Quantum antiferromagnetism and high $T_C$ superconductivity: a close connection between the $t$-$J$ model and the projected BCS Hamiltonian

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A connection between quantum antiferromagnetism and high $T_C$ superconductivity is theoretically investigated by analyzing the $t$-$J$ model and its relationships to the Gutzwiller-projected BCS Hamiltonian. After numerical corroboration via exact diagonalization, it is analytically shown that the ground state of the $t$-$J$ model at half filling (i.e., the 2D antiferromagnetic Heisenberg model) is entirely equivalent to the ground state of the Gutzwiller-projected BCS Hamiltonian with strong pairing. Combined with the high wavefunction overlap between the ground states of the $t$-$J$ model and the projected BCS Hamiltonian at moderate doping, this equivalence provides strong support for the existence of superconductivity in the $t$-$J$ model. The relationship between the ground state of the projected BCS Hamiltonian and Anderson's resonating valence bond state (i.e., the projected BCS ground state) is discussed.

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I. INTRODUCTION

There are many reasons as to why high $T_C$ superconductivity has attracted so much attention. Aside from the obvious (but very important) prospects for technological applications of high $T_C$ materials, a very salient reason is the mysterious nature of the pairing mechanism. Since the bare electron-electron interaction is strongly repulsive, it seems that there are two ingredients essential to electron pairing: (i) how to overcome the Coulomb repulsion and (ii) how to generate an attraction between quasiparticles.

In “low” $T_C$ superconductivity described well by the standard BCS theory, the pairing mechanism is roughly as follows: Electrons form a Fermi liquid in which the strong Coulomb interaction is renormalized into a screened interaction between dressed quasiparticles which interact very weakly; with the strong repulsion gone, quasiparticles can form pairs through the exchange of phonons, which gives rise to a time-delayed attraction between quasiparticles. This intuition, while valid for standard BCS superconductors, is not correct for high $T_C$ materials.

First, in contrast to low $T_C$ superconductors which are metallic in the normal state, cuprates are insulators at low doping, and thus it is not a priori clear whether high $T_C$ superconductivity in cuprates has anything to do with the Landau-Fermi liquid description of the normal state in metallic systems. In fact, this suspicion is reinforced by many non-Fermi liquid behaviors of cuprates including pseudogap phenomena and stripe excitations. In other words, it is not clear how the strong Coulomb repulsion can be overcome by standard quasiparticle screening mechanisms.

Second, there is a wealth of evidence suggesting that pairing might be induced by a source other than the phonon exchange. While certainly the high energy scale of $T_C$ in the cuprates itself is difficult to explain in terms of the phonon exchange mechanism, probably one of the most persuasive pieces of evidence for a non-phonon pairing mechanism is the destruction of superconductivity (or the strong suppression of $T_C$) when even a small concentration of Cu atoms (in the Copper oxide plane) are replaced by non-magnetic impurities such as Zn. This is very suggestive of pairing with magnetic origin. Also, very important in this context is the $d$-wave symmetry of the gap function, which is explained most naturally in terms of pairing due to magnetic interactions. Therefore, it seems reasonable to assume that magnetic interactions have something to do with high $T_C$ superconductivity. However, the precise relationship between magnetism and high $T_C$ superconductivity is not very well understood; it is not clear exactly how the magnetic interaction generates an attraction between electrons, especially at low doping. Also, from a fundamental point of view, this attraction is very puzzling since, after the phonon-exchange mechanism (i.e., interaction between electrons and ions) is ruled out, it is hard to appreciate how the remaining microscopic interaction could be substantially different from the completely repulsive bare electron-electron interaction.

Despite the seemingly unrelated nature of the above two ingredients, they are, in fact, very closely connected. Specifically, it can be shown that the magnetic (antiferromagnetic, to be precise) interaction is a natural consequence of the strong repulsive interaction between electrons at low doping, a process known as super-exchange. The precise mathematical derivation of super-exchange can be carried out in the framework of model Hamiltonians. To this end, consider the Hubbard model with
repulsive on-site interaction $U$: \[ H_{\text{Hub}} = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) + U \sum_i n_i \downarrow n_i \uparrow \] where $\sigma = \uparrow, \downarrow$ is the spin index, and $\langle i,j \rangle$ indicates that $i$ and $j$ are nearest neighbors. All models studied throughout this paper are defined on the square lattice. It has been shown\(^\text{10,11,12,13}\) that, exactly at half filling, the Hubbard model becomes identical to the antiferromagnetic Heisenberg model in the limit of large $U$: \[ H_J = J \sum_{\langle i,j \rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - n_i n_j/4) \] where $J = 4t^2/U$. $\mathbf{S}_i$ and $n_i$ are, respectively, the spin and the electron-number operators at the site $i$. Physically speaking, the derivation of the Heisenberg model is as follows: The zeroth order effect of $t$ for large $U$ is to completely prevent the double occupancy of any site, thereby minimizing the large on-site interaction energy cost, which, in turn, gives rise to a low-energy Hilbert space in which sites are only singly occupied. This low-energy Hilbert space, however, is hugely degenerate since all states with single occupancy have exactly the same energy. Therefore, one has to investigate the next order effect of $t$. Exactly at half filling, there is no effect first order in $t$ because, when it acts on the degenerate Hilbert space mentioned above, the hopping term in Eq. (1) always creates a doubly occupied site which is outside the low-energy Hilbert space. The antiferromagnetic Heisenberg model emerges through the second-order contribution which is the virtual hopping process (hence, $J \propto t^2/U$). Note that the virtual hopping process minimizes the kinetic energy cost in the presence of the strong on-site Coulomb repulsion.

Away from half filling with addition of holes, the Heisenberg model generalizes to the $t$-$J$ model: \[ H_{t,J} = \hat{\mathcal{P}}_G (H_t + H_J) \hat{\mathcal{P}}_G, \] where $H_J$ is given in Eq. (2) and \[ H_t = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}). \]

The Gutzwiller projection operator, $\hat{\mathcal{P}}_G$, imposes the no-double-occupancy constraint, which handles the strong on-site interaction. It is important to note that, to order $t^2/U$, the rigorous derivation of the $t$-$J$ model from the Hubbard model requires the omission of three-site hopping terms\(^\text{14}\), which can be justified at low doping because the hopping terms have zero matrix elements exactly at half filling and their contribution is roughly proportional to the hole concentration away from half filling. In some sense, there are two small expansion parameters involved in deriving the $t$-$J$ model from the Hubbard model: $t/U$ and the hole concentration, $x$. The three-site hopping terms may become sizable when either parameter is not small.

As shown in the above, antiferromagnetism is a natural consequence of the strong Coulomb repulsion at low doped regimes. This is, of course, consistent with experimental findings that there is a well-defined long-range antiferromagnetic order (also known as Néel order) at low doping. The next question, then, is when and if antiferromagnetism can generate pairing; specifically, whether the $t$-$J$ model contains superconductivity in realistic parameter regimes (with non-zero doping). It is the goal of this paper to provide evidence for the existence for superconductivity in the $t$-$J$ model. To this end, we investigate the connection between the $t$-$J$ model and the Gutzwiller-projected BCS Hamiltonian. Note that the Gutzwiller-projected BCS Hamiltonian is nothing but the BCS Hamiltonian in the presence of the strong on-site repulsion.

The viewpoint advocated in this paper that antiferromagnetism and high $T_C$ superconductivity are intimately connected is shared by many of previous theories including the $SO(5)$ theory\(^\text{15}\). The central hypothesis of the $SO(5)$ theory is that antiferromagnetism and superconductivity are just two different manifestations of a single object called superspin which combines the three-dimensional antiferromagnetic order parameter and the two-dimensional superconducting order parameter. Apart from the phenomenological appeal of this idea, it is crucial from the microscopic point of view that one should be able to derive an effective superspin model from well-known microscopic models such as the $t$-$J$ model in a reliable manner. One of such attempts was to use some form of the renormalization-group transformation\(^\text{15}\). In this paper, however, we take a different approach, as outlined below.

This paper is organized as follows: The precise mathematical form of the Gutzwiller-projected BCS Hamiltonian is given in Sec. \(\text{II}\) where we discuss the physical motivation for studying its connection to antiferromagnetism. We also discuss the relationship between the ground state of the Gutzwiller-projected BCS Hamiltonian and Anderson’s resonating valence bond (RVB) states\(^\text{16}\) (i.e., the Gutzwiller-projected BCS ground state). In Sec. \(\text{III}\) by computing the wavefunction overlap via exact diagonalization in finite systems, we provide evidence suggesting that the ground state of the $t$-$J$ model is closely connected to the ground state of the Gutzwiller-projected BCS Hamiltonian. In particular, we emphasize that, within the limits of numerical accuracy, the ground state of the antiferromagnetic Heisenberg model (i.e., the $t$-$J$ model at half filling) is equivalent to that of the Gutzwiller-projected BCS Hamiltonian with strong pairing. In fact, this equivalence can be derived analytically. In Sec. \(\text{IV}\) we provide an analytic derivation for the equivalence between the Heisenberg model and the Gutzwiller-projected BCS Hamiltonian with strong pairing. We conclude in Sec. \(\text{V}\) by discussing physical implications of the Gutzwiller-projected BCS Hamiltonian.
II. THE GUTZWILLER-PROJECTED BCS HAMILTONIAN

We begin by providing a physical motivation for studying the connection between the $t$-$J$ model and the projected BCS Hamiltonian. For this purpose, it is convenient to write the pairing term of the BCS Hamiltonian in real space:

$$H_{\text{pair}} \equiv c_{i \uparrow} ^ {\dagger} c_{j \downarrow} + c_{i \downarrow} ^ {\dagger} c_{j \uparrow} + \text{H.c.}$$  \hspace{1cm} (5)

which creates a resonance of the singlet pair between the site $i$ and $j$: $| \uparrow_{i} \downarrow_{j} \rangle - | \downarrow_{i} \uparrow_{j} \rangle$. On the other hand, the singlet pair is energetically preferred by the antiferromagnetic exchange term in the $t$-$J$ model: $S_{i} \cdot S_{j}$ for $J > 0$. Therefore, despite their different appearances, the pairing term and the antiferromagnetic exchange term seem to have a similar physical effect; they both prefer singlet pairs (at least, between nearest neighbors). This similarity serves as a motivation to investigate whether there is a connection between the $t$-$J$ model and some form of the BCS Hamiltonian. In this paper, we take the Gutzwiller-projected BCS Hamiltonian$^{17}$:

$$H_{\text{BCS}}^{G} = \mathcal{P}_{G} H_{\text{BCS}} \mathcal{P}_{G}$$

$$= \mathcal{P}_{G} (H_{t} + H_{\Delta}) \mathcal{P}_{G},$$  \hspace{1cm} (6)

where $H_{t}$ is given in Eq. (3). Also, the pairing term is

$$H_{\Delta} = \sum_{\langle i,j \rangle} \Delta_{ij} \left( c_{i \uparrow} ^ {\dagger} c_{j \downarrow} - c_{i \downarrow} ^ {\dagger} c_{j \uparrow} + \text{H.c.} \right)$$  \hspace{1cm} (7)

where we are primarily interested in a pairing with $d$-wave symmetry, where $\Delta_{ij} = \Delta$ if $j = i + \hat{x}$ and $-\Delta$ if $j = i + \hat{y}$. However, we also examine the pairing with extended $s$-wave symmetry, where $\Delta_{ij} = \Delta$ for both $j = i + \hat{x}$ and $i + \hat{y}$, and the Hamiltonian is denoted as $H_{\text{BCS}}^{G}$. Note that $H_{\text{BCS}}^{G}$ in Eq. (6) has a very similar structure as $H_{lJ}$ in Eq. (3). The only change is that $H_{\Delta}$ in $H_{\text{BCS}}^{G}$ replaces $H_{J}$ in $H_{lJ}$, which is motivated by the possible correspondence between the pairing term and the antiferromagnetic exchange term. Note that $H_{t} + H_{\Delta}$ is the usual BCS Hamiltonian in the real space representation, and hence $H_{\text{BCS}}^{G} = H_{t} + H_{\Delta}$.

