducting media

We begin our DMFT analysis by writing an effective impurity-bath Hamiltonian for the BCS + $U$ model:

$$
H_{i-b} = \varepsilon_c c_\sigma^\dagger c_\sigma + U n_{c_\uparrow} n_{c_\downarrow} \\
+ \sum_l (a_{l\uparrow}^\dagger a_{l\downarrow}) \begin{pmatrix} \tilde{\varepsilon}_l & \tilde{\Delta}_l \\ \tilde{\Delta}_l & -\tilde{\varepsilon}_l \end{pmatrix} \begin{pmatrix} a_{l\uparrow}^\dagger \\ a_{l\downarrow}^\dagger \end{pmatrix} \\
+ \sum_l V_l (c_\sigma^\dagger a_\sigma + c_\sigma a_\sigma) \\
+ \sum_l W_l (a_{l\uparrow}^\dagger c_{\downarrow}^\dagger - a_{l\downarrow}^\dagger c_{\uparrow}^\dagger + \text{H.c.}),
$$

where $c_\sigma$ and $a_\sigma$ are the annihilation operators for the impurity and the bath orbitals, respectively. The core energy, $\varepsilon_c$, is minus the chemical potential. $V_l$ is the usual hybridization parameter for hopping between the impurity and the bath, while $\tilde{\varepsilon}_l$ is the energy of the $l$th bath orbital. Note that there are two new additions in our theory: (i) $\tilde{\Delta}_l$, the pairing amplitude of the $l$th bath orbital, and (ii) $W_l$, the anomalous hybridization parameter for pairing between the impurity and the bath.

To ensure that $H_{i-b}$ is a faithful effective Hamiltonian for the BCS + $U$ model, unknown parameters, $\tilde{\varepsilon}_l$, $\tilde{\Delta}_l$, $V_l$ and $W_l$, should be determined appropriately. This is done by imposing the DMFT self-consistency condition that the impurity Green’s function is entirely equivalent to the local Green’s function of the original lattice problem:

$$
\hat{G}(i\omega) = \sum_k \hat{G}_k(i\omega),
$$

where

$$
\hat{G}_k^{-1}(i\omega) = \begin{pmatrix} i\omega - \varepsilon_{k} & \Delta_k \\ \Delta_k & i\omega + \varepsilon_{k} \end{pmatrix} - \hat{\Sigma}(i\omega),
$$

in which $\varepsilon_k$ and $\Delta_k$ are given by the bare dispersion; $\varepsilon_k = -2t(\cos k_x + \cos k_y)$ and $\Delta_k = 2\Delta(\cos k_x - \cos k_y)$. In the above, the self-energy correction, $\hat{\Sigma}(i\omega)$, is defined as the difference
between the inverse of the impurity Green’s function for \( U = 0 \) (called the Weiss field), \( \hat{G}_0^{-1}(i\omega) \), and the inverse of the full impurity Green’s function for finite \( U \), \( \hat{G}^{-1}(i\omega) \):

\[
\hat{\Sigma}(i\omega) = \hat{G}_0^{-1}(i\omega) - \hat{G}^{-1}(i\omega),
\]

where

\[
\hat{G}(i\omega) = \begin{pmatrix} G(i\omega) & F(i\omega) \\ F(i\omega) & -G^*(i\omega) \end{pmatrix},
\]

and here \( G(i\omega) \) and \( F(i\omega) \) are the normal and anomalous impurity Green’s function, respectively.

Technically important is the fact that the Weiss field, \( \hat{G}_0(i\omega) \), can be expressed in terms of the effective parameters, \( \tilde{\varepsilon}_l, \tilde{\Delta}_l, V_l \) and \( W_l \):

\[
\hat{G}_0^{-1}(i\omega) = (i\omega - \varepsilon_c - \tilde{\varepsilon}_l - i\omega + \epsilon_c - \tilde{\Delta}_l),
\]

where \( \Gamma(i\omega) \) and \( \Lambda(i\omega) \) are the normal and anomalous corrections in the impurity Green’s function after integrating out all bath orbitals. Explicitly,

\[
\begin{align*}
\Gamma(i\omega) &= \sum_l \left( V_l^2 G_l - W_l^2 G_l^* + 2V_l W_l F_l \right), \\
\Lambda(i\omega) &= \sum_l \left[ (V_l^2 - W_l^2) F_l - V_l W_l (G_l + G_l^*) \right],
\end{align*}
\]

where \( G_l \) and \( F_l \) are, respectively, the normal and anomalous Green’s functions of the \( l \)th bath orbital:

\[
\begin{align*}
G_l(i\omega) &= \frac{i\omega + \tilde{\varepsilon}_l}{(i\omega)^2 - \tilde{\varepsilon}_l^2 - \tilde{\Delta}_l^2}, \\
F_l(i\omega) &= \frac{-\tilde{\Delta}_l}{(i\omega)^2 - \tilde{\varepsilon}_l^2 - \tilde{\Delta}_l^2}.
\end{align*}
\]

Solving the DMFT self-consistency equation in equation (3) requires computing the full impurity Green’s function for a given set of effective parameters. This is done via exact diagonalization in our study, which uses a finite number of orbitals. The number of orbitals is ten throughout this paper. Computing the full impurity Green’s function is technically difficult and numerically expensive in general, but is particularly time consuming in our study since \( H_{i-b} \) does not conserve the particle number so that different number-sectors mix. Therefore, \( H_{i-b} \) needs to be diagonalized in the Hilbert space containing all different possible number configurations. Once the impurity Green’s function is computed for a given parameter set, effective parameters in \( H_{i-b} \) can in turn be updated for a next iteration step in a similar manner to the method invented by Caffarel and Krauth [19]. The impurity Green’s function obtained in the converged iteration is taken to be the final solution.

