Spin Charge Recombination in Projected Wave Functions.

Hong-Yu Yang and Tao Li

Center for Advanced Study, Tsinghua University, Beijing 100084, P.R.China

Abstract

We find spin charge recombination is a generic feature of projected wave functions. We find this effect is responsible for a series of differences between mean field theory prediction and the result from projected wave functions. We also find spin charge recombination plays an important role in determining the dissipation of supercurrent, the quasiparticle properties and the hole - hole correlation.
Superconductivity results from Bose condensation of charged particles. In the BCS theory of superconductivity, Fermionic electrons are paired into Bosonic Copper pairs whose condensation lead to superconductivity. Soon after the discovery of high temperature superconductors, Anderson proposed an exotic way toward superconductivity in this class of materials. His way is to fractionalize the electron rather than pair them up\[1\],[2],[3]. The parent compounds of high temperature superconductors are antiferromagnetic insulators. Anderson argued that doping holes into such antiferromagnetic insulators would generate a spin liquid state which can be envisioned as coherent superposition of spin singlet pairs. He also argued that the excitations on the spin liquid state are fractionalized. Specifically, the spin and charge quantum number of the electron are now carried separately by two kinds of excitations, namely a spin-1/2 chargeless Fermionic excitation called spinon and a spinless Bosonic charged excitation call holon. In such a spin-charge separated system, the charged holon is liberated from the Fermionic statistics of the original electron and are ready to condense into a superfluid.

One main problem for such a proposal lies in the fact the predicted $T_c$ is too high\[4],[5]. There is just no sufficient dissipation to suppress the holon supercurrent. In the BCS theory, the supercurrent is suppressed by quasiparticle excitation. These charged Fermionic excitation form the normal fluid and cause dissipative response in external electromagnetic(EM) field. However, in an ideal spin charge separated system, the Fermionic spinon excitation dose not carry charge and do not cause dissipation in an external EM field while the bosonic excitation of the holon system is much less effective in dissipate the supercurrent.

The spin charge separation idea is nicely embodied in the slave Boson scheme of $t - J$ model. In this scheme, the electron operator $c_{i\sigma}$ is written as $f_{i\sigma}b_i^\dagger$, where $f_{i\sigma}$ and $b_i$are Fermionic spinon operator and Bosonic holon operator. Within this scheme, Lee and Wen proposed that the spinon - holon recombination may hold the key for the problem of overestimated $T_c$\[6]. Through such a recombination, the Fermionic spinon excitation acquire charge and can cause dissipation in EM field, or, a charged hole regain Fermionic statistics and is transformed into a normal carrier out of the condensate. However, it is not clear what is the cause and nature of such a spinon - holon recombination. Wen and Lee argued that the recombination may be related the unbroken $U(1)$ gauge structure in their $SU(2)$ gauge theory of high temperature superconductivity\[7]. The problem of spinon - holon recombination is also discussed phenomenologically by Lee et. al.\[8] and Ng\[9].
Here we point out that spinon - holon recombination is a generic feature in projected wave functions. First we mention some clues that imply this. As our first example, we consider the motion of holon in the so called uniform RVB state on square lattice. The uniform RVB state is generated by the following mean field ansatz

\[ H_f = - \sum_{\langle ij \rangle, \sigma} \langle f_{i,\sigma}^\dagger f_{j,\sigma} + h.c. \rangle - \mu_f \sum_{i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} \]

in which the sum is over nearest neighboring (NN) sites on the square lattice. At the mean field level, the motion of a holon in such a spin background is described by the mean field Hamiltonian

\[ H_h = -t\chi \sum_{\langle ij \rangle} (b_{i}^\dagger b_{j} + h.c.) - \mu_b \sum_i b_i^\dagger b_i \]

in which \(\chi\) is the mean field hopping matrix element in such a spin background and is given by \(\chi = \sum_{\sigma} \left\langle f_{i,\sigma}^\dagger f_{j,\sigma} \right\rangle\), in which \(i\) and \(j\) are NN sites. At the mean field level, the ground state of the system is given by