In order to provide evidence for the close connection between the $t$-$J$ model and the Gutzwiller-projected BCS Hamiltonian, we will pursue two approaches with one being numerical (Sec. III) and the other being analytical (Sec. IV). But, before presenting our results, we would like to briefly discuss the relationship between the ground state of the Gutzwiller-projected BCS Hamiltonian and the RVB state proposed by Anderson$^{16}$, which is just the Gutzwiller-projected BCS ground state:

$$\psi_{\text{RVB}} = \tilde{\mathcal{P}} \psi_{\text{BCS}},$$  \hspace{1cm} (8)

where $\tilde{\mathcal{P}}$ is the previously introduced Gutzwiller projection operator imposing the no-double-occupancy constraint. $\mathcal{P}_{N}$ is the electron-number projection operator which is necessary for constructing states with definite electron number from the BCS ground state, $\psi_{\text{BCS}}$, that has an intrinsic fluctuation in particle number.

In general, $\psi_{\text{RVB}}$ is not the exact ground state of $H_{\text{BCS}}^{G}$ since the Gutzwiller projection does not commute with the BCS Hamiltonian, $H_{\text{BCS}}$: $[\mathcal{P}_{G}, H_{t} + H_{\Delta}] \neq 0$. The difference between $\psi_{\text{RVB}}$ and the ground state of $H_{\text{BCS}}^{G}$ is particularly severe at half filling because, as shown in the later sections, the ground state of $H_{\text{BCS}}^{G}$ has long-range antiferromagnetic order (Néel order) at half filling, while $\psi_{\text{RVB}}$ does not. Since the exact ground state of the $t$-$J$ model has Néel order at half filling, it seems that $\psi_{\text{RVB}}$ cannot be a good ansatz wavefunction for the $t$-$J$ model at least for regimes very close to half filling. This was one of the reasons why $\psi_{\text{RVB}}$ was proposed as a candidate for the ground state of models with sufficiently strong “quantum frustration” (to destroy Néel order), examples of which include models with the next-nearest-neighbor exchange coupling, $J'_{ij}$ and antiferromagnetic models on the triangular lattice$^{16}$. Also, $\psi_{\text{RVB}}$ was conjectured to be a good ansatz wavefunction for the $t$-$J$ model at moderate, non-zero doping. Its validity, however, has remained very controversial even after many years of active research$^{18,19,20,21,22,23,24}$.

The situation is different for the ground state of $H_{\text{BCS}}^{G}$. In addition to the possession of Néel order at half filling, the ground state of $H_{\text{BCS}}^{G}$ also has a very high overlap with the ground state of the $t$-$J$ model at moderate doping (in fact, unity overlap at half filling), as shown in the next section. Therefore, the ground state of $H_{\text{BCS}}^{G}$ can be taken as a good ansatz wavefunction for the ground state of the $t$-$J$ model at general doping. Now, this brings up an interesting question: how is the ground state of $H_{\text{BCS}}^{G}$ related to the RVB state at non-zero doping? In Sec. IV, it is argued that, despite severe differences at half filling, the RVB state is, in fact, qualitatively similar to the ground state of $H_{\text{BCS}}^{G}$ in doped regimes sufficiently away from half filling.

III. NUMERICAL EVIDENCE

In this section, we present numerical evidence for the close connection between the $t$-$J$ model and the Gutzwiller-projected BCS Hamiltonian. While some numerical results are available in a previous paper by the authors$^{17}$, more details are given in this section along with new results. Before we provide detailed evidence, we would like to emphasize two important aspects of the numerical approach used in this paper. The first aspect pertains to the computing technique while the second issue concerns what to compute.

First, we use exact diagonalization as the computing technique. Exact diagonalization offers an unbiased approach, as opposed to other methods with biased assumptions or guesses, which include the large $N$ (or $S$) expansion$^{14,25}$ and variational Monte Carlo simulation$^{18,19,20,21,24}$. Uncontrolled approximations in
techniques mentioned above require an independent verification of the involved assumptions. In contrast, exact diagonalization can determine the exact ground state wavefunction without bias. The problem is, however, that its application is limited to studies of finite systems with relatively small spatial size. This limitation motivates the second aspect of the numerical approach in this paper.

The second aspect of our numerical approach concerns what to compute. In general, evidence for long-range order is provided by relevant correlation functions. In the case of superconductivity, the relevant correlation function is the pairing correlation function:

\[
F_{\alpha\beta}(r - r') = \langle c^\dagger_r c^\dagger_{r'} (r + \alpha) c^\dagger_{r'} c_r (r' + \beta) \rangle, \tag{9}
\]

where \(\alpha, \beta = \hat{x}, \hat{y}\). True off-diagonal long-range order (ODLRO) can be claimed only when \(F_{\alpha\beta}\) remains non-zero in the limit of large distance \(|r - r'|\). Unfortunately, however, the small spatial size of finite systems accessible via exact diagonalization makes the distinction between true long-range order and short-range order (present even in normal states) ambiguous. Therefore, a measure of pairing order that is unambiguous even in finite system studies is needed.

An inspiration comes from the fractional quantum Hall effect (FQHE), where our understanding of the subject is significantly advanced by the direct comparison between ansatz wavefunctions and exact states. It is well accepted by now that all essential aspects of the FQHE are explained by the composite fermion (CF) theory, which is a general theory of the FQHE including the Laughlin states as a subset. While there are various (both experimental and theoretical) verifications of the composite fermion theory, arguably the most significant is the amazing agreement between the exact ground state and the CF wavefunction: the overlap is practically unity for various short-range interactions including the Coulomb interaction. Indeed, as was crucial in establishing the CF theory for the FQHE, we would in turn like to achieve the same methodological clarity for the \(t-J\) model.

In order to give a perspective on the significance of wavefunction overlap in finite system studies, consider two randomly-chosen states in a Hilbert space with \(N_{\text{basis}}\) basis states. Then, the possibility for having a large wavefunction overlap between those two states is roughly \(1/N_{\text{basis}}\). So, roughly speaking, if the square of the overlap between an ansatz state and the exact state is significantly higher than \(1/N_{\text{basis}}\), it can be argued that the ansatz state is a good representation of the exact state. The main finite system studied in this paper is the \(4 \times 4\) square lattice system, whose Hilbert space has \(10^3 - 10^5\) basis states depending on the number of holes (even after translational symmetries are implemented as reported in this paper). Therefore, in our system, the possibility for having a large wavefunction overlap between two random states by chance is roughly 0.1% - 0.001%. We will show in the following sections that the square of the overlap between the ground states of the \(t-J\) model and the Gutzwiller-projected BCS Hamiltonian is very close to unity at optimal parameter ranges (typically 90% - 100% depending on parameters).

While it may seem straightforward at first to compute wavefunction overlap by exactly diagonalizing the \(t-J\) model and the Gutzwiller-projected BCS Hamiltonian, there is a subtle, but physically important twist in applying exact diagonalization to the BCS Hamiltonian. The subtlety arises from the fact that there is a (coherent) fluctuation in particle number due to the pairing term in \(H_\text{BCS}\) which has matrix elements mixing the Hilbert space of \(N_e\) and \(N_e \pm 2\) electrons. In order to incorporate the particle-number fluctuation into finite system studies, we diagonalize \(H_{\text{BCS}}^\text{Gutz}\) in the combined Hilbert space of \(N_e\) and \(N_e \pm 2\) electrons, which, in turn, invariably requires a careful treatment of the chemical potential. In essence, the chemical potential is adjusted so that the kinetic energy plus the chemical potential energy of the \(N_e\) particle ground state is the same as that of the \(N_e \pm 2\) particle ground state. Once the chemical potential is set this way, the mixing with other particle-number sectors such as the \(N_e + 2\) and \(N_e \pm 4\) sectors can be shown to be negligibly small, even if it is allowed. For more details, readers are referred to discussions in the following sections.

Finally, the following notations are defined for future convenience: \(\psi_{\text{BCS}}^{G}(N_h, N_h + 2|N)\) denotes the ground state of the Gutzwiller-projected BCS Hamiltonian obtained from the combined Hilbert space of \(N_h\) and \(N_h + 2\) holes in the system of \(N\) sites. (Note that the sum of the number of electrons and holes equals the number of sites: \(N_e + N_h = N\)). \(\bar{P}_{N_h=N_0}\) denotes the number projection operator which projects states onto the Hilbert space of states with \(N_0\) holes, and renormalizes the projected states. \(\psi_{t-J}(N_h|N)\) is the exact ground state of the \(t-J\) model in the Hilbert space of \(N_h\) holes in \(N\) sites.

Numerical evidence for the close connection between the ground states of the \(t-J\) model and the Gutzwiller-projected BCS Hamiltonian is presented as follows: In Sec. 14A the symmetry of the Gutzwiller-projected BCS Hamiltonian with \(d\)-wave pairing is discussed. Then, the wavefunction overlap between \(\psi_{t-J}(N_h|N)\) and the appropriately number-projected \(\psi_{\text{BCS}}^{G}(N_h, N_h + 2|N)\) is computed in Sec. 14B for the case of undoped regime, which is followed by similar calculations in Sec. 14C for the optimally doped regime, and in Sec. 14D for the overdoped regime.

A. Symmetry

In general, before solving any Hamiltonian, one has to examine the symmetry of the Hamiltonian. Incorporating symmetry is particularly important when two different Hamiltonians are compared since it is possible for their ground states to have completely different symmetries from each other. The BCS Hamiltonian with \(d\)-wave pairing is particularly tricky in this respect because (i)
it does not conserve the particle number and (ii) it is not invariant under diagonal reflection, i.e., $x \leftrightarrow y$ (or, equivalently, under rotation in space by $\pi/2$). Therefore, it does not conserve parity with respect to diagonal reflection. Surprisingly, however, the effects of the above two properties cancel and can be eliminated simultaneously by applying the number projection operator to the ground state of the Gutzwiller-projected BCS Hamiltonian, as explained below. (As far as parity is concerned, it is not important whether the BCS Hamiltonian is Gutzwiller-projected; the Gutzwiller projection commutes with diagonal reflection.)

