Properties of the doped spin 3/2 Mott insulator near half filling

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Abstract

We develop an exact generalized Bogoliubov transformation for the spin 3/2 Hubbard model with large anti-Hunds rule coupling near half filling. Since our transformation is unitary, we can thereafter employ standard approximate mean field theory methods in the full Hilbert space to analyze the doped Mott insulator, in contrast to a conventional approach based on truncated Hilbert spaces complemented with hard core constraints. The ground state at exactly half filling is an insulating (Mott) singlet, and according to our analysis a non-Fermi liquid order parameter $\Delta$ usually associated with extended s-wave superconductivity, will appear self-consistently as soon as a finite density $n$ holes are introduced. The non-Fermi liquid behavior is a consequence of the nonlinear nature of the unitary transformation mapping the Mott singlet state to a Fock vacuum which introduces anomalous terms such as $\Delta n$ in the effective Lagrangian. Our analysis uses an approach that generalizes readily to multi-band Hubbard models and could provide a mechanism whereby a non-Fermi liquid order parameter proportional to density is developed in Mott insulators with locally entangled ground states. For more complicated systems, such an order parameter could coexist naturally with a variety of other order parameters.

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I. INTRODUCTION

A Mott transition is expected to occur when the overlap between atomic orbitals in an insulator becomes large enough for the hopping energy to overcome the energy associated with charge fluctuations. To understand this transition has turned out to be a very difficult problem that has been attacked by a variety of means, with dynamic mean field theory being an important recent contribution \[1, 2, 3, 4, 5, 6, 7\]. In the present work we will develop an alternative approach, more in the spirit of BCS theory, which is appropriate for understanding doped Mott insulators where the parent state has an even number of electrons, and thus integer spin, at each state. Such models have been considered for instance in two-band Hubbard models in the context of ruthenate alloys \[8\], and multi-band Hubbard models in the theory of doped \[C_60\] \[2, 3, 6, 9, 10\]. We will present evidence for non-Fermi liquid behavior in these systems even for weak doping. We shall focus on the simplest system to which our conclusions apply, namely the spin 3/2 Hubbard model on a square lattice with anti-Hunds rule couplings \[8, 9, 10, 11, 12, 13\].

We define the local particle number by \(n_r = \sum_s c_{s,r}^+ c_{s,r}\) and the spin by \(S_r = \sum_s c_{s,r}^+ S_{s,s'} c_{s',r}\), where \(-\frac{3}{2} \leq s \leq \frac{3}{2}\) and \(S_{s,s'}\) are the generators of spin 3/2 rotations. Furthermore, we define the operator \(P^\dagger_{2,m}(r)\) which creates an \(l = 2, l_z = m\) state with two fermions \[12\], \(P^\dagger_{2,m}(r) = \sum_{\alpha,\beta} \langle \frac{3}{2}\frac{3}{2}\alpha\beta | \frac{3}{2}\frac{3}{2}; 2, m \rangle c_{\alpha,r}^+ c_{\beta,r}^+\). We also define the \(SU(2)\) invariant \(P^2_r = \sum_m P^\dagger_{2,m}(r) P_{2,m}(r)\). The Hamiltonian containing the maximal number of onsite terms permitted by symmetry is

\[
H = -t \sum_{r,\delta} c_{s,r}^+ c_{s,r+\delta} + \sum_r \left( U n_r(n_r - 2) + J P^2_r \right),
\]

where an arbitrary chemical potential is absorbed in \(U\). Another term which can be considered is of course \(S^2_r\), but for spin 3/2 this obeys \(P^2_r = \frac{1}{3} S^2 - \frac{5}{2} n + \frac{5}{4} n^2\), so there is no loss of generality in the onsite term of our Hamiltonian aside from ignoring the possibility of an arbitrary term proportional to \(n^3\). We will consider the case \(J > 2U \gg t\), thus the singlet state is heavily favored near \(n = 2\).

The single site spectrum consists of sixteen states: an empty site, four equivalent spin 3/2 singly charged states, a singlet and five spin 2 doubly charged sites, four spin 3/2 charge three states and a charge four singlet. If \(E_g(n)\) is the atomic ground state for \(n\) particles we find \(E_g(0) = E_g(2) = 0\), \(E_g(1) = -U\), \(E_g(3) = 5J + 3U\), \(E_g(4) = 10J + 8U\) and the quintet
state has energy $2J$. The lowest energy states obey $E_g(n + 1) + E_g(n - 1) - 2E_g(n) \geq U \gg 0$ so there is no tendency for superconducting pair formation from any of the local interactions.

With our choice of parameters, standard arguments imply that the ground state for $n = 2$ and small $t$ should be a spin singlet. For small doping near zero filling, the ground state will most likely be a normal Fermi liquid. This statement may be violated if $U$ and $J$ are sufficiently large, and a spin-symmetry breaking state may appear according to the Stoner criterion. Whether or not this happens depends on the density of states, which at least in the case of two dimensions remains finite even down to $n = 0$. Numerical simulations indicate the tendency toward spin ordering is grossly exaggerated in mean field theory. In any case a deeper discussion of this point is not within the scope of the present article, which is to investigate the analog of a Fermi liquid near half filling.