Before moving onto the results, it is worthwhile to mention symmetry properties of the effective impurity-bath Hamiltonian with d-wave pairing. These properties are also technically important since one can use them to remove unnecessary degrees of freedom when choosing initial values for the effective parameters in the iterative method. Specifically, the d-wave pairing symmetry imposes a constraint on the effective parameters so that two identical parameter sets
for $\tilde{\epsilon}_i$, $V_i$ and $W_i$ always come in pairs with the opposite sign of $\tilde{\Delta}_i$, i.e. $(\tilde{\epsilon}_i, \tilde{\Delta}_i, V_i, W_i)$ and $(\tilde{\epsilon}_i, -\tilde{\Delta}_i, V_i, W_i)$. At half filling, there is an additional constraint due to particle–hole symmetry: for a given set $(\tilde{\epsilon}_i, \tilde{\Delta}_i, V_i, W_i)$, there exists a corresponding set of $(-\tilde{\epsilon}_i, \tilde{\Delta}_i, V_i, W_i)$.

4. Results

4.1. Local duality of the BCS + $U$ model

In this section, we discuss a peculiar property of the BCS + $U$ model at half filling: a duality in the local dynamics of the BCS + $U$ model with respect to the exchange between the hopping parameter, $t$, and the pairing amplitude, $\Delta$. We would like to prove this statement here.

To this end, let us first rewrite the BCS + $U$ Hamiltonian as follows:

$$
H_{\text{BCS+U}}(\{t, \Delta, \mu, U\}) = H_{\text{hop}}(\{t, \Delta\}) + H_{\text{pair}}(\{\Delta, -\Delta\}) + H_{\text{chem}}(\mu) + H_{\text{inter}}(U),
$$

where

$$
H_{\text{hop}}(\{t, \Delta\}) = -t \sum_{i, j = i + \hat{z}} \left( c_{i\sigma}^\dagger c_{j\sigma}^\uparrow + \text{H.c.} \right) - t \sum_{i, j = i + \hat{y}} \left( c_{i\sigma}^\dagger c_{j\sigma}^\downarrow + \text{H.c.} \right),
$$

$$
H_{\text{pair}}(\{\Delta, -\Delta\}) = \Delta \sum_{i, j = i + \hat{z}} \left( c_{i\sigma}^\dagger c_{j\sigma}^\dagger - c_{i\sigma}^\dagger c_{j\sigma}^\downarrow + \text{H.c.} \right) - \Delta \sum_{i, j = i + \hat{y}} \left( c_{i\sigma}^\dagger c_{j\sigma}^\dagger - c_{i\sigma}^\dagger c_{j\sigma}^\uparrow + \text{H.c.} \right),
$$

$$
H_{\text{chem}}(\mu) = -\mu \sum_{i} c_{i\sigma}^\dagger c_{i\sigma},
$$

$$
H_{\text{inter}}(U) = U \sum_{i} n_{i\uparrow} n_{i\downarrow}.
$$

Now, the chemical potential needs to be appropriately determined in order to fix the electron density. Unfortunately, there is an ambiguity in choosing the value of the chemical potential exactly at half filling, at least for sufficiently large $U$. This is fundamentally due to the fact that the ground state becomes a Mott insulator for sufficiently large $U$, in which case an excitation gap develops and the chemical potential becomes discontinuous below and above half filling. This situation can be dangerous since what happens exactly at half filling can be different from that at infinitesimal doping. This difference can, in principle, give rise to significant changes when different particle-number sectors are coupled, which is exactly our current situation with the superconducting ground state.

To accentuate this issue, consider the large-$U$ limit of the BCS + $U$ model. As mentioned in the introduction, it is shown in [11] that, at half filling, the Gutzwiller-projected BCS model is entirely equivalent to the Heisenberg model in the limit of strong coupling. Consulting the above reference, however, one may notice that there is a slight difference between the Gutzwiller-projected BCS model and the naive large-$U$ limit of the BCS + $U$ model. While the fact that double occupancy is removed is the same, the difference is in the choice of the chemical potential. That is, the chemical potential is set to zero in the Gutzwiller-projected BCS model at half filling while it is $U/2$ in the large-$U$ limit of the BCS + $U$ model. This may seem like a minor technical detail. There is, however, numerical evidence showing that the above two
different choices of the chemical potential can and do produce completely distinct results in a non-bipartite lattice [20]. Fortunately, in the square lattice, the naive large-$U$ limit of the BCS + $U$ model generates the identical energy eigenstate structure to that of the Gutzwiller-projected BCS model. Below, we provide an argument for this.

To begin with, it is important to note that the chemical potential for half filling is uniquely defined to be $\mu = U/2$ so long as $U$ is smaller than a critical value, $U_c$, that causes the Mott transition. Now, let us imagine a situation where $U$ is slightly below $U_c$. As mentioned before, once $U$ crosses $U_c$, the chemical potential becomes discontinuous. However, it is likely that the ground state itself is still continuously connected since both the ground states slightly below and above $U_c$ are almost entirely composed of the lower Hubbard band. Increasing $U$ only separates the lower Hubbard band further away from the upper one without changing the nature of the ground state much. On the other hand, the chemical potential in the limit of infinitesimal doping is the one that is needed to move the upper tip of the lower Hubbard band to zero energy. This also does not change the nature of the ground state. Therefore, the physics does not depend on the choice of the chemical potential between the two different limits of half filling. Note that the validity of our argument is restricted to the square-lattice system where the nature of the Mott transition is well known. From now on, we set the chemical potential to be $\mu = U/2$.