First, the non-conservation of particle number is, of course, a direct consequence of the pairing term in the BCS Hamiltonian, $c_d^\dagger c_d + c_d c_d^\dagger$. At first glance, the uncertainty in particle number may seem as a theoretical artifact in the BCS Hamiltonian. But, the coherent fluctuation in particle number is essential for superconductivity since it is vital to the superfluid phase coherence. (The coherent fluctuation in superconductors stands in sharp contrast with the incoherent fluctuation in thermodynamic ensembles.) On the other hand, when a precise comparison with number eigenstates (such as the ground state of the $t$-$J$ model) is required, the ground state of the BCS Hamiltonian should be projected onto the Hilbert space of states with a definite particle number. The number projection operator, $\mathcal{P}_N$, performs this task.

Second, the non-conservation of parity with respect to diagonal reflection is due to the sign difference in space of states with a definite particle number. The relative sign difference between distinct Hilbert spaces does not alter the hopping term since $H_d$ does not mix Hilbert spaces with different particle numbers.

Now, let $\hat{R}_d$ act on both sides of Eq.(12):

$$\hat{R}_d H_{BCS}^G(t, \Delta) \hat{R}_d = H_{BCS}^G(t, -\Delta)$$

where $\hat{R}_d$ is the diagonal reflection operator and $H_{BCS}^G(t, \Delta)$ is the Gutzwiller-projected BCS Hamiltonian given in Eq.(9) with the dependence on $t$ and $\Delta$ shown explicitly. Note the sign change of $\Delta$ in $H_{BCS}^G$ in the right-hand side of Eq.(11). Now, for convenience, Eq.(11) is re-written as follows:

$$\hat{R}_d H_{BCS}^G(t, \Delta) \hat{R}_d = H_{BCS}^G(t, -\Delta) \hat{R}_d$$

(11)

since $\hat{R}_d^2 = 1$. What we want to prove in this section is that a number-projected eigenstate of $H_{BCS}^G$ is also a parity eigenstate.

We begin by defining $|\Psi\rangle$ as an eigenstate of $H_{BCS}^G(t, \Delta)$:

$$H_{BCS}^G(t, \Delta)|\Psi\rangle = E|\Psi\rangle.$$  

(12)

Also, for convenience, let us write $|\Psi\rangle$ in vector form showing amplitudes in each individual particle-number sector. That is,

$$|\Psi\rangle = \left(\cdots, C_\alpha^{N_e}, \cdots, C_\beta^{N_e+2}, \cdots\right),$$  

(13)

where $C_\alpha^{N_e}$ is the amplitude for the $\alpha$-th basis element in the $N_e$-particle Hilbert space. Similarly, $C_\beta^{N_e+2}$ is the amplitude for the $\beta$-th basis element in the $N_e+2$ particle Hilbert space.

Now, it is not too difficult to show that

$$H_{BCS}^G(t, -\Delta)|\tilde{\Psi}\rangle = E|\tilde{\Psi}\rangle,$$

(14)

where $E$ is the same energy as in Eq.(12) and

$$\langle \tilde{\Psi} | = \left(\cdots, -|N_e\rangle C_\alpha^{N_e}, \cdots, -|N_e+2\rangle C_\beta^{N_e+2}, \cdots\right).$$

(15)

where $N_e$ is restricted to even numbers since we are interested only in paired states. What accounts for the form of Eq.(14) is that the pairing term, $H_\Delta$, always mixes the Hilbert spaces with particle numbers differing by two. Attaching the relative sign according to the particle number (i.e., $-|N_e\rangle$ and $-|N_e+2\rangle$ for $N_e$ and $N_e+2$ Hilbert space, respectively) is tantamount to changing the sign of $\Delta$ in $H_\Delta$. Note that a relative sign difference between distinct Hilbert spaces does not alter the hopping term since $H_d$ does not mix Hilbert spaces with different particle numbers.

Now, let $\hat{R}_d$ act on both sides of Eq.(12):

$$\hat{R}_d H_{BCS}^G(t, \Delta) |\Psi\rangle = E\hat{R}_d |\Psi\rangle,$$

(16)

which, with aids of Eq.(11), becomes

$$H_{BCS}^G(t, -\Delta) \hat{R}_d |\Psi\rangle = E\hat{R}_d |\Psi\rangle.$$  

(17)

Then, by comparing Eq.(14) and (17), one is able to conclude that

$$\hat{R}_d |\Psi\rangle = \lambda |\tilde{\Psi}\rangle,$$

(18)

where $\lambda$ is a constant which is almost (though not quite yet) an eigenvalue. After acting on both sides by $\mathcal{P}_{N=N_e}$, the above equation becomes

$$\hat{R}_d \mathcal{P}_{N=N_e} |\Psi\rangle = \lambda' \mathcal{P}_{N=N_e} |\tilde{\Psi}\rangle.$$  

(19)

(Note that $\mathcal{P}_{N}$ commutes with $\hat{R}_d$. Also, there is no loss of generality in choosing $N = N_e$.) Moreover, since

$$\mathcal{P}_{N=N_e} |\tilde{\Psi}\rangle = (-1)^{\frac{N_e}{2}} \mathcal{P}_{N=N_e} |\Psi\rangle,$$

(20)

Eq.(19) becomes

$$\hat{R}_d \mathcal{P}_{N=N_e} |\Psi\rangle = \lambda' \mathcal{P}_{N=N_e} |\Psi\rangle,$$

(21)

where $\lambda' = (-1)^{\frac{N_e}{2}} \lambda$. Consequently, $\mathcal{P}_{N} |\Psi\rangle$ is an eigenstate of the parity with respect to the diagonal reflection.

Until now, only the spatial symmetry has been investigated. (Note that $H_{BCS}^G$ is invariant under the spatial translation, and therefore linear momentum is conserved.) Now, we would like to briefly consider spin rotation symmetry. The hopping term is obviously invariant under spin rotation. In addition, the pairing term can be also shown to be invariant under the spin rotation: $[H_\Delta, S_{\text{tot}}] = 0$ where the total spin is $S_{\text{tot}} = \sum_i S_i$. The essential physics of the spin-rotational invariance of the pairing term is the fact that $H_\Delta$ concerns only spin-singlet pairs, which are rotationally invariant.
B. Undoped regime (half filling)

In this section, we provide numerical evidence indicating that, at half filling, the ground state of the Gutzwiller-projected BCS Hamiltonian is actually equivalent to the ground state of the t-J model in the limit of strong pairing, i.e., $\Delta/t \to \infty$. To this end, the wavefunction overlap between the two ground states is computed as a function of $\Delta/t$ via a modified Lanczos method for exact diagonalization. Note that the ground state of the t-J model is uniquely determined at half filling without any dependence on $J/t$, while the ground state of the Gutzwiller-projected BCS Hamiltonian depends on $\Delta/t$. The reason for the former is that, at half filling, the t-J model becomes the antiferromagnetic Heisenberg model where $J$ is just an overall scale factor.

As mentioned previously, the main finite system studied in this paper is the $4 \times 4$ square lattice system with periodic boundary conditions. The $4 \times 4$ system is one of the most studied systems in numerical treatments because it is accessible via exact diagonalization, yet large enough to contain essential many-body correlations. We have checked that our results for the t-J model are in complete agreement with previous numerical studies for all available cases. Using notations defined earlier in Sec. III, the ground state of the t-J model is denoted as $\psi_{t-J}(0|16)$ for half filling: 0 holes (16 electrons) in the $4 \times 4$ system. Also, the ground state of the Gutzwiller-projected BCS Hamiltonian at half filling is obtained by applying $\mathcal{P}_{N_h=0}$ to $\psi_{BCS}^G(0,2|16)$. Note that $\psi_{BCS}^G(0,2|16)$ is the ground state of the combined Hilbert space of 0 and 2 holes (16 and 14 electrons, respectively) in the $4 \times 4$ system.

At half filling, the overlap between the ground states of the t-J model and the Gutzwiller-projected BCS Hamiltonian is given by $\langle \psi_{t-J}(0|16)|\mathcal{P}_{N_h=0}\psi_{BCS}^G(0,2|16) \rangle$, the square of which is plotted in Fig. 1 as a function of $\Delta/t$. As one can see from Fig. 1, the overlap is very high even for $\Delta/t \approx 1$, and saturates very quickly to unity as $\Delta/t$ increases further. For sufficiently large values of $\Delta/t$, the overlap is indistinguishable from unity to within numerical accuracy (We have actually studied $\Delta/t$ values ranging as high as 1000). Therefore, as far as our finite system is concerned, the ground state of the Gutzwiller-projected BCS Hamiltonian is exactly identical to the ground state of the t-J model in the limit of strong pairing, i.e., $\Delta/t \to \infty$. In view of the fact that there are roughly $10^3$ basis states in the Hilbert space for the $4 \times 4$ system at half filling even after translational symmetries are implemented, the high overlap is particularly salient. We have also checked that the above result also holds in the 4-site ($2 \times 2$) and the 10-site ($\sqrt{10} \times \sqrt{10}$) systems. It should be emphasized that the equivalence between the ground state of the t-J model and that of the projected BCS Hamiltonian with strong pairing does not necessarily mean strong superconductivity since, despite strong pairing, there is little charge fluctuation near half filling, and therefore little phase coherence.

The equivalence between the ground states of the projected BCS Hamiltonian and the t-J model at half filling has a very important physical implication for the origin of high $T_C$ superconductivity supporting a long-standing conjecture. The conjecture is that electrons are already paired at half filling, and therefore form a condensate. However, electrons cannot superconduct (or, for that matter, even conduct) at half filling because there is no room for them to travel. But, away from half filling, it seems natural that removing some fraction of electrons (i.e., doping) may trigger superconductivity by mobilizing electrons (and also causing charge fluctuations).

C. Optimally doped regime

In this section, we present numerical results for the wavefunction overlap between the ground states of the projected BCS Hamiltonian and the t-J model at a moderate, non-zero doping. Specifically, we study the situation in which there are 2 holes in the $4 \times 4$ system, which roughly corresponds to the optimally doped regime. Using notations defined earlier, the overlap is given by $\langle \psi_{t-J}(2|16)|\mathcal{P}_{N_h=2}\psi_{BCS}^G(0,2|16) \rangle$ for the Hilbert space with 2 holes. An alternative representation of the overlap for this Hilbert space can be obtained from $\langle \psi_{t-J}(2|16)|\mathcal{P}_{N_h=2}\psi_{BCS}^G(2,4|16) \rangle$ which, however, leads to essentially the same conclusion, as shown later in this section.

Fig. 2 displays square of the overlap defined by $|\langle \psi_{t-J}(2|16)|\mathcal{P}_{N_h=2}\psi_{BCS}^G(0,2|16) \rangle|^2$. Note that the overlap now is a function of two parameters: $\Delta/t$ for the projected BCS Hamiltonian and $J/t$ for the t-J model. For better visualization, a three-dimensional plot of the overlap is also given in Fig. 3. As shown in Fig. 2 and...
Fig. 2: Square of the overlap between the ground states of the $t$-$J$ model and the projected BCS Hamiltonian in the $4 \times 4$ system with 2 holes (which roughly corresponds to the optimally doped regime).