The Mott singlet $\ket{\Phi_s(r)} = \Delta^\dagger_r \ket{0}$ at site $r$ is created from the vacuum by the operator $\Delta^\dagger_r$, given by

$$\Delta^\dagger_r = \frac{1}{2\sqrt{2}} \sum_s e^{i\pi(s + \frac{1}{2})} c^\dagger_{s,r} c^\dagger_{-s,r} . \tag{2}$$

A natural first attempt to understand the system for small hole doping is to try the same method as for the nearly half filled spin $1/2$ Hubbard model, i.e., to make a particle-hole transformation $\hat{c}^\dagger_{s,r} = c_{-s,r}$, where $\hat{c}^\dagger_{s,r}$ and $c_{s,r}$ are new local fermionic creation and destruction operators. In contrast to the case of the filled spin $1/2$ Hubbard model however, this canonical transformation fails a number of criteria if the Mott singlet is to act as a vacuum for the new operators. In particular, we see that

$$\hat{c}_{s,r} \ket{\Phi_s(r)} \neq 0 \tag{3}$$

$$\langle \Phi_s(r) | \hat{c}_{s,r} \hat{c}^\dagger_{s,r} | \Phi_s(r) \rangle \neq 1 \tag{4} .$$

The first inequality is perhaps not so severe; after all the operator $\hat{c}_{s,r}$, being fundamentally a fermion creation operator creates a state with three fermions on site $r$, and we could argue that we could ignore this problem by suitably projecting the states on those with two or less particles. This is in fact the approach usually taken in attempts to perturbatively construct a new vacuum at $n = 2$. The second inequality is much worse; it is a consequence of the singlet being entangled, i.e. it cannot be written as a product state in any one-particle basis. As a result, the putative creation operator does not generate a normalized state from the vacuum. The entanglement property implies that the destruction operator on the cre-
ated state does not recreate the ground state—not even in the two particle space since it projects into the $S = 2$ two-particle states.

II. CANONICAL TRANSFORMATION TO THE MOTT SINGLET VACUUM

We now show how to systematically construct creation and annihilation operators that have the correct local properties. We seek a canonical transformation that fulfills the following criteria: (a) it maps $|\Phi_s(r)\rangle$ to $|0\rangle$, and (b) it maps the singly charged states to themselves. Due to our choice of interaction parameters, where $J > 2U$, we also expect that the state composed of two holes will play the same role in the hole doped Mott insulator near $n = 2$, as the doubly charged singlet does for small filling. The canonical transformation that we desire therefore has the property that it interchanges the Mott singlet and the vacuum, leaving all other states invariant. The $S = 2$ doubly charged states will have the same charge as the Mott singlet. However, due to the constraints imposed by a canonical transformation utilizing only the spin $3/2$ fermion operators, these doubly charged states must be obtained by two applications of the new creation operator, while the singlet created by another double combination of these creation operators forms a state with relative charge minus two. These considerations force the canonical transformation to be charge non-conserving.

The canonical transformation that accomplishes this and similar mappings can be systematically obtained through the method in Ref. [15]. However, we can obtain it without much formalism through the following argument. Our desired operator is “almost” $\Delta_r^\dagger$. The problem is that this operator generates unwanted side effects in the $n = 1$ and $n = 2$ particle subspaces by mapping these to new states with $n = 3$ and $n = 4$. We can get rid of these unwanted overlaps by using a projection operator, and therefore define $Q_r^\dagger$ by $Q_r^\dagger = \Delta_r^\dagger(1 - n)(1 - \frac{n}{2})$. It is straightforward to check that $Q_r^\dagger |0\rangle = |\Phi_s(r)\rangle$, that $Q_r |\Phi_s(r)\rangle = |0\rangle$, and that $Q_r$ and $Q_r^\dagger$ annihilate all other states. A canonical transformation that rotates the states $|0\rangle$ and $|\Phi_s(r)\rangle$ at each site $r$ into each other without affecting the other states is provided by the unitary operator

$$U(\tilde{\phi}_r) \equiv e^{iG(\tilde{\phi}_r)} = \prod_r U_r(\tilde{\phi}_r)$$

$$U_r(\tilde{\phi}_r) \equiv e^{iG_r(\tilde{\phi}_r)} = e^{i(\tilde{\phi}_r Q_r^\dagger + \phi^*_r Q_r)}$$

(5)
where \( \tilde{\phi}_r \equiv \phi_r e^{i\chi_r} \) (\( \phi_r \) and \( \chi_r \) are real). On \( \mid 0 \rangle \) and \( \mid \Phi_s(r) \rangle \) the transformation becomes

\[
U_r(\tilde{\phi}_r)|0,0 \rangle = \cos \phi_r + i \sin \phi_r (e^{i\chi_r} Q_r^\dagger + e^{-i\chi_r} Q_r),
\]

(6)

whereas it is unity on all other states. Choosing \( \phi_r = \pi/2 \), for all \( r \), we obtain the canonical transformation that fulfills our criteria, i.e. it interchanges the empty state and the Mott state at each site without affecting the other states.