Now, we show that a series of unitary transformations can generate the exchange operation between $t$ and $\Delta$ in the BCS + $U$ model. To this end, let us first consider the following unitary transformation:

$$
\begin{align*}
    c_{i \uparrow} &\rightarrow c'_{i \uparrow}, & c_{i \downarrow} &\rightarrow c'_{i \downarrow} & \text{for } i \in A, \\
    c_{j \uparrow} &\rightarrow c'_{j \downarrow}, & c_{j \downarrow} &\rightarrow -c'_{j \uparrow} & \text{for } j \in B,
\end{align*}
$$

(15)

where $A$ and $B$ indicate two different sublattices of the bipartite lattice, as shown in figure 1(a). By denoting this transformation as $\hat{T}_b$, one can rewrite the above equation more formally:

$$
\begin{align*}
    \hat{T}_b c_{i \sigma} \hat{T}_b^\dagger &= c'_{i \sigma} & \text{for } i \in A, \\
    \hat{T}_b c_{j \sigma} \hat{T}_b^\dagger &= \sigma c'_{j \sigma} & \text{for } j \in B,
\end{align*}
$$

(16)

where $\sigma$ can be $\uparrow = 1$ or $\downarrow = -1$. Then, a straightforward algebra shows that

$$
\begin{align*}
    \hat{T}_b H_{\text{hop}}(\{t, t\}) \hat{T}_b^\dagger &= H'_{\text{pair}}(\{-t, -t\}), \\
    \hat{T}_b H_{\text{pair}}(\{\Delta, -\Delta\}) \hat{T}_b^\dagger &= H'_{\text{hop}}(\{\Delta, -\Delta\}),
\end{align*}
$$

(17)

where $H'$ indicates that $H$ is written in terms of $c'$. Similarly, one can transform $H_{\text{chem}}$ and $H_{\text{inter}}$:

$$
\begin{align*}
    \hat{T}_b H_{\text{chem}}(\mu) \hat{T}_b^\dagger &= -\mu \left[ \sum_{i \in A} n_i' + \sum_{j \in B} (2 - n_j') \right], \\
    \hat{T}_b H_{\text{inter}}(U) \hat{T}_b^\dagger &= U \left[ \sum_{i \in A} n_i' n_i' + \sum_{j \in B} (1 - n_j')(1 - n_j') \right],
\end{align*}
$$

(18)
where \( n' = n'_\uparrow + n'_\downarrow \). Adding the above two equations leads to the following expression:

\[
\hat{T}_b[H_{\text{chem}}(\mu) + H_{\text{inter}}(U)]\hat{T}_b^\dagger = H'_{\text{chem}}(U - \mu) + H'_{\text{inter}}(U) + (U - 2\mu)N_B,
\]

(19)

where \( N_B \) is the number of \( B \) sublattice sites. As mentioned previously, \( \mu = U/2 \) at half filling, in which case the above equation simply becomes

\[
\hat{T}_b[H_{\text{chem}}(U/2) + H_{\text{inter}}(U)]\hat{T}_b^\dagger = H'_{\text{chem}}(U/2) + H'_{\text{inter}}(U).
\]

(20)

In conclusion, by combining all components of \( H_{\text{BCS+U}} \), we arrive at the following equation:

\[
\hat{T}_bH_{\text{BCS+U}}([t, t], \{\Delta, -\Delta\}, \mu = U/2, U)\hat{T}_b^\dagger = H''_{\text{BCS+U}}([\Delta, -\Delta], \{-t, -t\}, \mu = U/2, U).
\]

(21)

The second unitary transformation is performed as follows:

\[
c'_{i\sigma} \rightarrow c''_{i\sigma} \quad \text{for } i \in C,
\]
\[
c'_{j\sigma} \rightarrow -c''_{j\sigma} \quad \text{for } j \in D,
\]

(22)

where \( C \) and \( D \) indicate two different sublattices shown in figure 1(b). Let us denote this transformation as \( \hat{T}_s \). Note that \( \hat{T}_s \) flips the relative sign of the electron operators in the nearest-neighboring sites separated in the \( y \)-direction. Therefore,

\[
\hat{T}_sH''_{\text{BCS+U}}([\Delta, -\Delta], \{-t, t\}, \mu = U/2, U)\hat{T}_s^\dagger = H''_{\text{BCS+U}}([\Delta, \Delta], \{t, -t\}, \mu = U/2, U).
\]

(23)

The last unitary transformation is the diagonal reflection that performs an exchange between the \( x \)- and \( y \)-axes. By denoting this transformation as \( \hat{T}_d \),

\[
\hat{T}_d c''_i \hat{T}_d^\dagger = \tilde{c}_i,
\]

(24)

where \( \tilde{i} = i_x \hat{x} + i_y \hat{y} \) when \( i = i_x \hat{x} + i_y \hat{y} \). Consequently, applying the diagonal reflection operation to \( H''_{\text{BCS+U}} \) results in the following equation:

\[
\hat{T}_dH''_{\text{BCS+U}}([\Delta, \Delta], \{-t, t\}, \mu = U/2, U)\hat{T}_d^\dagger = \tilde{H}_{\text{BCS+U}}([\Delta, \Delta], \{t, -t\}, \mu = U/2, U).
\]

(25)
Now, let us combine all of the three previous unitary transformations into one:

$$\hat{T} \equiv \hat{T}_d \hat{T}_s \hat{T}_b.$$  \hfill (26)

Using this operator, we arrive at an important step toward the main goal of this section:

$$\hat{T} H_{\text{BCS+U}}(\{t, t\}, \{\Delta, -\Delta\}, \mu = U/2, U) \hat{T}^\dagger = \tilde{H}_{\text{BCS+U}}(\{\Delta, \Delta\}, \{t, -t\}, \mu = U/2, U),$$  \hfill (27)

which proves that $t$ and $\Delta$ can be exchanged through a unitary transformation. What is left is to show that the local dynamics is indeed invariant with respect to the exchange between $t$ and $\Delta$. More precisely, we would like to prove that the local Green’s function is invariant.