Fig. 3: Three-dimensional plot for the square of the overlap as a function of $\Delta/t$ and $J/t$ in the $4 \times 4$ system with 2 holes. While this plot is essentially the same as Fig. 2, the existence of two distinct regions of high overlap is more easily visualized.

Fig. 4: Square of the overlap for the $4 \times 4$ system with 2 holes, which is in the same regime as Fig. 2. But, the ground state of the projected BCS Hamiltonian in this plot, $\mathcal{P}_{N_h=2}|\psi^G_{BCS}(2,4|16)\rangle$, is obtained from the combined Hilbert space of 2 and 4 holes in the $4 \times 4$ system, as opposed to the combined Hilbert space of 0 and 2 holes in Fig. 2. It is important to note that qualitative features of this plot are basically identical to Fig. 2 while there are some quantitative differences.

There are two distinct regimes of high overlap: a weak-coupling regime ($J/t \lesssim 0.08$ and $\Delta/t \lesssim 0.1$) and a strong-coupling regime ($J/t \gtrsim 0.08$ and $\Delta/t \gtrsim 0.1$). These two regimes are qualitatively different in the sense that the symmetry of the ground states with respect to a spatial rotation by $\pi/2$ changes from $s$-wave to $d$-wave at the boundary $J/t \simeq 0.08$ for the ground state of the $t$-$J$ model, and at the boundary $\Delta/t \simeq 0.1$ for the ground state of the projected BCS Hamiltonian. Note that, in a similar fashion for the case of parity with respect to diagonal reflection, the angular momentum associated with spatial rotation by $\pi/2$ can be shown to be conserved in the BCS Hamiltonian with $d$-wave pairing. Note also that, because of the symmetry change, the overlap in the regime defined by $J/t \gtrsim 0.08$ and $\Delta/t \lesssim 0.1$ is precisely zero.

The high overlap in the weak-coupling regime is rather trivial because, in this regime, both the projected BCS Hamiltonian and the $t$-$J$ model Hamiltonian are reduced basically to the same Hamiltonian which is just the hopping Hamiltonian, $H_0$, with the Gutzi"{u}ller projection; hence, we regard the equivalence at small $J/t$ and $\Delta/t$ as a self-consistency check for the techniques used in this paper. The high overlap in the strong-coupling regime, on the other hand, cannot be trivially explained. As seen in Fig. 2, the maximum value of the overlap (as a function of $\Delta/t$) approaches unity as $J/t$ increases, which can be also seen in Fig. 3 in the form of a rising ridge as $J/t$ increases. The high overlap in the strong-coupling regime is therefore not accidental, but rather is connected to the unity overlap in the limit of strong coupling, which is in turn due to an intrinsic connection between antiferromagnetism and superconductivity.

Finally, as mentioned before, we study the overlap defined by $\langle \psi(t,J)(2|16)|\mathcal{P}_{N_h=2}|\psi^G_{BCS}(2,4|16)\rangle$. This alternative definition is also valid because the ground state of the projected BCS Hamiltonian can be obtained in two different ways: one can apply $\mathcal{P}_{N_h=2}$ either to the ground state of the combined Hilbert space of 0 and 2 holes, or to that of the combined Hilbert space of 2 and 4 holes. While, strictly speaking, these two definitions become identical only in the thermodynamic limit, it would be an assuring self-consistency check of our approach if they produce similar results even in the finite system studies that we study. We find that this is indeed the case. Fig. 4 depicts $|\langle \psi(t,J)(2|16)|\mathcal{P}_{N_h=2}|\psi^G_{BCS}(2,4|16)\rangle|^2$ showing that the essential features are basically identical to those in Fig. 2 while there are some minor quantitative differences.
D. Overdoped regime

We now present numerical results for the case of 4 holes in the $4 \times 4$ system, which roughly corresponds to an overdoped regime. In this regime, it is not strictly appropriate to regard the $t$-$J$ model as the large-$U$ limit of the Hubbard model due to the omission of three-site hopping terms mentioned in the introduction. Experimentally, however, superconductivity is weakened and eventually destroyed as the hole concentration increases. Hence, it is natural to expect that the overlap between the ground states of the projected BCS Hamiltonian and the $t$-$J$ model becomes small in this regime. We show in Fig. 5 that this trend does indeed occur.

Fig. 5 displays $|\langle \psi_{t,J}(4|16)|\hat{P}_{\text{NS}}|\psi_{\text{BCS}}^{G}(2,4|16)\rangle|^2$, which shows that the overlap is, in general, negligibly small except for the trivial case of $J/t = 0$ and $\Delta/t = 0$. Therefore, in the overdoped regime, the ground state of the projected BCS Hamiltonian is no longer a good representation of the ground state of the $t$-$J$ model.

IV. ANALYTIC DERIVATION OF THE EQUIVALENCE AT HALF FILLING

It has been shown numerically in the previous section that, at half filling, the ground state of the Gutzwiller-projected BCS Hamiltonian is equivalent to the exact ground state of the $t$-$J$ model in the limit of strong pairing, i.e., $\Delta/t \rightarrow \infty$. While the numerical evidence is quite strong (the overlap between the two ground states is indistinguishable from unity to within numerical accuracy), questions regarding the validity of finite-system studies linger: especially, whether the overlap is actually equal to unity, or just very close to unity. If only the latter is true, the overlap will diminish and will eventually vanish as the system size increases.

We emphasize that, even if it is true that the overlap does vanish in the thermodynamic limit, the high wavefunction overlap for the finite system still provides strong support for the ansatz wavefunction by demonstrating that it contains the correct physics. This situation is, in fact, very similar to what happens in the FQHE: the overlap between the Laughlin wavefunction (the CF wavefunction, in general) and the exact ground state of the Coulomb interaction decreases as the system size increases, and eventually vanishes in the thermodynamic limit. The vanishing overlap in the thermodynamic limit is an inevitable consequence of the fact that the two ground states are not precisely identical. For example, while the Laughlin state at the lowest-Landau-level filling factor $\nu = 1/3$ is the exact ground state of the short-range interaction given by $\nabla^2 \delta(r)^{11-12}$, it is still an approximation for the exact ground state of the Coulomb interaction (relevant for experiments) albeit an extremely good one.

In this paper, it will be shown that the overlap at half filling is actually unity in the strong-pairing limit; in other words, we will prove that, at half filling, the ground state of the Gutzwiller-projected BCS Hamiltonian with strong pairing is identical to the ground state of the Heisenberg model. We will also prove a stronger statement that the two Hamiltonians do not merely share the same ground state, but also have in common the same low-energy physics. Note that the Hamiltonian for the Heisenberg model is $H_J$ in Eq. (2) and the Gutzwiller-projected BCS Hamiltonian with strong pairing is given by $H_{\text{BCS}}^G$ in Eq. (4) with $t = 0$, which is nothing but $H_\Delta$ with the Gutzwiller projection:

$$H_\Delta^G = \hat{P}_G \left[ \sum_{\langle i,j \rangle} \Delta_{ij} (c^\dagger_{i \uparrow} c^\dagger_{j \downarrow} - c^\dagger_{i \downarrow} c^\dagger_{j \uparrow} + \text{H.c.}) \right] \hat{P}_G. \quad (22)$$

Note that the strong-coupling limit, i.e. the large-$\Delta/t$ limit, is equivalent to the situation in which $t = 0$ since $t/\Delta = 0$ is not a singular point.

A. Gutzwiller projection as the large-$U$ limit and Lieb’s theorem

We begin our analytic derivation for the equivalence at half filling by writing the BCS Hamiltonian with finite, repulsive on-site interaction $U$:

$$H_{\text{BCS}+U}(t, \Delta_0) = H_t + H_{\Delta_0} + U \sum_i n_{i \uparrow} n_{i \downarrow}, \quad (23)$$

where $H_t$ is defined in Eq. (1). It is very important to note that $H_{\Delta_0}$ is given in Eq. (4) with a bare pairing amplitude, $\Delta_0$, instead of a fully renormalized pairing amplitude, $\Delta$. The relationship between $\Delta_0$ and $\Delta$ should become clear at the end of the analytic derivation: we mention in advance, however, that $\Delta \propto \Delta_0^2/U$. 

FIG. 5: Square of the overlap between the ground states of the $t$-$J$ model and the projected BCS Hamiltonian in the $4 \times 4$ system with 4 holes (which roughly corresponds to an overdoped regime).
Our study of $H_{\text{BCS+U}}$ is motivated by the fact that, in the large-$U$ limit, $H_{\text{BCS+U}}$ reduces to the Gutzwiller-projected BCS Hamiltonian. In addition, treating the Gutzwiller projection as the large-$U$ limit instead of working directly with the projection facilitates the analysis. Motivated by numerical studies given in the previous section, we are particularly interested in $H_{\text{BCS+U}}$ with strong pairing:

\[
H_{\Delta_0+U} = H_{\text{BCS+U}}(t = 0, \Delta_0) = H_{\Delta_0} + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{24}
\]

which, in the large-$U$ limit, becomes $H^G_{\Delta}$ in Eq. 22. What we strive to prove is that, in the limit of large $U/\Delta_0$, $H_{\Delta_0+U}$ has exactly the same low-energy physics (i.e., the same ground state and the same low-energy excitations) as the Hubbard model, $H_{\text{Hub}}$, in the limit of large $U/t$. This, in turn, means that the low-energy physics is identical for both $H_{\Delta}$ and $H_J$ since $H_{\text{Hub}}$ becomes $H_J$ in the large-$U/t$ limit.

It is important to note a subtle, but very crucial difference between the large-$U$ behavior of the Hubbard model and that of the strong-pairing Gutzwiller-projected BCS Hamiltonian. To appreciate this distinction, let us rewrite the Hamiltonian for the Hubbard model as follows:

\[
H_{\text{Hub}} = H_t + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_{\text{BCS+U}}(t, \Delta_0 = 0), \tag{25}
\]

which shows that $H_{\text{Hub}}$ is a special case of $H_{\text{BCS+U}}$ with $\Delta_0 = 0$, while $H_{\Delta+U}$ was also a special case of $H_{\text{BCS+U}}$ but with $t = 0$. Hence, there is a parallel between $H_{\text{Hub}}$ and $H_{\Delta+U}$. Specifically, the equivalence between the low-energy physics of $H^G_{\Delta}$ and $H_J$ can be recast as the equivalence between the low-energy physics of two different parameter points (i.e., between those of $t/\Delta_0 = 0$ and $t/\Delta_0 = \infty$) of the same Hamiltonian, $H_{\text{BCS+U}}(t, \Delta_0)$, in the large-$U$ limit.