Applying the unitary transformation Eq. 5 with \( \phi_r = \pi/2 \), the true vacuum state, \( \mid 0 \rangle \), is mapped onto the Mott insulator at half-filling \( \mid \Phi_s \rangle \). The phase factors \( e^{i\chi_r} \) enter this state only as an overall phase \( \sum_r \chi_r \), and can be neglected. In general, however, it is obvious from Eq. 5 that the unitary transformation gives a state where the phase factors enter in a non-trivial way. In particular, this is the case for the slightly doped Mott insulator, which we will be interested in below. This will be mapped onto a state near the true vacuum state, which can then be analyzed with standard methods.

Note that the phase factors, \( e^{i\chi_r} \), are crucial to retain local gauge symmetry in the same way as the complex phases introduced into the Bogoliubov transformations are necessary to restore gauge invariance in BCS theory.

### III. A VARIATIONAL ANSATZ

We now turn to a systematic variational analysis of the slightly doped Mott insulator using the canonical transformation in Eq. 5 and use computer algebra to handle the complicated fermion polynomials that occur. In analogy with ordinary Fermi liquid theory, as well as the BCS theory of superconductivity, we will then search for a variational state with particle number given by \( n = 2 - \delta \) that is obtained from the vacuum by a canonical transformation \( e^{i\mathcal{G}_u} \) depending on a set of parameters \( u \). We define the functions \( E(u) \) and \( N(u) \) by

\[
E(u) = \langle 0 \mid e^{-i\mathcal{G}_u} H e^{i\mathcal{G}_u} \mid 0 \rangle \quad \text{(7)}
\]

\[
N(u) = \langle 0 \mid e^{-i\mathcal{G}_u} N e^{i\mathcal{G}_u} \mid 0 \rangle \quad \text{(8)}
\]

The values \( \{u\} \) which minimize \( E(u) \) define our variational ground state \( e^{i\mathcal{G}_u} \mid 0 \rangle \) with particle number \( N(u) \). We have seen that for \( n = 2 \), the transformation \( \mathcal{G}_u \) is simply \( G(\chi_r) \equiv G_0(\chi_r) \) given by Eq. 5. We therefore expect that near the Mott insulator, the relevant transformation will be given by a further transformation close to the identity. We therefore make the ansatz \( e^{i\mathcal{G}_u} = e^{iG_0(\chi_r)} e^{i\mathcal{G}'_u} \equiv U_0 U' \).
Note that since we can continuously rotate the Mott state at \( n = 2 \) to the true vacuum by letting \( \phi \) go from \( \pi/2 \) to zero, we can generate a Mott singlet on a site either by having \( U'_r = 1 \) and \( \phi_r = \pi/2 \), or by having \( U'_r = U_r(\pi/2) \) and \( \phi_r = 0 \). In general, we can make a coherent superposition of empty and doubly occupied singlet sites, both by letting \( \phi \) vary and by adding an onsite s-wave order parameter. As could be expected, this indeterminacy leads to a numerical instability in the variational equations which we resolve by simply taking \( \phi_r = \pi/2 \) for all \( r \), and not further exploiting these variational parameters.

In order to construct an ansatz for \( e^{iG_n} \) we first work out \( e^{-iG_0(\chi_r)} H e^{iG_0(\chi_r)} \). This operator is obtained by replacing each occurrence of the fermion operator \( c^\dagger_{r,s} \) by \( e^{-iG_0(\chi_r)} c^\dagger_{r,s} e^{iG_0(\chi_r)} \) and similarly for \( c_{s,r} \). This expression is complicated, but it can nonetheless be worked out exactly in terms of polynomials of \( c_{s,r} \) and \( c^\dagger_{s,r} \), since the fermion algebra at a site is closed. The exact expression, written here for reference only, is given by

\[
\begin{align*}
  c^\dagger_{s,r} \rightarrow c^\dagger_{s,r} & \left( (\Delta^\dagger e^{-2i\chi} (1 - n) - e^{2i\chi} \Delta) + \left( \frac{S^2}{3} + n + \frac{n^4}{6} \right) \right) + \\
  & (-1)^{(s+\frac{1}{2})} e^{2i\chi} 2^{-\frac{1}{2}} \left( -1 + e^{-2i\chi} \Delta^\dagger + \left( \frac{S^2}{3} + n + \frac{n^4}{4} \right) \right) c_{-s,r},
\end{align*}
\]

where the subscripts are dropped on the right hand side. The notation : \( O : \) is used to indicate a normal ordered operator, \( i.e. \) strings of fermion operators where all creation operators are anticommutated to the left and annihilation operators to the right taking only into account the sign of the permutation. In this case, : \( n^2 := n^2 - n \) and : \( S^2 := S^2 - 15n/4 \).