\[ |FS\rangle = (b_{q=0}^\dagger)^{N_h} \prod_{k<k_f} f_{k\uparrow}^\dagger f_{-k\downarrow}^\dagger 0\rangle \]

where \(N_h\) is the number of holon, \(k_F\) is the spinon Fermi surface (FS). In the mean field ground state, \(\chi = \sum_{k<k_F} (\cos(k_x) + \cos(k_y))\) and is nonzero. Thus each holon has a kinetic energy of order \(t\chi\). Now we project the mean field ground state into the physical subspace of no double occupancy. The projection of the spinon wave function lead to the uniform RVB state (the projection of the holon condensate only contribute a constant)

\[ |U - RVB\rangle = P_G |FS\rangle = P_G \left( \sum_{i,j} a_{ij} f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger \right)^{N_f/2} |0\rangle \]

with the RVB amplitude \(a_{ij}\) given by \(\sum_{k<k_F} e^{ik(i-j)}\). At half filling, the RVB amplitude \(a_{ij}\) has the important characteristics that it is nonzero only for sites \(i\) and \(j\) belonging to different sublattices. Thus, contrary to our expectation from mean filed theory, the holon in fact can not hop between NN sites in such a spin background. One would argue that the spin wave function should be modified upon hole doping. According to mean field theory,
the most natural guess on the modification is to remove \( N_b \) spinon below the spinon Fermi surface. For two holes, the modified mean filed state is given by

\[
|MF'\rangle = (b_{q=0}^\dagger)^2 f_{k_0\uparrow} f_{-k_0\downarrow} \prod_{k<k_F} f_{k\uparrow} f_{-k\downarrow} |0\rangle = f_{k_0\uparrow} f_{-k_0\downarrow} |FS\rangle
\]

in which \( k_0 \) and \(-k_0\) are momentums below the spinon Fermi surface where a pair of spinons are removed. This wave function represents a state with two holons at \( q = 0 \) and two spinon excitations (more exactly, two holes of spinon) at \( k_0 \) and \(-k_0\) on the half filled uniform RVB background. Projecting this mean field state into the subspace of no double occupancy, we get a RVB state with a modified RVB amplitude \( a'_{ij} = \frac{1}{N} \sum_{k<k_F, k≠k_0} e^{ik(i-j)} \). The change of the RVB amplitude caused by the spinon excitation is vanishingly small (of order \( 1/N \), where \( N \) is number of lattice sites) and it seems that the hole motion between NN sites is still blocked. However, by direct calculation of kinetic energy in the modified RVB state, we find such an expectation is wrong. The kinetic energy per hole is of order \( t \) rather than vanishingly small. The only explanation for this surprising result is that the spinon excitation is bound to the moving holon. If the spinon excitation and the holon are independent of each other, the change of the local spin background around the moving holon caused by the spinon excitation would be of order \( 1/N \) and would not be able to release to NN kinetic energy.

The uniform RVB state is quite special. However, the spinon - holon recombination is quite generic in projected wave functions. Now we consider the d-wave RVB state on the square lattice generated by the ansatz

\[
H_f = -\sum_{\langle ij \rangle, \sigma} (f_{i\sigma}^\dagger f_{j\sigma} + h.c.) + \sum_{\langle ij \rangle} \Delta_{ij} (f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger + f_{j\uparrow}^\dagger f_{i\downarrow}^\dagger + h.c.) - \mu_f \sum_{i, \sigma} f_{i\sigma}^\dagger f_{i\sigma}
\]

in which \( \Delta_{ij} = \Delta \) and \(-\Delta\) for NN sites along \( x \) and \( y \) directions. The mean field ground state is given by

\[
|d - BCS\rangle = (b_{q=0}^\dagger)^{N_b} \prod_k (1 + \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}} f_{k\uparrow}^\dagger f_{-k\downarrow}^\dagger \}} |0\rangle
\]

in which \( \xi_k \) and \( \Delta_k \) are mean field kinetic energy and pairing gap of the spinon. Projecting \( |d - BCS\rangle \) into the subspace of no double occupancy generates a RVB state with

\[
a_{ij} = \sum_k \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}} e^{ik(i-j)}. \]