In fact, it has been shown by Affleck et al.\textsuperscript{33} that two apparently very different mean-field solutions of the half-filled Hubbard model are actually equivalent. The first mean-field solution is considered by Baskaran, Zou, and Anderson\textsuperscript{34} as well as by Ruckenstein, Hirschfeld, and Appel\textsuperscript{35} and later by Kotliar\textsuperscript{36}, who performed a quadratic factorization of $H_J$ assuming that $\langle c_{i\uparrow} c_{j\downarrow} \rangle \neq 0$ and $\langle c_{i\sigma} c_{j\sigma} \rangle = 0$ for nearest neighbor $i$ and $j$. On the other hand, the second mean-field solution, considered by Affleck and Marston\textsuperscript{37}, assumes the opposite situation: $\langle c_{i\uparrow} c_{j\downarrow} \rangle = 0$ and $\langle c_{i\sigma} c_{j\sigma} \rangle \neq 0$. It thus seems that the mean-field solution with $\langle c_{i\uparrow} c_{j\downarrow} \rangle \neq 0$ and $\langle c_{i\sigma} c_{j\sigma} \rangle = 0$, which corresponds to $H_{\text{BCS+U}}$ with $t = 0$, is equivalent to that with $\langle c_{i\uparrow} c_{j\downarrow} \rangle = 0$ and $\langle c_{i\sigma} c_{j\sigma} \rangle \neq 0$, which corresponds to $H_{\text{BCS+U}}$ with $\Delta_0 = 0$. In this paper, we prove that a stronger equivalence, not just between mean-field solutions, but also between the exact ground state of $H_{\text{BCS+U}}$ with $t = 0$ and with $\Delta_0 = 0$. We, however, emphasize that, despite their success in mean-field theory, approaches based on unitary transformations are not applicable in the exact treatment due to the fundamental difference in the large-$U$ behavior of $H_{\text{Hub}}$ and $H_{\Delta_0+U}$, which is discussed in greater detail below.

Consider the effect of a large $U$ in $H_{\text{Hub}}$. In this situation, the zeroth-order effect of $H_t$ corresponds to keeping only the on-site repulsion term, in which case the ground state energy is exactly the same for arbitrary spin configurations as long as there is a single electron per site. Therefore, there is a huge $2^N$ degeneracy in the low-energy Hilbert space which is, in fact, the Gutzwiller-projected space. Now, let us investigate the next order effect in the Gutzwiller-projected space. The first-order effect of $H_t$ does not contribute to the Gutzwiller-projected space since, at half filling, the hopping term always creates a doubly occupied site taking the state beyond the Gutzwiller-projected space. In other words, exactly at half filling,

\[
\hat{\mathcal{P}}_G H_t \hat{\mathcal{P}}_G = 0. \tag{26}
\]

The antiferromagnetic Heisenberg model, $H_J$, arises from the second-order virtual hopping processes.

Next, we consider the effect of a large $U$ in $H_{\Delta_0+U}$. The zeroth-order effect of $H_{\Delta_0}$ is, of course, the same as that of $H_t$ in $H_{\text{Hub}}$: the Gutzwiller-projected space is the low-energy Hilbert space. In contrast to $H_{\text{Hub}}$, however, there is a non-zero first-order effect of pairing term:

\[
H^G_{\Delta} = \hat{\mathcal{P}}_G H_{\Delta} \hat{\mathcal{P}}_G, \tag{27}
\]

where $\Delta$ is renormalized from the bare value $\Delta_0$. Physically speaking, the strong-pairing BCS Hamiltonian sets up the pairing resonance directly instead of by virtual processes. Therefore, it is not a priori clear why or if $H^G_{\Delta}$ has the same low-energy physics as $H_J$. In fact, the above real v.s. virtual contrast suggests that, if it exists, the equivalence between the low-energy physics of $H^G_{\Delta}$ and $H_J$ cannot be derived via a simple unitary transformation of the Hamiltonian. Instead, the equivalence must be connected to intricate physics.

An essential point is that the large-$U$ behavior of $H_{\Delta_0+U}$ and $H_{\text{Hub}}$ can be dealt with systematically in our approach where we analyze finite-$U$ models and take the large-$U$ limit as the Gutzwiller projection. There is no singular behavior in the large-$U$ limit of $H_{\Delta_0+U}$ (because $H^G_{\Delta}$ is non-zero). However, it is not obvious whether the ground state of the antiferromagnetic Heisenberg model is adiabatically connected to those of the Hubbard model with finite $U$. In fact, it can be proven by Nagaoka's theorem\textsuperscript{38} that, infinitesimally away from half filling, the ground state of the Gutzwiller-projected hopping term, $\hat{\mathcal{P}}_G H_t \hat{\mathcal{P}}_G$, (which, in a naive sense, is the large-$U$ limit of the Hubbard model) is ferromagnetic rather than antiferromagnetic. Therefore, one should be careful in how one takes this limit. Fortunately, there is a theorem by Lieb\textsuperscript{39} showing that the ground state of the Hubbard model is uniquely determined at any positive $U$ and, as
a corollary, the ground state in the large-$U$ limit is adiabatically connected to those of finite $U$. Therefore, the ground state of the antiferromagnetic Heisenberg model is adiabatically connected to ground states of the Hubbard model for which $U$ is finite. (We assume that this connection is also valid for low-energy excitations.)

We now present our analytic derivation step by step beginning with an outline summarizing each step: (i) We begin by separating $H_{\Delta_0+U}$ and $H_{\text{Hub}}$ into two parts: the saddle-point Hamiltonian ($H_{\Delta_0+U}$ and $H_{\text{Hub}}$, respectively) and the remaining Hamiltonian incorporating fluctuations around the saddle-point solution ($\delta H_{\Delta_0+U}$ and $\delta H_{\text{Hub}}$, respectively). The saddle-point Hamiltonian is chosen so as to capture a possible singular effect of the spin-density-wave (SDW) instability at $(\pi, \pi)$, which is inherent in $H_{\Delta_0}$ and $H_t$ in the presence of repulsive on-site interactions with arbitrary strength.

(ii) The ground states of $H_{\Delta_0+U}$ and $H_{\text{Hub}}$ are obtained for a general $U$. It is shown that, in both cases, the saddle-point ground state is separated from other excited states by an energy gap proportional to $U$ when $U$ is large. It is also shown that these two saddle-point ground states become identical in the large-$U$ limit. We denote this saddle-point ground state in the large-$U$ limit as $|\psi_0\rangle$.

(iii) In the large-$U$ limit, the low-energy Hilbert space for the full Hamiltonian (including the saddle-point and fluctuation part) is composed of only states that are connected to $|\psi_0\rangle$ via rigid spin rotations, $\{R_i\}$. We denote these states as $\{|\psi_i\rangle\}$. Then, we show that in the large-$U$ limit, all matrix elements of $\delta H_{\Delta_0+U}$ and $\delta H_{\text{Hub}}$ are precisely the same in the low-energy Hilbert space with the same being true for the matrix elements of the two saddle-point Hamiltonians.

(iv) Having shown that all matrix elements in the low-energy Hilbert space are precisely the same in the large-$U$ limit, we argue that the strong-pairing Gutzwiller-projected BCS Hamiltonian and the 2D antiferromagnetic Heisenberg model have identical low-energy physics. The situation is depicted schematically in Fig. 6.

Finally, the above discussion provides physical insight as to why the ground state of the Gutzwiller-projected BCS Hamiltonian is fundamentally different from Anderson’s RVB state at half filling. The difference originates from the singularity due to the SDW instability which occurs at half filling. This singularity cannot be captured by applying the Gutzwiller projection to the BCS wavefunction which, as constructed, intrinsically lacks long-range antiferromagnetic order. In fact, generally, no long-range order can be generated by applying local operators to states without long-range order. On the other hand, long-range antiferromagnetic order is fully captured in the ground state of the Gutzwiller-projected BCS Hamiltonian, as shown in the analytic derivation. It has been shown in numerical studies that the semi-classical Néel configuration has a finite weight in the ground state of the Gutzwiller-projected BCS Hamiltonian. Despite the difference at half filling, however, we argue in Sec. that, sufficiently away from half filling, the ground state of the Gutzwiller-projected BCS Hamiltonian is, in fact, intimately related to the RVB state.

B. Step (i)

It is well known that the nesting property of the Fermi surface at half filling induces an instability toward long-range antiferromagnetic order (i.e., Néel order) in the ground state of the Hubbard model. Nesting is mathematically defined as follows:

$$\epsilon_k = -\epsilon_{k+Q},$$  \hspace{1cm} (28)

where $\epsilon_k = -2t(\cos k_x + \cos k_y)$ is the kinetic energy due to hopping, $Q = (\pi, \pi)$ is the nesting vector. The strong-pairing BCS Hamiltonian with $d$-wave pairing symmetry has precisely the same nesting property for the gap function:

$$\Delta_k = -\Delta_{k+Q},$$  \hspace{1cm} (29)

where $\Delta_k = 2\Delta_0(\cos k_x - \cos k_y)$ is the gap function for $d$-wave pairing. Therefore, in analogy with the Hubbard model, the nesting property of $\Delta_k$ generates a SDW instability at $(\pi, \pi)$. Note that, for both Hamiltonians, the chemical potential is set to zero at half filling. Away from half filling, the chemical potential becomes non-zero, in which case the perfect nesting is ruined and the SDW instability disappears.

In order to study spin orders, it is convenient to re-write the on-site interaction Hamiltonian in terms of spin
operator, $S_i = \frac{1}{2} c_{i\alpha}^\dagger \sigma_{ab} c_{ib}$:

$$U \sum_i n_{i\uparrow} n_{i\downarrow} = -\frac{2U}{3} \sum_i S_i^2 + \frac{U}{6} \sum_i (n_{i\uparrow} + n_{i\downarrow})$$  \tag{30}$$

where the last term becomes constant if the total number of electrons is fixed, and will henceforth be suppressed except when its consideration is necessary.

Keeping in mind that there is an intrinsic SDW instability at half filling, we decompose the spin operator into the stationary and fluctuation part: $S_i = \langle S_i \rangle + (S_i - \langle S_i \rangle)$. Then, by retaining all terms up to first order in $S_i - \langle S_i \rangle$, one obtains the saddle-point Hamiltonian, $H_{\Delta_0 + U}$:

$$H_{\Delta_0 + U} = \Delta_0 \sum_i (c_{i\uparrow}^\dagger c_{i+\hat{x},\downarrow} - c_{i\downarrow}^\dagger c_{i+\hat{x},\uparrow} + \text{H.c.})$$

$$- \Delta_0 \sum_i (c_{i\uparrow}^\dagger c_{i+\hat{y},\downarrow} - c_{i\downarrow}^\dagger c_{i+\hat{y},\uparrow} + \text{H.c.})$$

$$+ \frac{3}{8U} \sum_i \phi_i^2 + \sum_i \phi_i \cdot S_i,$$ \tag{31}

where the $d$-wave pairing symmetry is explicitly written in real space and $\phi_i \equiv -\frac{3U}{4} (S_i)_{\Delta_0 + U}$ is the spin expectation value for the ground state of $H_{\Delta_0 + U}$. The remaining terms form the fluctuation Hamiltonian, $\delta H_{\Delta_0 + U}$:

$$\delta H_{\Delta_0 + U} = -\frac{2U}{3} \sum_i \left( S_i + \frac{3}{4U} \phi_i \right)^2.$$ \tag{32}

Similarly, the Hubbard Hamiltonian, $H_{\text{Hub}}$, can be decomposed into two parts:

$$H_{\text{Hub}} = -t \sum_{\langle ij \rangle} (c_{i\alpha}^\dagger c_{j\alpha} + \text{H.c.})$$

$$+ \frac{3}{8U} \sum_i \phi_i^2 + \sum_i \phi_i \cdot S_i,$$

$$\delta H_{\text{Hub}} = -\frac{2U}{3} \sum_i \left( S_i + \frac{3}{4U} \phi_i \right)^2,$$ \tag{33}

where $\phi_i \equiv -\frac{4U}{3} (S_i)_{\text{Hub}}$ is the spin expectation value for the ground state of $H_{\text{Hub}}$.