The onsite interaction is zero in the vacuum and two particle singlet subspace. Since these are the only two states affected by the canonical transformation, this interaction remains invariant, while the chemical potential transforms according to

\[
n \rightarrow 2 - \left( n - \frac{5n^2}{4} - \frac{3S^2}{3} + \frac{n^4}{6} \right).
\]

Anticipating a mean field calculation under the assumption of no spontaneously broken global symmetries, we do a Wick decomposition of the onsite term, and calculate the expectation value according to

\[
\langle U_n(n-2) + J P^2_r \rangle = -\hat{n}U + \hat{n}^2 \left( \frac{5J}{8} + \frac{3U'}{4} \right) + 2 \hat{\Delta}^2 U,
\]

where a hat indicates the expectation value of an operator composed of ordinary fermion operators evaluated in the state \( U' | 0 \rangle \) near the physical vacuum. Similarly, the expectation
values for the density and s-wave order parameter $\Delta^\dagger$, become exactly

\[ \langle \Delta^\dagger \rangle = \frac{(\hat{\Delta}^*)^2}{2} e^{-i\chi} \hat{\Delta} e^{2i\chi} \left( 1 + \left| \frac{\hat{\Delta}}{2} - \frac{\hat{n}}{2} + \frac{\hat{n}^2}{16} \right| - \hat{\Delta}^* \left( \left| \hat{\Delta} \right|^2 - \frac{\hat{n}}{2} + \frac{\hat{n}^2}{8} \right) \right) \]  

(12)

\[ \langle n \rangle = \hat{n} + 2 \left( 1 - \frac{\hat{n}}{4} \right)^2 \left( 1 - \frac{\hat{n}}{2} \right) - \frac{\hat{n}^2}{2} \left( 1 + \left| \hat{\Delta} \right|^2 \right) \]  

(13)

We now derive a similar expansion of the hopping operator. In this case the expressions become a terrible mess—far too complicated to write down in their entirety. It is however possible to construct a systematic expansion in the number of fermion operators, which is appropriate for small doping. To this respect, we take the entire expression, and rewrite it exactly as a sum of normal ordered terms. We then truncate this expression at fourth order in fermion operators and keep expectation values of on-site and nearest neighbor s-wave pairing amplitudes, ordinary hopping and density operators. Defining

\[ \Delta^\dagger_{r,r'} = \sum_s \frac{(-1)^{(s+\frac{1}{2})}}{2\sqrt{2}} c^\dagger_{s,r} c_{-s,r'} \]  

(14)

\[ h_{r,r'} = \sum_s c^\dagger_{s,r} c_{s,r'}, \]  

(15)

we find that the hopping operator, truncated to fourth order in fermion operators, becomes

\[ \langle h_{r,r'} \rangle = -\frac{5t}{4} \hat{n} \left( e^{2i\chi_r} \Delta_{r,r'} - e^{2i\chi_{r'}} \Delta^*_{r,r'} + \frac{1}{2} e^{2i(\chi_r - \chi_{r'})} \right) \]  

(16)

Decomposing the s-wave order parameters as,

\[ \Delta_{r,r'} = e^{-i\eta_{r,r'}} \tilde{\Delta}_{r,r'} \]  

(17)

\[ \Delta_r = e^{-i\eta_r} \tilde{\Delta}_r, \]

where $\tilde{\Delta}_{r,r'}$ is real, we obtain,

\[ \langle h_{r,r'} \rangle = -te^{i(\chi_r - \chi_{r'})} \left[ \frac{5}{4} \hat{n} (e^{i(\chi_r + \chi_{r'} - \eta_{r,r'})} \tilde{\Delta}_{r,r'} + \text{h.c.}) - \frac{1}{2} (1 - \hat{n}) e^{i(\chi_r - \chi_{r'})} h_{r,r'} \right] \]  

(18)

\[ + \left\{ (e^{2i(\chi_r - \eta_r)} \tilde{\Delta}_r - \text{h.c.}) (e^{i(\chi_r + \chi_{r'} - \eta_{r,r'})} \tilde{\Delta}_{r,r'} + \text{h.c.}) \right\} \]  

\[ + \ldots . \]

Written in this way, the invariance under local gauge transformations is manifest (of course provided that the original hopping term is supplemented with the usual electromagnetic phase factor $\exp(\int \frac{d^2\pi}{2} \cdot \vec{A}(\vec{r})$)).

Note that the combinations $\chi_r + \chi_{r'} - \eta_{r,r'}$ and $\chi_r - \eta_r$ are gauge invariant, so it is physically meaningful to fix them to some value — this corresponds to locking the phase of
the order parameter to those of the on-site s-wave density, i.e. the phase of the local Mott singlets. Similarly, by virtue of Eq. 13, the combination \( e^{i(\chi_r - \chi_{r'} \hat{h}_{r,r'}} \) is also gauge invariant. In the following, we shall set \( \chi_r + \chi_{r'} - \eta_{r,r'} = \chi_r - \eta_r = 0 \).

The full set of variational parameters are now \( \chi_r \), which characterize the transformation \( U_0 \), together with the parameters \( \{U\} \), used to characterize \( U' = e^{iG_u} \). In the subsequent mean field calculation, these will be \( \hat{n}, \Delta_{r,r'}, \tilde{\Delta}_r \) and \( h_{r,r'} \), where \( \tilde{\Delta}_r \) is the amplitude of the local s-wave order parameter.