In the d-wave RVB state, the NN hopping is not suppressed. However, the matrix element for next nearest neighboring (NNN) and next next nearest
neighboring(NNNN) hopping is very small near half filling. This is reasonable since the mean field matrix element for hoping between sites on the same sublattice is exactly zero when \( \mu_f = 0 \). Lee et. al. find the kinetic energy due to NNN and NNNN hopping can be released by creating spinon excitation at appropriate momentums on the d-wave RVB state. For the case of two holes, they find the NNN and NNNN kinetic energy is released in a state with \( a'_{ij} = \sum_{k \neq k_0} \frac{\Delta_k}{\xi_k + \sqrt{\xi_k^2 + \Delta_k^2}} e^{i k (i-j)} \). It is easy to check that this state can be generated by projecting \( |MF'\rangle = f_{k_0 \uparrow} f_{-k_0 \downarrow} |d - BCS\rangle \) and thus represent a state with two spinon excitations. Thus once again we see the creation of an individual spinon excitation can make an order of one change on the hopping matrix element of holon. This again indicate that the spinon excitation is bound to the moving holon.

The spinon - holon recombination can be inferred also from the quasiparticle weight. In the slave Boson mean field theory, the quasiparticle weight is proportional to the holon condensate and vanish with hole density. After projection, the quasiparticle weight can have a nonzero value even at vanishingly small hole density. As a trivial example in this respect, we consider doping a hole into a fully polarized spin background. Since the spin is fully polarized, the system is in fact in a free particle state and the quasiparticle weight should be exactly one. As we will show below, the difference between the prediction from the mean filed theory and that from the projected wave function can be understood as a result of spinon - holon recombination. In fact, the spinon excitation and holon are totally combined in the fully polarized spin background in the sense that they sit at the same site and bind into a real electron. A a less trivial example we consider doping a hole into a spin background with antiferromagnetic long range order. As we will show below, the spinon excitation and the holon will form well defined bound state in such a spin background. This bound state has a nonzero overlap with a bare electron. Thus the quasiparticle weight do not vanish near half filling in this case.

Now we define the spinon - holon recombination more concretely. For simplicity, we consider the uniform RVB state and dope only one hole into the system. The mean field wave function for the doped system is

\[
|k_0, \uparrow\rangle = b_{q=0}^\dagger f_{-k_0 \downarrow} \prod_{k < k_F} f_{k \uparrow}^\dagger f_{-k \downarrow}^\dagger |0\rangle = \frac{1}{N} \sum_{i,j} e^{i k_0 (i-j)} b_i^\dagger f_{j \downarrow} \prod_{k < k_F} f_{k \uparrow} f_{-k \downarrow} |0\rangle
\]
This wave function represents a state with a holon at \( q = 0 \) (created by \( b_{q=0}^\dagger \)) and a spinon excitation at \(-k_0\) (created by \( f_{-k_0} \)) on the half filled RVB background. In this mean field state, the spinon excitation and the holon are independent of each other. Now we discuss how they are correlated in the projected wave function. Here we define the site on which \( f_{j+} \) operate as the location of the spinon excitation and study how the spinon excitation is distributed when the holon is located on site \( i \). In fact, it suffers from some ambiguity to talk about the location of the spinon excitation on the projected wave function, especially when the RVB amplitude is long ranged\[11\]. Although suffers from such ambiguity, the correlation function defined above is still of great value for understanding the difference between mean field theory and projected wave functions. For example, if the correlation function reduce to a delta function, then the spinon operator \( f_{j+} \) and the holon operator \( b_i^\dagger \) act on the same site and as a whole is equivalent to the operation of a bare electron operator \( c_{i+} \). In this case, the spinon and the holon are recombined into a real electron.