Since we are interested in the SDW singularity at $(\pi, \pi)$, we set both $\phi_0 = \phi_0 \cos (Q \cdot r_i) \hat{x}$ and $\phi_i = \phi_0 \cos (Q \cdot r_i) \hat{x}$ with $Q = (\pi, \pi)$. Finally, the saddle-point solution is completed by the determination of the optimal value of $\phi_0$ ($\phi_0$) by minimizing the ground state energy of $H_{\Delta_0 + U}$ ($H_{\text{Hub}}$) with respect to $\phi_0$ ($\phi_0$). Note that the optimization of the ground energy amounts to the saddle-point condition for the auxiliary field in the path integral formulation, hence the label “the saddle-point Hamiltonian”.

C. Step (ii)

It is convenient to re-write $H_{\Delta_0 + U}$ in momentum space:

$$H_{\Delta_0 + U} = \frac{3}{8U} \phi_0^2 + \int \frac{d^2 k}{(2\pi)^2} \Delta_k \left( c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \text{H.c.} \right)$$

$$+ \frac{\phi_0}{4} \int \frac{d^2 k}{(2\pi)^2} \left( c_{k+Q,a}^\dagger \sigma_{ab}^\sigma c_{k,b} + \text{H.c.} \right), \tag{34}$$

where the Einstein sum rule is applied on the $\sigma$ indices. Moreover, by defining a spinor field $\Psi_k$:

$$\Psi_k = \left( \begin{array}{c} c_{k\uparrow} \\ c_{k+Q,k\uparrow} \\ c_{k\downarrow}^\dagger \\ c_{k+Q,k\downarrow}^\dagger \end{array} \right), \tag{35}$$

one can re-write $H_{\Delta_0 + U}$ in a convenient $4 \times 4$ form:

$$H_{\Delta_0 + U} = \frac{3}{8U} \phi_0^2 + \int \frac{d^2 k}{(2\pi)^2} \Psi_k^\dagger \mathcal{M}_k \Psi_k,$$ \tag{36}

where

$$\mathcal{M}_k = \left( \begin{array}{cc} \frac{\phi_0}{2} \sigma_x & \Delta_k \sigma_z \\ \Delta_k \sigma_z & \frac{\phi_0}{2} \sigma_x \end{array} \right). \tag{37}$$

The momentum integration, $\int \frac{d^2 k}{(2\pi)^2}$, covers half of the Brillouin zone, which, for convenience, we choose to be the area in $k$-space bounded by $k_y = k_x \pm \pi$ and $k_y = -k_x \pm \pi$.

While it is straightforward to obtain eigenvalues of $\mathcal{M}_k$, it is instructive to diagonalize $\mathcal{M}_k$ in two steps. First, we apply the following unitary transformation onto $\mathcal{M}_k$:

$$\mathcal{M}_k' = \left( \begin{array}{cc} U & 0 \\ 0 & U^{-1} \end{array} \right) \mathcal{M}_k \left( \begin{array}{cc} U & 0 \\ 0 & U^{-1} \end{array} \right)^\dagger \tag{38}$$

where

$$U = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & 1 \\ -1 & 1 \end{array} \right) \tag{39}$$

which also defines $\gamma_{\pm}(k)$:

$$\begin{pmatrix} \gamma_{+\uparrow}(k) \\ \gamma_{-\downarrow}(k) \\ \gamma_{+\downarrow}(-k) \\ \gamma_{-\uparrow}(-k) \end{pmatrix} = \left( \begin{array}{cc} U & 0 \\ 0 & U^{-1} \end{array} \right) \Psi_k. \tag{40}$$

Second, $\mathcal{M}_k'$ is diagonalized via Bogoliubov transformation:

$$\begin{pmatrix} \omega_{\pm\uparrow}(k) \\ \omega_{\pm\downarrow}(-k) \end{pmatrix} = \begin{pmatrix} u_{\pm}(k) & v_{\pm}(k) \\ v_{\pm}(k) & u_{\pm}(k) \end{pmatrix} \begin{pmatrix} \gamma_{\pm\uparrow}(k) \\ \gamma_{\pm\downarrow}(-k) \end{pmatrix} \tag{41}$$

where $\omega_{\pm\uparrow}(k)$ and $\omega_{\pm\downarrow}(-k)$ are the energy eigenvalues in the $\pm\uparrow$ and $\pm\downarrow$ channels, respectively.
where

\[ u^2_\pm(k) - v^2_\pm(k) = \pm \frac{\phi_0}{2} E_k, \]

\[ -2u_\pm(k)v_\pm(k) = \pm \frac{\Delta_k}{E_k}, \tag{42} \]

and

\[ E_k = \sqrt{\Delta_k^2 + (\phi_0/2)^2}. \tag{43} \]

Then, it can be shown that the ground state is a vacuum of the Bogoliubov quasiparticles:

\[ \alpha_{\pm,\sigma}(k)|\psi^r_{\Delta + \epsilon_U}\rangle = 0, \tag{44} \]

which is satisfied by the following wavefunction:

\[ |\psi^r_{\Delta_0 + U}\rangle = \prod_{k \in \Omega} [u_+(k) + v_+(k)\gamma^r_{\uparrow \downarrow}(k)\gamma^r_{\downarrow \uparrow}(-k)] \]

\[ \times [u_-(k) + v_-(k)\gamma^r_{\uparrow \downarrow}(k)\gamma^r_{\downarrow \uparrow}(-k)]|0\rangle. \tag{45} \]

Moreover, minimizing the ground state energy with respect to \( \phi_0 \) leads to the saddle-point equation for \( \phi_0 \):

\[ \frac{3}{2U} = \int_{\Omega} \frac{d^2k}{(2\pi)^2} \frac{1}{\sqrt{\Delta_k^2 + (\phi_0/2)^2}}. \tag{46} \]

The saddle-point equation in Eq. (46) has a remarkable property that the solution exists for arbitrary values of \( U \). Especially intriguing is that the solution is singular in the small-\( U \) limit: \( \phi_0 \propto -\Delta_0/U \) for \( U \to 0 \). As a consequence, there is a large-range antiferromagnetic order (i.e., \( \phi_0 \neq 0 \)) even for an arbitrarily weak interaction \( U \), which is, in turn, adiabatically connected to the large-range order in the large-\( U \) limit.

In the large-\( U \) limit, \( \phi_0 \) is proportional to \( U \): \( \phi_0 = 2U/3 \). The excitation spectrum \( E_k \), therefore, has a large energy gap proportional to \( U \). Consequently, in the large-\( U \) limit, the ground state, \( |\psi^r_{\Delta_0 + U}\rangle \), is completely separated from other excitations as far as the saddle-point Hamiltonian, \( H_{\Delta_0 + U} \), is concerned. Furthermore, one can show that the situation is exactly the same for the Hubbard model: the ground state of \( H_{\text{Hub}} \), is separated from other excitations by an energy gap proportional to \( U \) in the large-\( U \) limit. Low-energy fluctuations must, then, come from the fluctuation Hamiltonians, \( \delta H_{\Delta_0 + U} \) and \( \delta H_{\text{Hub}} \).

Before we discuss the effect of fluctuations, however, we analyze \( H_{\text{Hub}} \) to show that, in the large-\( U \) limit, the ground state of \( H_{\Delta_0 + U} \) is identical to that of \( H_{\text{Hub}} \).

The saddle-point solution of the Hubbard model was discovered long ago \( 22,26 \); the ground state of \( H_{\text{Hub}} \) is a fully filled Fermi sea state of the “negative-energy-mode quasiparticles”, associated with \( \beta_- \), while it is a vacuum for the “positive-energy-mode quasiparticles”, associated with \( \beta_+ \). The precise definition of \( \beta_\pm \) is given by:

\[
\begin{pmatrix}
\beta_+(k) \\
\beta_-(k) \\
\beta^+_{\uparrow}(k) \\
\beta^-_{\downarrow}(k)
\end{pmatrix} = \begin{pmatrix}
\xi_k & -\eta_k & 0 & 0 \\
\eta_k & \xi_k & 0 & 0 \\
0 & 0 & \xi_k & \eta_k \\
0 & 0 & -\eta_k & \xi_k
\end{pmatrix} \begin{pmatrix}
c_{k\uparrow} \\
c_{k\downarrow} \\
c_{k+Q\uparrow} \\
c_{k+Q\downarrow}
\end{pmatrix}. \tag{47}
\]

where

\[ \xi_k - \eta_k = \frac{\epsilon_k}{\xi_k}, \]

\[ -2\xi_k\eta_k = \frac{\phi_0/2}{\xi_k}, \tag{48} \]

and

\[ \xi_k = \frac{\epsilon_k^2 + (\phi_0/2)^2}{\xi_k}. \tag{49} \]

The ground state of \( H_{\text{Hub}} \) is, then, given by

\[
|\psi^r_{\text{Hub}}\rangle = \prod_{k \in \Omega} \beta^r_{\uparrow}(-k)\beta^r_{\downarrow}(-k)|0\rangle. \tag{50}
\]

Similar to what was done in the case of the strong-pairing BCS Hamiltonian, minimizing the ground state energy leads to the saddle-point equation for \( \varphi_0 \), which is given by

\[ \frac{3}{2U} = \int_{\Omega} \frac{d^2k}{(2\pi)^2} \frac{1}{\sqrt{\epsilon_k^2 + (\varphi_0/2)^2}}. \tag{51} \]

It can be shown from Eq. (51) that, in the large-\( U \) limit, \( \varphi_0 \) becomes proportional to \( U \); more precisely \( \varphi_0 = 2U/3 \), in which case \( \xi_k = -\eta_k = 1/\sqrt{2} \) [See Eq. (45)]. At the same time, for the strong-coupling BCS Hamiltonian, \( \varphi_0 \) is also proportional to \( U \) in the large-\( U \) limit so that \( u_+(k) = 1, v_+(k) = 0, u_-(k) = 0, \) and \( v_-(k) = 1 \) [See Eq. (42)], which results in the following ground state:

\[
|\psi_0\rangle = \prod_{k \in \Omega} \beta^r_{\uparrow}(-k)\beta^r_{\downarrow}(-k)|0\rangle. \tag{52}
\]

As one can see, \( |\psi_0\rangle \) is identical to the ground state of \( H_{\text{Hub}} \) in Eq. (50) if the large-\( U \) limit is taken (Note that \( \beta^r_{\downarrow}(-k) = \gamma^\downarrow_{\uparrow \downarrow}(k) \) in the large-\( U \) limit).