It is now clear that in order to evaluate the expression in Eq. 18 we must have some information about the phases \( \chi_r \). In the undoped Mott state, they only contribute to an overall phase, and are thus completely random. If this would be true also in the doped state, both terms in Eq. 18 would average to zero because of the phase factor \( e^{i(\chi_r - \chi_{r'})} \). In the doped state, however, it is reasonable to assume that some short range correlation is generated among the phases \( \chi_r \). This would correspond to having

\[
\langle e^{i\chi_r} e^{-i\chi_{r'}} \rangle = f(\vec{r} - \vec{r'}) .
\]  

Really, this should be shown by including the phases \( \chi_r \) in the variational calculation, but this is technically very hard to do, so we shall instead simply assume Eq. 19 to hold and set \( f(\vec{r} - \vec{r'}) = 1 \) for nearest neighbors. Under this assumption, Eq. 16 simplifies to,

\[
\langle h_{r,r'} \rangle = \frac{1}{2} \hat{h}_{r,r'} (1 - \hat{n}) - \frac{\alpha}{2} \tilde{\Delta}_{r,r'} \hat{n} + ... - \frac{1}{16} \tilde{\Delta}_r \hat{n}^2 ,
\]  

where for future reference we have included the lowest higher order term which couples linearly to \(\tilde{\Delta}_r\). We therefore find that the Hamiltonian expectation value to be minimized is given by the sum of Eq. 11 and Eq. 20, subject to total particle number given by Eq. 13. This effective Hamiltonian looks very much like an ordinary BCS Hamiltonian, corresponding to Eq. 1 but with one dramatic difference, namely the presence of a term proportional to \(\tilde{\Delta}_{r,r'} \hat{n}\), as well as a higher order term which couples linearly to the s-wave pairing operator.

**IV. MEAN FIELD ANALYSIS**

The mean field Hamiltonian can be analyzed by several equivalent methods. In the spirit of what was just developed, we could e.g. make a Bogoliubov-Valatin canonical transformation and minimize the energy of the retransformed vacuum. This variational procedure
would precisely correspond to the canonical transformation \( e^{iG_u} \) alluded to earlier. The method we actually use generalizes easily to finite temperatures and arbitrary large number of terms in the polynomial expansion of the mean field Hamiltonian. It uses that the density matrix \( \rho = e^{\beta(\Omega(T,\mu)-(H-\mu N))} \) minimizes the free energy \( F = \langle H - \mu N \rangle_\rho - kT \langle S \rangle_\rho \) for all values of \( \rho \) (\( e^{-\beta \Omega} \) is the partition function and \( S \) the entropy). We can then take \( \rho \) to be the exponential of an expression linear in \( \hat{n}_r, \hat{\Delta}_{rr'}, \hat{\Delta}_r \) and \( \hat{h}_{rr'} \), where the prefactors are varied to minimize \( F \). This method yields the ordinary BCS theory when applied to a Hamiltonian of the form in Eq. 1 and gives a more complicated self-consistent calculation when more terms are kept.

We have performed the mean field analysis numerically, both using the truncated expressions given explicitly above and the full mean field theory containing polynomials to seventh order. Since we construct an effective Hamiltonian, we define the hatted operators whose expectation values give the values \( \hat{\Delta}_r^\dagger \) in Eq. 16. The corresponding operators \( \hat{\Delta}_{rr'}^\dagger, \hat{\Delta}_{r,r'}^\dagger, \hat{h} \) are therefore formally \( \hat{\Delta}_r^\dagger = e^{-i\vec{g}_u \Delta_{rr'}^\dagger} e^{i\vec{g}_u} \) etc. but in the calculation this involves simply reinterpreting the original operator in Eq. 13 in terms of quasiparticle fermion operators. For the density matrix \( \rho \propto e^{-\beta H_{eff}} \) we choose the Hamiltonian \( H = H_{eff} \) as

\[
H_{eff} = \sum_{r,r'} (t' \hat{h}_{rr'} + 2\hat{\Delta}_{rr'}^\dagger) - \sum_r (\mu' n_r + 2\gamma_2 \hat{\Delta}_r^\dagger) + (CC) \quad (21)
\]

Our approximation is reasonable for small doping, and we confine the mean field analysis to this regime. We let \( \epsilon_k = (2 - \cos k_x - \cos k_y) \) in two dimensions with a similar expression for \( D = 3 \). With \( \mu' = Dt' + \delta \mu \) and \( \gamma_2 = D\gamma + \delta \gamma \) we define \( \epsilon_k = t' \epsilon_k + \delta \mu, d_k = \gamma \epsilon_k + \delta \gamma \) and \( E_k = \sqrt{\epsilon_k^2 + d_k^2} \). The energy gap \( \Delta \) is the minimum in \( E_k \), and it is easy to verify that for small doping an excellent approximation is given by \( \Delta = \frac{|\gamma \delta_{k_x} - \delta \gamma t'|}{\sqrt{\gamma^2 + (t')^2}} \). We define the momentum space sums as \( \tilde{f}(k) = \sum_k \frac{|v' f(k)|}{E_k} \). Taking into account that there are four spin values we find the following expression for the doping \( \delta \approx \hat{n} \), where expectation values of operators are dropped when the context is clear,

\[
\hat{n} = 4 \times \frac{1}{2} \int \left( 1 - \frac{\epsilon_k}{E_k} \right) d^2 k = 2 - 2 \tilde{c}_k / |t'| \quad (22)
\]

The expressions for \( t' \) and \( \gamma \) can be read off to lowest order from Eq. 20

\[
t' = -\frac{1}{2} t(1 - \hat{n}) \quad (23)
\]

\[
\gamma = -\frac{5\hat{n} t}{4\sqrt{2}} \quad (24)
\]
while the definition of the on-site s-wave order parameter can be read off from Eq. \ref{eq:onsite_nonspec}

\[ D\gamma - \delta \gamma = 2\sqrt{2}U\Delta_r. \]  