The desired correlation function can be evaluated easily. Suppose the holon sit on site \( i \) while the spinon sit on a different site \( j \). Since all sites besides \( i \) are singly occupied after the projection, site \( j \) must be doubly occupied before the action of \( f_{j+} \) while site \( i \) must be empty. Thus the probability for such a spinon - holon configuration is given by the probability of finding site \( i \) empty and site \( j \) doubly occupied and with all other sites singly occupied in the mean field state \(|FS\rangle\). At the same time, the probability for the holon and the spinon to sit on the same site is given by the probability of finding site \( i \) occupied by a down spin and with all other sites singly occupied in \(|FS\rangle\). The ratio between the two probability \( P_{ij} \) and \( P_{ii} \) is given by

\[
\frac{P_{ij}}{P_{ii}} = \frac{\sum_\beta |\psi_\beta|^2}{\sum_\alpha |\psi_\alpha|^2} = \frac{\sum_\alpha |\psi_\alpha|^2}{\sum_\beta |\psi_\beta|^2}
\]

Here, \( \alpha \) denotes an arbitrary configuration with all sites singly occupied, \( \beta \) denotes an arbitrary configuration with site \( i \) empty and site \( j \) doubly occupied and with all other sites singly occupied. In deriving this formula, we have used the fact that each configuration \( \beta \) can be generated from two configuration \( \alpha \) through electron hopping from site \( i \) to site \( j \). This statistical sum can be evaluated easily with Variational Monte Carlo method.

Now we present the result for the spinon - holon correlation function in various projected
wave functions. Figure 1 shows the correlation function for the projected one dimension Fermi sea. The projected one dimensional Fermi sea is found to be a very good variational guess on the ground state of one dimensional $t - J$ model\textsuperscript{12}. We see the spinon - holon correlation function decay as $1/r$ at large distance in this state. This power law decay (which is not integrable) lead to a vanishingly small quasiparticle weight near half filling. Figure 2 show the result for the two dimensional d-wave RVB state. The correlation function in this case also decay with power law at large distance and is not integrable. Thus the quasiparticle weight in this case also vanishes near half filling. However, numerically the power law decaying tail is quite small for both the one dimension projected Fermi sea and the d-wave RVB state. The power law tail is hardly visible in Figure 2 due to its numerical smallness. In Figure 3 we plot the the dependence of correlation at the largest distance of the lattice as a function of the lattice size. From this plot we see the spinon - holon correlation decay approximately as $1/r^{3/2}$ at large distance in the d-wave RVB state.

Now we show some examples with more tightly bound spinon - holon pairs. The first example is the fully polarized state. In this state, the probability of finding a doubly occupied site is zero. Thus the spinon and the holon must occupy the same site and recombine into a bare electron. Hence the quasiparticle weight is exactly one. As our second example, we consider states with antiferromagnetic long range order. In this case, the configuration with site $i$ empty and site $j$ doubly occupied is separated from the configuration with all sites singly occupied in energy by a gap proportional to the SDW order parameter. Thus, we expect the spinon - holon correlation function to decay exponentially at large distance. Our calculation do find such an exponential decay as shown in Figure 4 and 5. This exponential decay indicates that the spinon and the holon form well defined bound state and has a finite overlap with a bare electron. Calculation of Lee \textit{et. al.} do find a finite quasiparticle weight on such a state.

Another consequence of the spinon - holon recombination is the change of statistics of the charge carrier. In the absence of the spinon excitation, the holon is a bosonic excitation which move coherently in the RVB background. In the presence of the spinon excitation, the holon tend to bind with the spinon. The composite object of spinon - holon pair then acquire Fermi statistics and become normal carrier. This is especially true when the spinon - holon bound state is well defined. In the case of power law decaying spinon - holon correlation, there is no well defined bound state and the statistics is in a strict sense not
defined. However, when the energy scale involved is not too small, assigning Fermi statistics to the composite object of spinon - holon pair is reasonable since the power law decaying tail is numerically very small.