To compute the local Green’s function, we first consider the following quantity:

$$\langle \psi | c_{j\uparrow}(\tau) c_{j\downarrow}^\dagger (0) | \psi \rangle,$$  \hfill (28)

where $|\psi\rangle$ is the ground state of $H_{\text{BCS+U}}$. By inserting several $\hat{T}^\dagger \hat{T}$ inside the bracket, we obtain that

$$\langle \psi | c_{j\uparrow}(\tau) c_{j\downarrow}^\dagger (0) | \psi \rangle = \langle \psi | \hat{T}^\dagger \hat{c}_{j\uparrow}(\tau) \hat{T} \hat{c}_{j\downarrow}^\dagger (0) \hat{T}^\dagger \hat{T} | \psi \rangle$$

$$= \langle \tilde{\psi} | \hat{T} \hat{c}_{j\uparrow}(\tau) \hat{T}^\dagger \hat{c}_{j\downarrow}^\dagger (0) \hat{T}^\dagger | \tilde{\psi} \rangle$$

$$= \begin{cases} 
\langle \tilde{\psi} | \tilde{c}_{j\uparrow}(\tau) \tilde{c}_{j\downarrow}^\dagger (0) | \tilde{\psi} \rangle & \text{for } j \in A, \\
\langle \tilde{\psi} | \tilde{c}_{j\downarrow}(\tau) \tilde{c}_{j\uparrow}^\dagger (0) | \tilde{\psi} \rangle & \text{for } j \in B, 
\end{cases}$$  \hfill (29)

where the following two facts are used. Firstly, being equal to $\hat{T} | \psi \rangle$, $| \tilde{\psi} \rangle$ is the ground state of $\tilde{H}_{\text{BCS+U}}$. Secondly, for $j \in B$,

$$\hat{T} \hat{c}_{j\uparrow}(\tau) \hat{T}^\dagger = \hat{T} e^{i H} c_{j\uparrow}(0) e^{-i H} \hat{T}^\dagger$$

$$= \hat{T} e^{i H} \hat{T}^\dagger \hat{c}_{j\uparrow}(0) \hat{T} e^{-i H} \hat{T}^\dagger$$

$$= e^{i \hat{H}} \hat{c}_{j\uparrow}(0) \hat{T} e^{-i \hat{H}}$$

$$= e^{i \hat{H}} \tilde{c}_{j\uparrow}(0) e^{-i \hat{H}}$$

$$= \tilde{c}_{j\uparrow}(\tau),$$  \hfill (30)

where we drop the subscript, BCS + $U$, for $H$. Similarly, for $j \in A$, $\hat{T} \hat{c}_{j\uparrow}(\tau) \hat{T}^\dagger = \tilde{c}_{j\uparrow}(\tau)$. It is important to note that the conditional sign change due to $\hat{T}_s$ is ignored in the above since it is exactly cancelled by that induced from $\hat{T} \hat{c}_{j\uparrow}(0) \hat{T}^\dagger$.

Then, by using equation (29), it is not too difficult to show that the local Green’s function at the $j$th site, $G_j(i\omega)$, is given by

$$G_j(i\omega) = \begin{cases} 
\tilde{G}_{j\uparrow}(i\omega) & \text{for } j \in A, \\
-\tilde{G}_{j\downarrow}(-i\omega) & \text{for } j \in B, 
\end{cases}$$  \hfill (31)

which achieves the main goal of this section: the local dynamics of the BCS + $U$ model is dual with respect to the exchange between $t$ and $\Delta$. Note that the particle–hole symmetry
enforces $-\tilde{G}(-i\omega) = \tilde{G}(i\omega)$. Also, note that we assume a paramagnetic solution where $G$ is spin independent.

So far, it has been shown that the BCS + $U$ model is locally dual with respect to the exchange between $t$ and $\Delta$. Now, we show that the single-site DMFT formalism is properly equipped to represent the same duality. To this end, it is important to note that the self-energy is given by the inverse difference between the Weiss field, $\tilde{\Gamma}_0$, and the full Green's function, $\tilde{G}$ (see equation (5)). Also important is the fact that the Weiss field is completely determined by $\Gamma$ and $\Lambda$, which depend on the effective parameters in $H_{t-b}$ (see equations (7) and (8)).

In the last paragraph of section 3.1, it is mentioned that there are two symmetry constraints on the effective parameters at half filling. That is, at half filling, the effective parameters always come in pairs as (i) $(\tilde{\varepsilon}_i, \tilde{\Delta}_i, V_i, W_i)$ and $(-\tilde{\varepsilon}_i, \tilde{\Delta}_i, V_i, W_i)$ and (ii) $(\tilde{\varepsilon}_i, -\tilde{\Delta}_i, V_i, W_i)$ and $(\tilde{\varepsilon}_i, -\tilde{\Delta}_i, V_i, W_i)$. Utilizing this property, one can then show that

$$\Gamma(i\omega) = \sum_i \left( V_i^2 G_i - W_i^2 G_i^* + 2V_i W_i F_i \right)$$

$$= \sum_i \left( V_i^2 + W_i^2 \right) \frac{i\omega}{(i\omega)^2 - \tilde{\varepsilon}_i^2 - \tilde{\Delta}_i^2},$$

and $\Lambda(i\omega)$ is zero. As one can see, $\Gamma(i\omega)$ is invariant with respect to the exchange operation of $(\tilde{\varepsilon}_i, V_i) \leftrightarrow (\tilde{\Delta}_i, W_i)$. Bearing in mind the physical meaning of each effective parameter, one can see that the above operation corresponds to the exchange between hopping and pairing, i.e. between $t$ and $\Delta$. Consequently, it is shown that the Weiss field is consistent with local duality.