(25)

In writing Eq. \ref{eq:onsite_nonspec} we neglected the non-local repulsive interactions of type \( n_r n_{r'} \) that will certainly be present in any realistic model with screened Coulomb interaction. Assuming a nearest neighbor term, \( U_1 n_r n_{r'} \) and using the identity \( \langle n_r n_{r'} \rangle = 1 + \frac{1}{2} \hat{\Delta}_{r,r'} \hat{\Delta}_{r,r'}^\dagger - \frac{1}{4} h_{r,r'} h_{r',r} - 2(\hat{n}_r + n_{r'}) + \frac{5}{2} (n_r^2 + n_{r'}^2) + n_r n_{r'} \), Eq. \ref{eq:onsite_nonspec} would change to

\[ \gamma = -\frac{5\hat{n}t}{4\sqrt{2}} + \sqrt{2} U_1 \hat{\Delta}_{r,r'}^\dagger \]  

(26)

Below we argue that this would not qualitatively change our conclusions.

As usual, self-consistency implies a gap equation which here reads,

\[ \Delta_r = -\frac{1}{\sqrt{2}t'} \tilde{\Delta}_k. \]  

(27)

After expanding to lowest order in \( \delta \) and doing some some algebra this can be recast as

\[ \frac{t}{4U} \left( \frac{\Delta}{\sqrt{2}t} - \frac{5D\delta}{8} \right) = \frac{5\delta}{8} - \frac{\Delta}{t \sqrt{2}}, \]  

(28)

which is a closed equation that can be used to find the physical gap \( \Delta \) as a function of \( \delta \).

Using the self-consistent equations, we can find expressions for the extended and onsite s-wave pairing amplitudes:

\[ \tilde{\Delta}_{r,r'} \approx \left( \frac{5D\delta}{8} - \frac{\Delta}{\sqrt{2}t} \right) \]  

(29)

\[ \tilde{\Delta}_r \approx -\frac{t}{2U} \hat{\Delta}_{rr'} \]

Thus, not surprisingly we find that the onsite s-wave component is reduced by a factor \( t/U \) relative to the extended component. We note that the particular combination corresponding to \( \Delta_{rr'} \) occurs in the left hand side of Eq. \ref{eq:gap_eq} which is consistent with the onsite s-wave component vanishing while the nearest neighbor extended pairing remains finite in the limit \( U \to \infty \). We can now understand what would be the qualitative effect of adding extra repulsive interactions corresponding to the redefinition Eq. \ref{eq:gamma_red} of the variational parameter \( \gamma \). For large \( U_1 \), \( \gamma \) will effectively be put to zero corresponding to \( \tilde{\Delta}_{r,r'} \sim \frac{t}{U_1} \hat{n} \), rather than \( \tilde{\Delta}_{r,r'} \sim \delta \). We see that the scale of \( \tilde{\Delta}_{r,r'} \) changes but it is still non-zero for arbitrary small doping.
A. Asymptotic behavior of the gap in \( D = 2 \)

In two dimensions, the expression Eq. 22 can be approximated by

\[
\hat{n} \approx \frac{1}{\pi |t'|} (\delta_\mu + \sqrt{\delta_\mu^2 + \Delta^2}).
\]  

(30)

The expression for \( \tilde{1} \) is logarithmically singular but can be approximated by

\[
\tilde{1} \approx \frac{-1}{2\pi} \ln \left( \frac{-\delta_\mu + \sqrt{\delta_\mu^2 + \Delta^2}}{32 |t'|} \right) = \frac{1}{2\pi} \ln \left( \frac{32\hat{n}(t')^2}{\Delta^2} \right),
\]  

(31)

where Eq. 30 was used. In spite of the logarithmic singularity, the self-consistent equation Eq. 28 can be solved in closed form. Defining \( q = \Delta / (t\delta) \) the (inverse) equation is

\[
\delta \approx \frac{8\pi}{q^2} e^{\frac{4q^5 - 5q^3 + 2q}{8qU/t}}.
\]  

(32)

By plotting the pairs \((\delta, q\delta)\) according to the above formula as a function of \( q \), we find the gap as a function of \( \delta \), shown for values of \( U = (\infty, 10, 5, 1) \) in Fig. 1. We can see an almost linear behavior of the gap as a function of doping that is quite insensitive to the value of \( U \). For all values of \( \delta \) and \( U \) the approximation \( \Delta \approx t\delta \) is a surprisingly good approximation. A comparison with the numerical solution of the self-consistent equations is shown in Fig. 2.

B. Asymptotic solution for \( D = 3 \) and small doping

In the case \( D = 3 \), the vanishing density of states near \( k = 0 \) makes the integral \( \tilde{1} \) converge. In this case the self-consistent equation is Eq. 28 with \( D = 3 \), and constant \( \tilde{1} \). However, due to the vanishing density of states, even relatively small values of density lead to quite substantial values of \( \mu \) and \( \delta \) so the asymptotic value of this equation is far from being reached even for doping as low as .01. The corrections to \( \tilde{1} \) are rather slowly varying, so the linear dependence of the gap upon doping is obtained for the \( D = 3 \) case as well, as shown in Fig. 2.