It should not come as a surprise that \( |\psi_0\rangle \) is independent of parameters (such as \( U/t \) or \( U/\Delta_0 \)) since, in the large-\( U \) limit, the ground state, \( |\psi_0\rangle \), is uniquely determined without the dependence on \( U/t \) or \( U/\Delta_0 \). Remember that, in the large-\( U \) limit, the Hubbard model becomes the Heisenberg model which has a single scale factor \( J \). Therefore, the ground state (actually, any eigenstate) of the Heisenberg model is parameter free. The situation is similar for the strong-pairing Gutzwiller-projected BCS Hamiltonian, \( H^\Delta \).

So, at least superficially, it seems that taking the large-\( U \) limit entails simply making \( U \) infinite and ignoring any effect of \( t \) or \( \Delta_0 \). However, this is not correct because there is a reduction in the ground state energy due to finite \( \Delta_0 \) in \( H_{\Delta_0 + U} \). The ground state energy of \( |\psi^r_{\Delta_0 + U}\rangle \) has the following form:

\[
\frac{E^r_{\Delta_0 + U}}{N_e} = \frac{3}{8U} \phi_0^2 - 2 \int_{\Omega} \frac{d^2k}{(2\pi)^2} \sqrt{\Delta_k^2 + (\phi_0/2)^2} + U/6. \tag{53}
\]

where the last term \( U/6 \) comes from the constant term in Eq. (50). Then, it can be shown that, in the large-\( U \)
limit,

\[
\frac{E_{\Delta+U}^{\text{gt}}}{N_c} \simeq -\frac{2}{\phi_0} \int_{\Omega} \frac{d^2k}{(2\pi)^2} (\Delta_0^2 / U) \cos k_x \cos k_y \frac{\Delta_0^2}{U} \theta_0
\]

where we use the fact that \(\phi_0 = 2U/3\) in the large-\(U\) limit. As one can see, for finite \(\Delta_0\), there is a reduction in the ground state energy, which is proportional to \(\Delta_0^2 / U\). As long as \(\Delta_0\) is not zero, spin configurations are not random in the low-energy Hilbert space. This is the difference between the large-\(U\) limit and strictly infinite \(U\).

The situation is similar for the Hubbard model. The ground state energy of \(|\psi_{\text{Hub}}^{\text{gr}}\rangle\) is given by:

\[
\frac{E_{\text{Hub}}^{\text{gt}}}{N_c} = \frac{3}{8U} \theta_0^2 - 2 \int_{\Omega} \left( \frac{d^2k}{(2\pi)^2} \right) \sqrt{\Delta_0^2 / U} \left( \phi_0^2 / 2 \right) + \frac{U}{6},
\]

which, in the large-\(U\) limit, becomes

\[
\frac{E_{\text{Hub}}^{\text{gt}}}{N_c} \simeq -\frac{2}{\phi_0} \int_{\Omega} \frac{d^2k}{(2\pi)^2} (\Delta_0^2 / U) \cos k_x \cos k_y \frac{\Delta_0^2}{U} \theta_0
\]

Therefore, again, spin configurations of the low-energy states are not random.

D. Step (iii)

We have shown that the excitation spectra of \(H_{\Delta+U}\) and \(H_{\text{Hub}}\) are gapped with a very large energy gap of \(O(U)\) in the large-\(U\) limit. However, the true low-energy excitation should be gapless at half filling, as required by Goldstone’s theorem in two dimension where the spin rotation symmetry is broken by non-zero \((S_i)\). This dilemma is an artifact of the restriction of our attention to only a part of the full Hamiltonian.

The saddle-point ground state, \(|\psi_0\rangle\), is separated from other excitations of the saddle-point Hamiltonian. However, when the full Hamiltonian (including the saddle-point and fluctuation part) is considered, there are many other states which have exactly the same energy as \(|\psi_0\rangle\); these states are connected to \(|\psi_0\rangle\) by rigid spin rotations. We denote these states as \(|\psi_i\rangle \equiv R_i |\psi_0\rangle\) with \(\{R_i\}\) being spin rotation operators. The energy of \(|\psi_i\rangle\) is the same for an arbitrary spin rotation because

\[
\langle \psi_i | H | \psi_i \rangle = \langle \psi_0 | H | R_i^\dagger R_i | \psi_0 \rangle = \langle \psi_0 | H | \psi_0 \rangle,
\]

where \(H\), either \(H_{\Delta+U}\) or \(H_{\text{Hub}}\), is invariant under spin rotation. In the large-\(U\) limit, therefore, the low-energy Hilbert space is composed only of \(|\psi_i\rangle\). Note that, although linearly independent, the basis states in \(|\psi_i\rangle\) are not orthogonal to each other; \(|\psi_i\rangle\) forms an over-complete basis set, which is conceptually very similar to the coherent-state basis set for a spin representation.

Our task now is to evaluate matrix elements of the full Hamiltonian within the above low-energy Hilbert space. To this end, we first investigate the saddle-point equation. Eq. (51) is very similar to Eq. (46). In fact, when all quantities are properly scaled, Eq. (51) is exactly the same equation as Eq. (46) since the momentum, \(k\), is a dummy integration parameter and Eq. (51) can be obtained from Eq. (46) by translating \(k\) by \((\pi, 0)\). A constant translation in momentum does not affect the integral in the saddle-point equation. To be specific, if the solution of Eq. (51), \(\tilde{\phi}_0 / t\), is a function of \(U/t\):

\[
\tilde{\phi}_0 / U \simeq f(U/t),
\]

then the solution of Eq. (46), \(\tilde{\phi}_0 / \Delta_0\), is related to \(U / \Delta_0\) by the same function:

\[
\tilde{\phi}_0 / \Delta_0 \simeq f(U / \Delta_0).
\]

The precise functional form of \(f(x)\) is not important for general \(x\), but it is useful to know that \(f(x) = 2x / 3\) when \(x \gg 1\).

Now, considering the definition of \(\delta H_{\Delta+U}\) and \(\delta H_{\text{Hub}}\), it is not too difficult to show that effects of both fluctuation Hamiltonians become equivalent in the large-\(U\) limit since (i) \(\phi_0 = \tilde{\phi}_0\) for general \(U\), if \(t\) is set equal to \(\Delta_0\), and (ii) low-energy Hilbert spaces for both models reduce to the same Hilbert space, \(|\psi_i\rangle\}, in the large-\(U\) limit. So, in essence, it has been shown that, in the large-\(U\) limit, all matrix elements for both fluctuation Hamiltonians are the same in the low-energy Hilbert space. It is very important to note that we are interested in the the lowest-order, non-zero effect of finite \(\Delta_0\) and \(t\) in the limit of large \(U\). Since, in the large-\(U\) limit, eigenstates should be parameter free, lowest-order effects of finite \(\Delta_0\) and \(t\) must emerge through their effects on \(\phi_0\) and \(\tilde{\phi}_0\), respectively.

We now establish that matrix elements of both saddle-point Hamiltonians, \(H_{\Delta+U}\) and \(H_{\text{Hub}}\), are identical. We begin by considering two arbitrary states from the low-energy Hilbert space of the BCS Hamiltonian with finite \(U\), \(|\psi_j\rangle = R_j |\psi^{\text{gt}}_{\Delta+U}\rangle\) and \(|\psi_k\rangle = R_k |\psi^{\text{gt}}_{\Delta+U}\rangle\). The matrix element of \(H_{\Delta+U}\) between these two states is, then,

\[
\langle \psi_j | H_{\Delta+U} | \psi_k \rangle = \langle \psi_j | H_{\Delta_0} + 3 \frac{3}{SU} \sum_i \phi_i^2 + \sum_i \phi_i \cdot S_i | \psi_k \rangle
\]

\[
= \frac{E_{\Delta+U}}{N_c} \langle \psi_j | H_{\Delta_0} + R_j^\dagger R_k | \psi^{\text{gt}}_{\Delta+U}\rangle
\]

\[
+ \frac{E_{\Delta+U}}{N_c} \langle R_j^\dagger \left( \sum_i \phi_i \cdot S_i \right) R_k | \psi^{\text{gt}}_{\Delta+U}\rangle
\]

\[
- \frac{1}{2} \langle \psi_j | \left( \sum_i \phi_i \cdot S_i \right) | \psi^{\text{gt}}_{\Delta+U}\rangle, \quad (60)
\]
where \( E_{\text{Hub}}^{\text{SR}} = -3\Delta^2 / U \) and \( |\psi_{\text{SR}}^{\text{Hub}}(\Delta_0, t)| = |\psi_0^\Phi \) in the large-U limit. Note that the invariance of \( H_{\Delta} \) and \( \phi^2 \) under spin rotations is used. Similarly, in the large-U limit, the matrix element of \( H_{\text{Hub}} \) between the above states is as follows:

\[
\langle \psi_0 | H_{\text{Hub}} | \psi_k \rangle = E_{\text{Hub}}^{\text{SR}} \left\langle \psi_0 | R_i R_k | \psi_0 \right\rangle + \left\langle \psi_0 | R_i \left( \sum_i \varphi_i \cdot S_i \right) R_k | \psi_0 \right\rangle - \frac{1}{2} \left\langle \psi_0 | R_i R_k, \sum_i \varphi_i \cdot S_i | \psi_0 \right\rangle,
\]

where \( E_{\text{Hub}}^{\text{SR}} = -3\Delta^2 / U \) in the large-U limit. Therefore, it is clear from a comparison of Eq. (60) and (61) that the matrix elements are identical, provided that the large-U limit is taken while \( t \) is set equal to \( \Delta_0 \). Note that \( \phi_i = \varphi_i \) for general \( U \) if \( t = \Delta_0 \).

E. Step (iv)

We have learned two lessons from Step (ii) and (iii). First, the ground states of the saddle-point Hamiltonians, \( H_{\text{Hub}} \) and \( H_{\text{Hub}}^{\mathbf{k}+U} \), are identical in the large-U limit, and therefore low-energy Hilbert spaces (which are obtained by applying rigid spin rotations to the saddle-point ground states) are also identical in this limit. Second, in the low-energy Hilbert space, matrix elements for the fluctuation Hamiltonians are identical for both the Hubbard model and the strong-pairing BCS Hamiltonian with the same being true for the two saddle-point Hamiltonians. Therefore, we conclude that the strong-pairing Gutzwiller-projected BCS Hamiltonian at half filling is equivalent to the 2D antiferromagnetic Heisenberg model.

F. Relation to the projected BCS Hamiltonian with extended s-wave pairing: a corollary

In this section, we would like to discuss an interesting corollary of the analytic derivation given in previous sections. Our derivation is actually valid also for the strong-pairing BCS Hamiltonian with an extended s-wave pairing: \( \Delta_k / \Delta = 2 \cos k_x + \cos k_y \). This is due to the fact that the saddle-point equation for extended s-wave pairing is the same as that of d-wave pairing and, consequently, all matrix elements remain the same as obtained for d-wave case. Note that extended s-wave pairing is induced by nearest-neighbor pairing amplitudes with the same sign for the \( x \) and \( y \) directions in contrast to the opposite signs in d-wave pairing. However, despite this important distinction, it is proven as a corollary to our d-wave result that, at half filling, the strong-pairing Gutzwiller-projected BCS Hamiltonian with extended s-wave pairing is also equivalent to the antiferromagnetic Heisenberg model.