The full Green’s function, $\tilde{G}$, is too complicated to derive its dependence on the effective parameters in a closed form. It is, however, reasonable to assume that $\tilde{G}$ is also invariant with respect to the same exchange process since it is the local Green’s function for the BCS + $U$ model, albeit within the DMFT framework. As seen in the following sections, our DMFT analysis explicitly proves this to be true. In conclusion, it is shown that the single-site DMFT formalism is fully consistent with local duality.

At this point, it is interesting to note that the unitary transformation used in this section has similarities to the particle–hole transformation. In fact, there is a long history in investigating symmetry transformations of the Hubbard model. In particular, by using the particle–hole transformation, Singh and Scalettar [21] were able to show that the Nagaoka ferromagnet in the repulsive Hubbard model can be mapped onto Yang’s $\eta$-paired superconductor in the attractive counterpart. Despite similarities, however, there are crucial differences between our unitary and the usual particle–hole transformation as well. One of the most crucial ones is that, in our study, the particle–hole transformation is performed only on sites belonging to one sublattice (with an appropriate sign change depending on the spin) and the spin is simultaneously flipped at these sites.

Actually, there was a previous study by Affleck et al [22], who made use of a unitary transformation very similar to ours. In the above study, Affleck et al showed that, in the large-$U$ limit, two apparently very different mean-field theories of the repulsive Hubbard model proposed by Baskaran et al [23] (who assumed pairing order parameters to be non-zero) and by Affleck and Marston [24] (who assumed normal hopping order parameters to be non-zero) were actually equivalent. It is emphasized, however, that the main focus of our current study is on the exact local duality embedded in the general BCS + $U$ model (which includes the duality
between two extreme limits of \( t = 0 \) and \( \Delta = 0 \), not just on a symmetry between two mean-field solutions of the Hubbard model in the large-\( U \) limit. In a sense, our work provides a generalization of the results obtained by Affleck and collaborators.

In the next section, we analyze a limiting situation where \( t = 0 \). We call the model in this situation the strong-pairing BCS + \( U \) model. According to the local duality principle, the local dynamics of this model must be identical to that of the BCS + \( U \) model with \( \Delta = 0 \), i.e. the Hubbard model. The main goal of the next section is to investigate if this is indeed true.

### 4.2. Equivalence between the Hubbard and the strong-pairing BCS + \( U \) model

In this section, we compute the LDOS of the strong-pairing BCS + \( U \) model. Here, strong pairing means that there exists only the pairing amplitude with no hopping parameter, i.e. \( t = 0 \).

As mentioned previously, this model is physically meaningful at half filling due to the fact that, in the large-\( U \) limit, it has an energy spectrum precisely identical to that of the Heisenberg model [11].

Figure 2 presents the comparison between the LDOS of this model and that of the Hubbard model (which is nothing but the BCS + \( U \) model with \( \Delta = 0 \)). It is shown in this figure that the two models have essentially identical LDOS despite the difference in ‘global physics’. That is, the former model has a superconducting ground state at small \( U \) while the latter does not. The identity in the local dynamics is very important since it suggests that the DMFT framework can capture not only the fundamental equivalence between the two models in the large-\( U \) limit, but also their local duality at general \( U \).

In addition to local duality, it is interesting to investigate the nature of the insulating transition that occurs at a critical value \( U = U_c \). Two facts are important for this purpose. Firstly, the anomalous self-energy correction, \( S(i\omega) \), is zero. As mentioned before, at least at half filling, it is not too difficult to derive this property. It is basically due to the fact that the previously mentioned symmetry constraints on \((\tilde{\epsilon}_l, \tilde{\Delta}_l, V_l, W_l)\) make the anomalous coupling, \( \Lambda \), vanish, which in turn indicates that the Weiss field has zero off-diagonal matrix elements.

In this situation, the DMFT self-consistency equation is satisfied only when the off-diagonal element of the full Green’s function is also zero, which means that the off-diagonal element of the self-energy, \( S(i\omega) \), is zero as well. The situation is less clear at finite doping where \( S(i\omega) \) vanishes via an intricate adjustment of the relevant effective parameters in \( H_{\text{eff}} \). It is important to remember that only the local component of the anomalous Green’s function, \( \sum_k F_k(i\omega) \), is zero. For small \( U \), \( F_k(i\omega) \) itself is nonzero and a pure d-wave.

Secondly, within the metallic regime, \( \Sigma(i\omega) \) becomes linear in \( i\omega \) in the low-energy limit: \( \Sigma \simeq U/2 + (1 - 1/Z)i\omega \), where \( Z \) is the quasi-particle spectral weight. In this situation, the denominator of the normal Green’s function simply becomes \( \omega^2/Z^2 - \Delta_k^2 \) after analytic continuation. Note that the constant term of the normal self-energy exactly cancels the chemical potential at half filling. As a result, the pole occurs at \( \omega = \pm Z|\Delta_k| \), indicating that the pairing dispersion is effectively renormalized to be \( Z\Delta_k \). Figure 2 shows that \( Z \) decreases as a function of \( U \) and finally vanishes at \( U = U_c \), inducing the collapse of superconductivity (see figure 4 for explicit results). It is important to note that, according to the local duality principle, the nature of this transition process is exactly identical to that of the Hubbard model. What is different is that in the case of the strong-pairing BCS + \( U \) model, the transition occurs between a superconductor and a Mott insulator while, in the case of the Hubbard model, it is between a conductor and a Mott insulator.
Figure 2. Comparison between the LDOS of the Hubbard model ($\Delta = 0$) and that of the strong-pairing BCS + $U$ model ($t = 0$) at half filling as a function of on-site repulsive interaction, $U$. In the plot, $D = 4t$ and $D_\Delta = 4\Delta$. Note that the above calculations are performed at zero temperature so that we ignore the second DMFT solution that might occur in the vicinity of the insulating phase transition. The second DMFT solution is adiabatically connected to an insulating state and higher in energy than its metallic counterpart [12].