V. EFFECTIVE THEORY FOR SMALL \( \delta \)

After applying a transformation that rigorously preserves the full Fock space, we have obtained a non-Fermi liquid behavior for the doped spin 3/2 Mott insulator by using standard
mean field theory methods. Here we contrast this to an effective theory for the Hamiltonian in Eq. 1, derived in the limit of small doping \( \delta \ll 1 \) and small hopping \( t \ll U, J \), using the more conventional approach of projection on a low energy subspace. Ignoring hopping, \( t = 0 \), this low energy sector consists of states where each site is occupied by either a Mott singlet \(| \Phi_s \rangle \), which we choose as the Fock vacuum, \(| \Phi_s \rangle \rightarrow | 0 \rangle \), or by a single charge \(| s \rangle = c^\dagger_s | 0 \rangle \) with spin 3/2 (\( s = \pm 1/2, \pm 3/2 \)) – all other states are separated from these by a gap of order \( X \sim U, J \). Restricting to this low energy sector and including the hopping in perturbation theory gives to order \( t^2/X \), the effective Hamiltonian

\[
H_{\text{eff}} = -\tilde{t} \sum_{r,\delta,s} c^\dagger_{sr} c_{s,r+\delta} + \sum_{r,\delta,\alpha,\alpha',\beta,\beta'} \tilde{J}_{\alpha\alpha'\beta\beta'} c^\dagger_{\alpha,r} c_{\alpha'\beta,r+\delta} c_{\beta',r+\delta} (33)
\]

subject to the constraint \( \sum_s c^\dagger_{sr} c_{sr} \leq 1 \) (\( \tilde{J}_{\alpha\alpha'\beta\beta'} \) are \( SU(2) \) scalars). This \( t - J \)-type model describes four species of fermions with nearest neighbor hopping (\( \tilde{t} \sim t \)), nearest neighbor exchange couplings (\( \tilde{J} \sim t^2/X \)) and with the hard-core constraint that no two fermions occupy the same site. Second order perturbation theory guarantees a finite, albeit weak, attraction which opens the possibility of having a superconducting phase even for small doping. From this approach, however, we would expect such a phase to be destroyed by a nearest neighbor repulsion that is normally present in a realistic model. Thus, our previous mean field calculation is at odds with this approach. If the former turns out to be valid, it suggests that there are non-perturbative effects due to the hard-core constraints that are not easily accounted for in the conventional formulation. If on the other hand the hard-core constraints are not very important and the naive picture of four different species of weakly interacting fermions is essentially correct, it would suggest that our mean field treatment of the phase phase fluctuations does not capture the correct physics.

VI. DISCUSSION AND SUMMARY

A. The anomalous term \( \Delta_{r,r'} n_r \).

We see from Eq. 13 that in order to have a nonzero doping \( \delta = 2 - \langle n \rangle \), we must have \( \hat{n} > 0 \), in fact \( \hat{n} \approx \delta \) to lowest order in \( \delta \). Energetically we will also have \( \hat{h} \neq 0 \) for finite \( \delta \). According to Eq. 18 the extended s-wave pairing field \( \hat{\Delta}_{r,r'} \) cannot vanish and in fact will be proportional to doping. This in turn generates a (much smaller) on-site pairing
through the self-consistent equations. Note that this pairing field can never completely vanish because of the linear coupling to higher order terms. At finite temperature the mean field theory will presumably eventually break down via an $xy$-transition due to phase fluctuations that we have not taken into account. This has been discussed in a series of recent papers where the term “gossamer superconductivity” [16, 17, 18] has been used to describe a similar scenario.

It is admittedly not easy to understand the physical origin of these new anomalous terms of the type $\Delta_{r,r'} n_r$. On a technical level, they are forced by the fermion statistics which constrains the form of the canonical transformation necessary to map a local Mott ground state to the vacuum. In our case, this transformation must be (a) nonlinear in fermion operators and (b) charge non-conserving. Property (a) yields an effective interaction from the hopping term near a charged ground state and property (b) makes this interaction non-gauge invariant. Property (a) is a necessary consequence of mapping a locally entangled state to the vacuum and property (b) is a consequence of mapping a charged state to the vacuum which breaks gauge symmetry. Very general arguments relying on long range phase coherence and a finite range gap function then predict that the system should be a superconductor [19]. Our mean field calculation, which suggests a superconducting ground state, supports this picture, given our assumptions about phase coherence.