To test this assertion numerically, we compute the wavefunction overlap between the ground states of the Heisenberg model and the strong-pairing Gutzwiller-projected BCS Hamiltonian with extended s-wave pairing. As before, we analyze the 4 \( \times \) 4 square lattice system via exact diagonalization. To be specific, the strong-pairing Gutzwiller-projected BCS Hamiltonian with extended s-wave pairing is given by:

\[
H_{\text{BCS}}^{G} = \hat{P}_G (H_t + H_{s\Delta}) \hat{P}_G,
\]

where

\[
H_{s\Delta} = \Delta \sum_i (c_i^{\dagger} c_{i+\hat{x},\downarrow} - c_i^{\dagger} c_{i+\hat{x},\uparrow} + \text{H.c.}) + \Delta \sum_i (c_i^{\dagger} c_{i+\hat{y},\uparrow} - c_i^{\dagger} c_{i+\hat{y},\downarrow} + \text{H.c.}).
\]

Fig. 7 shows that, for sufficiently large \( \Delta / t \), the overlap indeed becomes essentially unity for both \( \Delta_k = 2 \Delta (\cos k_x + \cos k_y) \) [extended s-wave pairing] and \( 2 \Delta (\cos k_x - \cos k_y) \) [d-wave pairing].
evidence for the existence of superconductivity in the t-J model, which, in turn, may suggest that it is not only between the above, two examples. In both cases, dominantly non-interacting quasiparticles.

V. CONCLUSION

We conclude by discussing the physical implications of the close connection between the Gutzwiller-projected BCS Hamiltonian and the t-J model. There are practical implications as well as fundamental ones. Fundamentally, the close connection between the Gutzwiller-projected BCS Hamiltonian and the t-J model provides evidence for the existence of superconductivity in the t-J model, which, in turn, may suggest that it is not only possible, but rather natural that the pairing in high-temperature superconductors is caused purely by electronic correlations.

Now that we have reason to believe that the antiferromagnetic interaction is closely related to electron-electron pairing, the next natural question is how this connection can be used for the quantitative understanding of experiments. While it is in principle straightforward to apply exact diagonalization to the Gutzwiller-projected BCS Hamiltonian, exactly solving the Gutzwiller-projected BCS Hamiltonian is as complicated as solving the t-J model in the first place. The true practical advantage of analyzing the Gutzwiller-projected BCS Hamiltonian, however, lies in the fact that the Gutzwiller-projected BCS Hamiltonian is much more amenable to the ansatz wavefunction approach than the t-J model.

Ansatz wavefunction approaches have been very successful in various strongly correlated problems in condensed matter physics. Two very salient examples are the fractional quantum Hall effect (FQHE) and the liquid Helium. Despite their apparent difference in the physical context, there is actually a rather profound commonality between the above, two examples. In both cases, dominant short-range correlations are first separated from long-range correlations. Then, effects of the strong short-range correlations are captured by the attachment of the Jastrow factor. The specific functional form of the Jastrow factor, of course, depends on the nature of the problem at hand. After short-range correlations are taken into account via the Jastrow factor, it is assumed that residual long-range correlations are relatively much weaker so that the rest of the ansatz wavefunction describes essentially non-interacting quasiparticles.

Specifically, the ansatz wavefunction for the FQHE is given by the composite fermion (CF) wavefunction. In essence, the CF wavefunction is a product of the Jastrow factor, $\prod_{i<j}(z_i-z_j)^{2p}$ with $p$ an integer and $z_j=x_j+iy_j$, and a non-interacting fermionic wavefunction of new quasiparticles known as composite fermions. It is known that the above functional form of the Jastrow factor is most effective in minimizing the Coulomb repulsion between electrons in the lowest Landau level; the wavefunction overlap between the CF wavefunction and the exact ground state is practically unity for all available finite-system studies.

Another example is liquid Helium. The microscopic wavefunction for normal state $^4\text{He}$ is written in terms of an algebraic product of the Jastrow factor and the Slater determinant of plane-wave states,$^{24}$

$$\Psi_{^3\text{He}} = \exp \left[ -\sum_{i<j} u(r_i - r_j) \right] \text{Det} \left| e^{i\mathbf{k}\cdot\mathbf{r}} \right|$$

where $u(r)$ is determined by the interaction between He atoms: typically, $u(r) \propto 1/r^5$. While the Slater determinant provides the necessary antisymmetrization as well as the low-energy physics, the Jastrow factor captures dominant short-range correlations. Similarly, the ansatz wavefunction for superfluid $^4\text{He}$ is given by:

$$\Psi_{^4\text{He}} = \exp \left[ -\sum_{i<j} u'(r_i - r_j) \right]$$

where $u'(r)$ is basically identical $u(r)$ except for slight changes due to the mass difference between $^3\text{He}$ and $^4\text{He}$. Since the ground state wavefunction for non-interacting bosons is just a constant, the ansatz wavefunction for superfluid $^4\text{He}$ can be also viewed as the product of the Jastrow factor and a wavefunction for non-interacting bosons.

From the discussion so far, it seems promising that a range of strongly correlated problems can be attacked via the Jastrow-factor approach, provided that residual long-range correlations are weak so that, to a good approximation, they can be treated as those of non-interacting quasi-particles. One criterion for the weakness of residual interaction may be whether or not the residual interaction can cause an instability toward a new phase. In other words, as long as the ground state for the original interaction (causing the strong short-range correlation) is not completely different from that of weakly-interacting (emergent) quasi-particles, the Jastrow-factor approach can provide a good ansatz wavefunction.

The situation for the t-J model, or the Hubbard model in the large-$U$ limit, is quite intriguing. First, note that...
the Gutzwiller projection can be actually regarded as the Jastrow factor imposing the no-double-occupancy constraint that occurs because of the strong on-site repulsion in the large-$U$ limit. Keeping in mind that the $t$-$J$ model is the Hubbard model in the large-$U$ limit, it may be conjectured that the ground state of the $t$-$J$ model is described well by the Gutzwiller-projected Fermi-sea state. Unfortunately, however, this is not true at half filling. We have learned in Sec. IV C that, at half filling, the Gutzwiller-projected Fermi-sea state cannot be a good ansatz wavefunction.

On the other hand, away from half filling, the SDW instability disappears because perfect nesting is ruined with non-zero doping, as shown in Sec. IV B. One may assume now that the Gutzwiller-projected Fermi-sea state can be a good ansatz wavefunction for finite, non-zero doping. This is, however, not true either because there is another instability caused by electron-electron pairing. It is, in some sense, the goal of this paper to show that the $t$-$J$ model contains a pairing instability. Motivated by the fact that the Gutzwiller projection can play a role of the Jastrow factor for the Gutzwiller-projected BCS Hamiltonian, we now show that the Gutzwiller-projected BCS wavefunction (i.e., the RVB state) is, in fact, a good ansatz wavefunction for the Gutzwiller-projected BCS Hamiltonian at finite, non-zero doping, which, in turn, leads to the eventual connection between the ground state of the $t$-$J$ model and the projected BCS wavefunction.

While there have been studies showing that, for finite doping, the Gutzwiller-projected BCS wavefunction yields good agreement with experiments, we provide a more direct piece of evidence. Hasegawa and Poilblanc have shown that the overlap between the projected BCS wavefunction and the ground state of the $t$-$J$ model is high ($\sim 90\%$) for the case of 2 holes in the $\sqrt{10} \times \sqrt{10}$ lattice system. In order to make a direct comparison, we have computed the overlap between the ground state of the projected BCS Hamiltonian and that of the $t$-$J$ model in the same system; we find that the optimal overlap for the ground state of the projected BCS Hamiltonian is more than $98\%$ for the same $\sqrt{10} \times \sqrt{10}$ lattice system, as shown in Fig. 9. Therefore, it is shown (at least, in finite system studies) that the projected BCS wavefunction is a good ansatz wavefunction for the projected BCS Hamiltonian, as expected from the Jastrow-factor approach.

Regarding the work of Hasegawa and Poilblanc, it is interesting to note that they also computed the overlap between the projected BCS wavefunction and the ground state of the $t$-$J$ model in the $4 \times 4$ lattice system and they found that it was very low ($\sim 4\%$). This sudden drop in the overlap is a finite-system-size artifact due to the fact that the half-filled Fermi sea state (technically speaking, its chemical potential) is ill-defined in the $L \times L$ system with $L$ an even integer (e.g., the $4 \times 4$ system), while there is no such problem in the $L \times L + 1$ system with $L$ an odd integer (e.g., the $\sqrt{10} \times \sqrt{10}$ system when $L = 3$). It is important to note that the ground state of the projected BCS Hamiltonian in our approach does not suffer from the above problem regardless of site numbers.

The close relationship between the projected BCS wavefunction and the ground state of the projected BCS Hamiltonian at moderate doping is rather important since it provides additional support for the existence of superconductivity in the projected BCS Hamiltonian and, eventually, for that of the superconductivity in the $t$-$J$ model through the connection between the projected BCS Hamiltonian and the $t$-$J$ model; large-scale Monte Carlo simulation studies have shown that the projected BCS wavefunction has the long-range pairing correlation in the thermodynamic limit. In this perspective, the goal of our work in this paper is to show why the projected BCS wavefunction can be a good ansatz wavefunction for the $t$-$J$ model at moderate doping, while it is not true at half filling. The interrelationship between the ground state of the $t$-$J$ model, of the Gutzwiller-projected BCS Hamiltonian, and the RVB state is schematically shown in Table I.

| Condition   | Wavefunction Relationship |
|-------------|---------------------------|
| Half filling | $\psi_J = \psi_{BCS} \neq \psi_{RVB}$ |
| Moderate doping | $\psi_J \approx \psi_{BCS} \approx \psi_{RVB}$ |

TABLE I: Interrelationship between the ground state of the $t$-$J$ model, $\psi_J$, the ground state of the Gutzwiller-projected BCS Hamiltonian, $\psi_{BCS}$, and the RVB state, $\psi_{RVB}$.
ing the double occupancy with suppression weights:

$$\hat{P}_G^{\text{partial}} \equiv \prod_i (1 - \alpha n_i^\uparrow n_i^\downarrow)$$

$$= e^{-\beta \sum_i n_i^\uparrow n_i^\downarrow},$$

(66)

where $e^{-\beta} = 1 - \alpha$. The above expression suggests a very natural interpretation that the partial Gutzwiller projection is, in fact, also a specific form of the usual Jastrow factor. Incidentally, the Fermi sea state with partial Gutzwiller projection is, in fact, also a specific form of the usual Jastrow factor argument.

Finally, it is also interesting to note that, in one dimension where there is no instability for either spin-density-wave or pairing, the exact ground state of the antiferromagnetic Heisenberg model (i.e., Bethe ansatz solution\(^{15}\)) is actually very closely related to the Gutzwiller-projected Fermi-sea state\(^{12,36,47}\), as expected from the Jastrow-factor argument.

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