So far, we have discussed a special limit where $t = 0$. In the next section, we study the general BCS + $U$ model with neither $t$ nor $\Delta$ being zero, in which case the self-energy correction depends on both $U/t$ and $\Delta/t$.

4.3. Superconductor-to-insulator transition at half filling

Figure 3 shows the LDOS of the BCS+$U$ model at half filling with $\Delta/t = 0.5$ as a function of $U$. It is important to note that, due to pairing correlation, the density of states is reduced in the vicinity of the Fermi level (i.e. $\omega/D = 0$ in the plot), which in turn generates concomitant coherence peaks at two symmetric locations separated from the Fermi level by the ‘renormalized’ superconducting energy gap.

The existence of the coherence peak is a hallmark of superconductivity. It is thus worthwhile to mention how we determine such existence in our DMFT data. Without knowing what to look for, it is difficult to distinguish real superconducting coherence peaks from spurious ones. This is because the LDOS is obtained as a discrete series of sharp peaks within the DMFT framework using exact diagonalization as an impurity solver. The key is to focus on a continuous
evolution of the LDOS as a function of $U$. First, at $U = 0$, the BCS + $U$ Hamiltonian becomes bilinear and is solved exactly. The dotted curve in the top, left panel of figure 3 shows the LDOS in this case. As one can see, there exist two well-developed superconducting coherence peaks with a characteristic $V$-shaped LDOS in the middle. Then, by changing $U$ in a small increment, it is possible to continuously trace the evolution of the superconducting coherence peaks. In this way, the superconducting coherence peaks can be distinguished from spurious ones.

Note that the distance between the two superconducting coherence peaks decreases as $U$ increases. Eventually, the two coherence peaks collide and vanish at $U = U_c$ where superconductivity itself disappears. As a working definition, one may take the half distance between the two coherence peaks as the ‘renormalized’ (or physically observable) superconducting gap, $\Delta_{\text{ren}}$. In this definition, it can be seen that $\Delta_{\text{ren}}$ is strongly renormalized from the bare value, $\sim \Delta$, as $U$ increases.

Similar to the strong-pairing BCS + $U$ model discussed in the previous section, the superconductor-to-insulator transition in the general BCS + $U$ model is driven by the collapse of the quasiparticle spectral weight, $Z$. The difference is that $Z$ now depends on both $U/t$ and $\Delta/t$. Figure 4 plots $Z$ of the BCS + $U$ model with $\Delta/t = 0.5$ and 2 in comparison with that of the Hubbard model. As one can see, $Z$ is overall enhanced, resulting in a larger $U_c$: $U_c/D \simeq 3.5$ and 7 for $\Delta/t = 0.5$ and 2, respectively, while $U_c/D \simeq 3.0$ for $\Delta/t = 0$. Thus, when coexisting with hopping, pairing reduces interaction effects and delays the insulating phase transition (as a function of $U/D$).

In figure 5, we plot the renormalized superconducting gap, $\Delta_{\text{ren}}$, as a function of $U/D$ in comparison with $Z$. Bearing in mind that there are uncertainties caused by the discreteness of the LDOS peaks due to the finite-system size, two conclusions can be drawn from this figure. Firstly, while overall similar, $\Delta_{\text{ren}}$ has a $U$-dependence somewhat different from that of $Z$ for
Figure 4. Quasiparticle spectral weight, \( Z \), as a function of \( U \). Solid circles indicate \( Z \) of the BCS + \( U \) model with \( \Delta/t = 0.5 \) while empty squares denote that of the Hubbard model. Note that \( Z \) is determined by fitting \( \Sigma(i\omega) \) into a linear function of \( i\omega \) in the low energy limit. The fitting error bar is estimated to be smaller than the size of the symbol.

Figure 5. Renormalized superconducting gap, \( \Delta_{\text{ren}} \) (stars), in comparison with the quasiparticle spectral weight, \( Z \) (solid squares), as a function of \( U \). \( \Delta_{\text{ren}} \) is determined as half of the distance between coherence peaks in the LDOS. The bare pairing amplitude is constant in this figure: \( \Delta/t = 0.5 \). Note that ideally, in the limit of \( U/D \to 0 \), the coherence peak should be located at \( \Delta_{\text{ren}}/D \simeq 0.45 \), which is obtained via analytic evaluation of the LDOS of the non-interacting system.

For \( U/D < 3 \). We believe that this difference may occur since \( Z \) measures the slope of the self-energy at zero energy while \( \Delta_{\text{ren}} \) is affected by the self-energy around the energy scale of the gap itself. Secondly, for \( U/D > 3 \), \( \Delta_{\text{ren}} \) and \( Z \) have basically identical \( U \)-dependence, showing that the disappearance of the superconducting gap is essentially caused by the collapse of the \( Z \) factor.

It is interesting to note that, due to the local duality, \( Z \) for \( \Delta/t = 2 \) becomes exactly identical to that for \( \Delta/t = 0.5 \) when \( U/D \) is rescaled to become half. To see why this is so, let us remind ourselves of the local duality condition:

\[
H_{\text{BCS}+U}(t, \Delta, U) \leftrightarrow H_{\text{BCS}+U}(\Delta, t, U),
\]  

(33)

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where we use an abbreviated notation for the BCS + $U$ Hamiltonian defined in equation (10). Here, ↔ indicates that the two Hamiltonians are locally dual. Now, we rescale the Hamiltonian so that the hopping parameter becomes unity in proper units:

$$t \cdot H_{BCS+U}(1, \Delta/t, U/t) \leftrightarrow \Delta \cdot H_{BCS+U}(1, t/\Delta, U/\Delta),$$

which is reduced to the following for $\Delta/t = 0.5$:

$$t \cdot H_{BCS+U}(1, 0.5, U/t) \leftrightarrow \Delta \cdot H_{BCS+U}(1, 2, 2U/t).$$

Knowing that $Z$ is a local and dimensionless quantity, one can now see that

$$Z(1, 0.5, U/t) = Z(1, 2, 2U/t),$$

where $Z(a, b, c)$ indicates the quasiparticle spectral weight of the BCS + $U$ Hamiltonian with the hopping parameter being $a$, the pairing amplitude being $b$ and the interaction energy being $c$.