We already pointed out the contradiction between our main result and what would be expected based on a conventional analysis of the type leading to Eq. but also stressed the difficulties related to the hard core constraints inherent in the latter approach. Here we should note that more elaborate schemes for dealing with these non-holonomic hard core constraints face severe difficulties related to phase fluctuations. For example, in the spin 1/2 Hubbard model at half-filling, one can turn the no double occupancy constraint into a holonomic gauge constraint by introducing spinons and holons. The resulting phase depends crucially on the fluctuations in the related gauge fields. By working in the full Hilbert space, we avoid these difficulties, but nevertheless our conclusions are still dependent on certain assumptions about phase coherence. Without a more sophisticated analysis of the phase fluctuations, we cannot rule out that these will be important and e.g. destroy the superconducting state at low doping.
B. Range of validity and applicability

We now assume that our analysis is correct at low doping, and discuss its range of validity and applicability. At sufficiently large value of doping, the theory will yield a free energy which is unfavorable compared to that of a doped \( n = 1 \) Mott insulator. The mean field picture suggests there will be a coexistence region where a slightly hole doped \( n = 2 \) Mott insulator will coexist with a hole doped \( n = 1 \) Mott insulator. The \( n = 1 \) Mott insulator will presumably have some sort of magnetic order at low temperature that breaks the large spin degeneracy of the uncorrelated odd filling Mott insulator. If a coexistence region really exists, or whether an intermediate phase which breaks translational invariance may exist, is beyond the scope of the present analysis. Our calculation thus makes assumptions about \( U \) which leave open the question if this behavior could really be seen in a physical system. On the one hand, \( U \) must be large enough (and \( J \) even larger) so that a Mott insulating state occurs at \( n = 2 \) and furthermore triply occupied sites are effectively absent. On the other hand, \( U \) must be small enough so that the correlated state will have lower energy than a mixed state with an \( n = 1 \) Mott insulator and an \( n = 2 \) Mott insulator.

We should also ask how dependent our approximations are on our specific choice of parameters. In particular what would happen if we had taken \( J < 0 \) in the spin 3/2 model? According to the analysis in Ref. [12], the ground state at \( n = 2 \) is than \( SO(5) \) invariant and we could choose for instance \( c_{\frac{3}{2},r}^\dagger c_{\frac{1}{2},r}^\dagger |0\rangle \) as the Mott vacuum. However, this as well as the other states with \( m \neq 0 \) are not entangled, and the procedure discussed here results in a simple particle-hole transformation of pairs of fermion operators which does not generate any anomalous terms and the ordinary BCS-type analysis presented in these calculations should be valid. However, the state \( m = 0 \) is entangled, and it can be checked by the methods of Ref. [15] that the canonical transformation that maps this state to the vacuum will be nonlinear in fermion operators as well as charge nonconserving causing an effective interaction and superconductivity to appear at finite doping through a similar mechanism discussed here for the Mott singlet.

If we take the parameters as \( 0 < J < 2U \), which of course is more physically reasonable, the energetically most favorable state constructed with two quasicharge operators \( \hat{c}_{s,r}^\dagger \) from the Mott singlet will no longer be a singlet with relative charge minus two, but rather one of the \( l = 2 \) multiplets with zero relative charge. The extended s-wave order parameter
will still appear since it is a direct consequence of mapping the Mott singlet to the vacuum, but there will be a spin order parameter introduced that takes the place of the local s-wave superconducting order parameter. The presence of an additional order parameter together with spin degeneracy makes this calculation more difficult and it awaits further analysis.

Finally, it is relevant to ask whether the transformation used for the spin 3/2 case could be applied to the spin 1/2 systems. First consider the canonical transformation which maps between the $n=0$ and $n=2$ states. This is the ordinary particle-hole transformation which is not charge conserving. However, the doubly occupied singlet is created by $c_{r \uparrow}^\dagger c_{r \downarrow}^\dagger |0\rangle$ and hence is factorizable in fermion operators. The canonical transformation is therefore linear and no new interaction terms are introduced in the transformation. The physical properties of the system are symmetric under charge conjugation, which is sufficient for the particle-hole transformation not to generate any new behavior and the present analysis is uninteresting. In the case of the half-filled Hubbard model, the Mott ground state corresponds to one electron per site. This cannot be mapped to the vacuum through a canonical transformation without globally violating the Fermi anticommutation relations[15].

C. Summary

We have presented a new type of canonical transformation for the half-filled spin 3/2 Hubbard model that maps the Mott insulator at half filling to the vacuum. This canonical transformation is straightforward to generalize to multi-band Hubbard models with a local spin singlet Mott insulating ground state. At finite doping, a self-consistent mean field theory for such a system results in a phase with long range phase coherence. An order parameter that is usually identified with extended s-wave superconductivity appears and is proportional to doping. The calculation appears to be in contradiction to other methods of attacking these kinds of problems, and we pointed out the difficulties with both approaches. Our calculations bear a striking resemblance to the “gossamer superconductor” scenario that has been recently introduced by Lauglin and coworkers. Although we have only explored a specific half-filled spin 3/2 Hubbard model, we believe that our method could be useful for variety of similar models with locally entangled Mott insulating ground states.
FIG. 1: Values of $\Delta/t$ as a function of doping $\delta$ for $U = (\infty, 10, 5, 1)$ for $\delta \leq 0.1$, with the gap decreasing monotone with increasing $U$ at given $\delta$. 
FIG. 2: Values of $\Delta/t$ as a function of doping $\delta$ for $U/t = 10$ for $\delta < 0.05$. The upper curve is for $D = 3$ and the lower data points for $D = 2$. The solid line is the fit to the $2D$ asymptotic curve according to Eq. [32]. The $3D$ fits with no visible error to the curve $\Delta/t = 1.4848\delta$ corresponding to $\tilde{\nu}_1 = 0.18$. 

{gap vs doping D=2,3 for U/t = 10}
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