The spinon - holon recombination and the related change of statistics of charge carrier is essential for the dissipation of the supercurrent in a spin charge separated superconductor. The thermally excited spinon excitation would combine with the holon in the holon condensate. This combination would transform a superconducting charge carrier into a normal charge carrier. When the number of thermally excited spinon equals to the number of holon, all charge carrier in the superfluid are transformed into normal carrier and the superconductivity is gone. At low doping, the number of spinon excitation needed to destroy the superconductivity is small and it is thus expected that the spin state above $T_c$ is not significantly different from the RVB ground state. This may explain the normal state spin gap observed in underdoped cuprates.

As mentioned above, the spinon excitation can also be spontaneously generated in the d-wave RVB state by nonbipartite(for example NNN and NNNN) hopping term in the Hamiltonian. The spontaneously generated spinon will combine with the holon in the condensate and transform the latter into normal carrier. Thus, superconductivity is destroyed by the nonbipartite hopping term at low doping. This effect is recently studied by Shih et. al. [13] At higher doping level, the RVB background is modified so that the NNN and NNNN hoping are not suppressed and there is no need to generate spinon excitation. Then superconductivity will survive.

The spinon - holon recombination also modify the hole - hole correlation. When the spinon and the holon are tightly bound, the composite object of spinon - holon pair tend to avoid each other due to its Fermionic statistics. This change of hole - hole correlation is observed in numerical work of Lee et. al [10]. In their work, they calculated the correlation of a pair of holes in a state with coexisting d-wave RVB and SDW order. They find the holes tend to attract each other when there is no spinon excitation. When a pair of spinon excitations are generated, the hole - hole attraction disappear. Figure 6 and 7 show the hole - hole correlation calculated in the d-wave RVB state with and without spinon excitation. Although spinon and holon are less tightly bound in the d-RVB state, the influence of spinon - holon recombination on the hole - hole correlation function is still quite remarkable. From the figure we see clearly that the second hole is pushed away from the hole at the origin in
the presence of a pair of spinon excitations.

We conclude that spinon - holon recombination is a generic feature in projected wave functions. This effect play an important role in the dissipation of supercurrent in cuprates. The spinon - holon recombination also affect significantly the quasiparticle properties and hole - hole correlation in projected wave functions.

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[14] The state studied in [10] also has antiferromagnetic long range order. This order enhance the spinon - holon recombination.
[15] Another way to release the NNN and NNNN kinetic energy is to introduce NNN and NNNN hoping term in the mean field ansatz for the spinon. However, such nonbipartite term will cause fundamental change on the structure of spin wave function and result in significant increase of the exchange energy.
FIG. 1: Spinon - holon correlation function for projected one dimensional Fermi sea. The inset show the data in logarithmic scale.

FIG. 2: Spinon - holon correlation function for a d-wave RVB state with $\Delta = 0.25$. The calculation is done on a $20 \times 20$ lattice and the holon is located at (10,10).
FIG. 3: Power law decay of the spinon - holon correlation at large distance for d-wave RVB state. Here, L is the lattice size, $r_{\text{max}}$ is largest distance that can be defined in such a lattice.

FIG. 4: Spinon - holon correlation function in a spin background with both d-wave RVB and antiferromagnetic order. The SDW order parameter is $\Delta_{\text{AF}} = 0.1, \Delta = 0.25$. 
FIG. 5: Exponential decay of spinon - holon correlation at large distance in a spin background with antiferromagnetic order.

FIG. 6: Hole - hole correlation (normalized by its value for NN holes) in a d-wave RVB state with $\Delta = 0.25$ in the absence of spinon excitation. The calculation is done on $12 \times 12$ lattice and one the hole is located at (6,6).
FIG. 7: Hole - hole correlation in a d-wave RVB state with $\Delta = 0.25$ in the presence of a pair of spinon excitation.