Finally, it is important to recall that the pairing amplitude, $\Delta/t$, is set to be constant in the current analysis. Assuming that this ‘bare’ pairing amplitude is physically responsible for the spin singlet formation [3, 4, 11], a large renormalization of the pairing amplitude provides an explanation for pseudogap phenomena. In this view, the real superconducting gap is related to the ‘renormalized’ pairing amplitude, which can deviate from the bare value for sufficiently large $U$ so much that it can completely vanish at $U = U_c$. Therefore, for sufficiently large $U$, superconductivity is hidden at half filling while spin singlet pairs are inherently present due to the presence of a nonzero bare pairing amplitude. A natural question that follows is whether superconductivity can reemerge when electrons become mobile with doping. This is the main topic of the next section.

4.4. Reemergence of superconductivity with doping

We now turn to the doped BCS + $U$ model. As shown in the preceding sections, the superconducting gap is suppressed at half filling for sufficiently large $U$. The question is whether the suppressed superconductivity can resurface with hole doping that allows fluctuations in charge. Figure 6 shows the LDOS of the BCS + $U$ model with $\Delta/t = 0.5$ and $U/D = 3$: increasing the hole concentration indeed opens up a superconducting gap at the Fermi level. It is interesting to observe that, with the hole concentration increasing, the lower Hubbard band moves toward the Fermi level and provides a necessary density of states for the suppressed superconductivity to become reactivated.

It is mentioned in section 2 that the ground state of the Gutzwiller-projected BCS model has a high overlap with that of the $t-J$ model in an appropriate parameter range. For example, when $J/t \simeq 0.5–1.0$, the overlap becomes about 90% for $\Delta/t = 0.5$ in the doping range of $x \simeq 10–15%$. This range corresponds to somewhere between the fifth and the sixth panel from the top of figure 6.

5. Conclusion

In this paper, the repulsive BCS + $U$ model is analyzed within the DMFT framework. What is shown from this analysis is that the pairing amplitude can be strongly renormalized from the bare value, $\Delta$, for sufficiently large $U$. In fact, at half filling, the renormalized pairing amplitude
Figure 6. LDOS of the BCS + $U$ model with $\Delta/t = 0.5$ and $U/D = 3$ as a function of doping. The value of $U/D = 3$ is chosen so that the ground state at half filling is just about to enter the insulating phase, which corresponds to the almost fully Gutzwiller-projected regime. The top panel shows the LDOS at half filling, which is obtained at $\mu = \mu_0 \equiv U/2$. From the top to the bottom panel, the chemical potentials (the corresponding hole concentration, $x$) are $\mu_0$ (0%), $0.9\mu_0$ (1.65%), $0.8\mu_0$ (3.70%), $0.7\mu_0$ (6.42%), $0.6\mu_0$ (9.90%), $0.5\mu_0$ (14.10%), $0.4\mu_0$ (19.30%), $0.3\mu_0$ (25.13%) and $0.2\mu_0$ (31.53%), respectively.

completely vanishes at a critical value of $U$. Within the DMFT framework, the collapse of superconductivity is induced by the disappearance of the quasiparticle spectral weight, $Z$.

Physically speaking, the collapse of superconductivity can be understood in terms of the suppression in charge fluctuation, which induces the disappearance of the quasiparticle spectral weight and therefore generates the insulating phase transition. Note that, within the DMFT framework, both the collapse of superconductivity and the insulating phase transition occur at the same time. This viewpoint is consistent with the fact that the ‘hidden’ superconductivity at half filling reemerges with doping that allows fluctuations in charge.

In addition to the superconductor-to-insulator transition, the BCS + $U$ model has an intriguing property, which we named local duality. That is, at half filling, the local dynamics
of the BCS + $U$ model is dual with respect to the exchange between the hopping parameter, $t$, and the pairing amplitude, $\Delta$. Local duality provides a new insight on the precise equivalence between the Hubbard model ($\Delta = 0$) and the strong-pairing BCS + $U$ model ($t = 0$) at half filling in the large-$U$ limit. That is, we now understand that the fact that the Hubbard model is fundamentally connected to the strong-pairing BCS + $U$ model is a manifestation of local duality in the BCS + $U$ model.

Finally, we conclude by putting our theory in perspective. It is obviously beyond the scope of this paper to provide a comprehensive review on the theories of the pseudogap phenomenon. We thus select only a few theories that are closely related to our theory. In an overall scheme, our theory can be categorized into the theory with preformed pairs. This is because, in our theory, electrons are inherently paired due to the nonzero pairing amplitude. There are, however, many variations in the preformed-pair scenario. Pairs can be preformed by (i) the spin-charge separation $[25]$–$[27]$ involving a deconfined phase $[1]$, (ii) the formation of microscopic stripes $[28]$, (iii) the proximity to the long-range antiferromagnetic order $[29]$ (in the so-called nearly antiferromagnetic Fermi liquid theory), and so on. In our theory, preformed pairs exist because the ground state itself has nonzero (bare) pairing amplitude. Recall that the nonzero pairing amplitude is fundamentally related to the equivalence between the Heisenberg model and the strong-pairing Gutzwiller-projected BCS model at half filling. The dichotomy between the bare and real superconducting gap originates from strong renormalization effects of the large on-site repulsive interaction.

It is interesting to note that all of the above preformed-pair theories (including ours) can be separated into two sub-classes, as proposed by Lee et al. In their review paper $[1]$, Lee et al coined the words, ‘thermal explanation’ and ‘quantum explanation’ of the pseudogap. In the quantum explanation of the pseudogap, a fundamentally new quantum state is proposed. An example is the deconfined spin-liquid state in the spin-charge separation scenario, where the pseudogap is regarded as a high-frequency property of the spin-liquid state, seen at high temperature. A caveat is that the deconfined spin-liquid state might not be stable in the square-lattice $t$–$J$ model.

On the other hand, the thermal explanation refers to any theories viewing the pseudogap as a finite-temperature manifestation of the gap necessary for the spin-singlet formation. In this explanation, the ground state usually breaks a symmetry at zero temperature. Broken symmetries are lattice translation, spin rotation and global gauge invariance in the case of the stripe theory, the nearly antiferromagnetic Fermi liquid theory, and the fluctuating superconductivity theory (which conceptually includes our theory), respectively. The main difference between our theory and the others in this sub-class is that the real superconducting gap originates from the same spin gap while it is strongly renormalized by large $U$. Consequently, only the real superconducting gap is shown in the zero-temperature density of states while a signature for the pseudogap can be seen in the finite-temperature counterpart.

Finite-temperature behavior of the correlated superconducting state will be of importance. Strictly speaking, all results presented in this work concern only the symmetry-broken state at zero temperature. Therefore, implications for the pseudogap state are indirect in nature. To make a direct contact, it is imperative to investigate exactly how the correlated superconducting state behaves at finite temperature, especially in the range above critical temperature and below spin-gap energy scale. It is our future plan to pursue the answer to this question.

Finally, we conclude by providing a brief discussion on the results obtained in other DMFT formalisms. As mentioned at the beginning of section 3, various approximation
schemes have been proposed for extending the (single-site) DMFT to include non-local correlations. The CDMFT and the dynamic cluster approximation are among the most successful theories of this sort. In the context of this paper, it is worthwhile to mention that the relationship between the superconducting gap and the pseudogap is one of the main sources for current intensive research efforts in these approaches as well \([30, 31]\). On the other hand, in multi-orbital models with on-site s-wave pairing, it has indeed been shown by using the standard single-site DMFT formalism that pairing can survive and even be enhanced by correlations; moreover, this effect is actually accompanied by a pseudogap similar to that discussed in this paper \([32, 33]\).

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References

[1] Lee P A, Nagaosa N and Wen X-G 2006 Rev. Mod. Phys. 78 17
[2] Timusk T and Statt B 1999 Rep. Prog. Phys. 62 61
[3] Paramekanti A, Randeria M and Trivedi N 2001 Phys. Rev. Lett. 87 217002
Paramekanti A, Randeria M and Trivedi N 2004 Phys. Rev. B 70 054504
[4] Anderson P W, Lee P A, Randeria M, Trivedi N and Zhang F C 2004 J. Phys.: Condens. Matter 16 R755
[5] Curro N J, Imai T, Slichter C P and Dabrowski B 1997 Phys. Rev. B 56 877
[6] Loram J W, Mirza K A, Cooper J R and Liang W Y 1993 Phys. Rev. Lett. 71 174
[7] Norman M R et al 1998 Nature 392 157
[8] Homes C C, Timusk T, Liang R, Bonn D A and Hardy W N 1993 Phys. Rev. Lett. 71 1645
[9] Randeria M, Trivedi N, Moreo A and Scalettar R T 1992 Phys. Rev. Lett. 69 2001
[10] Emery V J and Kivelson S 1995 Nature 374 434
[11] Park K 2005 Phys. Rev. Lett. 95 027001
Park K 2005 Phys. Rev. B 72 245116
[12] Georges A, Kotliar G, Krauth W and Rozenberg M J 1996 Rev. Mod. Phys. 68 13
[13] Anderson P W 1987 Science 235 1196
[14] Kyung B and Tremblay A-M S 2006 Phys. Rev. Lett. 97 046402
[15] Capone M and Kotliar G 2006 Phys. Rev. B 74 054513
[16] Haule K and Kotliar G 2007 Phys. Rev. B 76 104509
[17] Poilblanc D and Scalapino D J 2002 Phys. Rev. B 66 052513
[18] Ohta Y, Shimozato T, Eder R and Maekawa S 1994 Phys. Rev. Lett. 73 324
[19] Caffarel M and Krauth W 1994 Phys. Rev. Lett. 72 1545
[20] Park K 2009 unpublished
[21] Singh R R P and Scalettar R T 1991 Phys. Rev. Lett. 66 3203
[22] Affleck I, Zou Z, Hsu T and Anderson P W 1988 Phys. Rev. B 38 745
[23] Baskaran G, Zou Z and Anderson P W 1987 Solid State Commun. 63 973
[24] Affleck I and Marston J B 1988 Phys. Rev. B 37 R3774

New Journal of Physics 11 (2009) 073027 (http://www.njp.org/)
[25] Kotliar G and Liu J 1988 Phys. Rev. B 38 5142
[26] Lee P A and Nagaosa N 1992 Phys. Rev. B 46 5621
[27] Lee P A and Wen X-G 1997 Phys. Rev. Lett. 78 4111
[28] Emery V J, Kivelson S A and Zachar O 1997 Phys. Rev. B 56 6120
[29] Millis A J, Monien H and Pines D 1990 Phys. Rev. B 42 167
[30] Maier T, Jarrell M, Pruschke T and Hettler M H 2005 Rev. Mod. Phys. 77 1027
[31] Civelli M, Capone M, Georges A, Haule K, Parcollet O, Stanescu T D and Kotliar G 2008 Phys. Rev. Lett. 100 046402
[32] Capone M, Fabrizio M, Castellani C and Tosatti E 2002 Science 296 2364
[33] Schiró M, Capone M, Fabrizio M and Castellani C 2008 Phys. Rev. B 77 104522