An Order Parameter for the Mott-Hubbard Transition in One Dimension

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We propose an order parameter for the one dimensional Mott-Hubbard transition and provide numerical evidence and general theoretical arguments for the correctness of our proposal. In addition, we discuss some of the implications of this picture of the one dimensional Mott-Hubbard transition and speculate about possible higher dimensional analogs.

The one dimensional Hubbard model:
\[ H_{1D \text{ Hubb}} = t \sum_{x, \sigma, \nu = \pm 1} c_{\sigma, x+\nu}^\dagger c_{\sigma, x} + U \sum_x n_{\uparrow, x} n_{\downarrow, x} \] (1)

is known to exhibit a \( T = 0 \) quantum transition between metal and insulator as a repulsive interaction in the model is turned on and an analogous transition is believed to occur in higher dimensions. These “transitions” are somewhat peculiar in that a physical, local order parameter has not been identified. Instead, following Kohn’s suggestion, the “order parameter” for these transitions is generally taken to be the weight in the zero frequency delta function in the electrical conductivity at zero temperature. In the metallic phase this weight is finite and in the insulator it vanishes, so that the proposed order parameter does in fact distinguish the two phases qualitatively as it should. However, the conductivity is clearly not locally defined, so that it is meaningless to speak of, for example, a diverging length scale in its correlation functions, and it leads to a qualitative distinction between metal and insulator only at zero temperature. In the limit of large spatial dimensions, the Hubbard model undergoes a finite temperature metal-insulator transition associated with a crossing of the free energies of two distinct phases; however, there is no order parameter distinguishing the phases in that case, and the transition line vanishes at a critical point, much like the liquid-gas transition of water. This is not expected to be the case for the metal insulator transition in one spatial dimension and may also not be generic for finite dimensions. Therefore, it would be desirable to define some local operator whose expectation value or correlations clearly distinguished the metallic and insulating phases; the purpose of this paper is to propose an operator which fulfills these requirements for the one-dimensional transition and to examine possible implications for higher dimensions.

The operator we propose is an extension of the operator introduced by us and P. W. Anderson as exhibiting off-diagonal long range order (ODLRO) in a wide variety of quantum spin chains. There we noted that the groundstate of a generic, gapless XXZ model on \( N + 2 \) sites has a finite overlap in the thermodynamic limit with the state obtained by taking the groundstate of the same model on \( N \) sites and tacking a singlet pair of spins onto the end. If we define an operator, \( O(i) \), which adds a pair of sites with their spins in a singlet configuration at site \( i \) into spin model, and its conjugate operator, \( O(i) \), which removes a pair of sites, \( i \) and \( i + 1 \), from the model if they are in a singlet configuration or else annihilates the wavefunction on which it acts, then, as a consequence of the overlap mentioned above, this operator has ODLRO in its correlation functions: \( \lim_{|i-j| \to \infty} \langle O(i)O(j) \rangle \neq 0 \).

However, \( \lim_{|i-j| \to \infty} \langle O(i)O(j) \rangle \neq C_1 \); rather, since the groundstates of generic XXZ models on \( N \) sites and \( N + 2 \) sites have momenta differing by \( \pi \), \( \langle O(i)O(j) \rangle \sim (-1)^{|i-j|} \) and our order parameter exhibits a broken \( Z_2 \) symmetry. This \( Z_2 \) is unconnected with the division of a Neel ordered state on a bipartite lattice into sublattices: there is no Neel order in one dimension even at zero temperature. However, the theorems of Mermin and Wagner and Coleman do allow the breaking of a discrete symmetry, such as the \( Z_2 \) breaking indicated by our order parameter.

What, then, is the nature of this broken symmetry? In we utilized the connection between the Heisenberg model and the large U Hubbard model to motivate the conjecture that the insertion of a single spin of spin species \( \sigma \) into a Heisenberg model at site \( j \) was equivalent in the Luttinger liquid description of that models low energy physics to the action of the operator \( i^j \exp[\Theta_{R,\sigma}(ja)] + (-i)^j \exp[\Theta_{L,\sigma}(ja)] \). This not only accounts for the ODLRO of the singlet insertion, but explains the behavior of the family of operators in which singlet pairs of spins are inserted into sites which are not adjacent. We have further investigated this proposal using exact diagonalization and Haldane and Shas-
try's [14] solution of the inverse squared exchange model, to show that spin insertion is essentially equivalent to spinon creation [11] or the annihilation of a spinon of the opposite spin species and the conjecture is now firmly supported. However, it leads to a rather peculiar picture for the cause of the broken symmetry. The “operator” responsible in Luttinger liquid description is $(-1)^j$, i.e. a $c$ number [11]. This suggests that the order is not the order of a spin model at all, and we propose that it should rather be thought of as the charge “order” which sets in when a Mott-Hubbard transition occurs in one dimension and the low energy effective theory is transformed from one of interacting fermions to one containing only spin degrees of freedom. In support of this, we note that all of the spin models for which we have demonstrated this order can be obtained as the low energy limits of fermion models which have undergone such a transition.

To check the proposal that the order in question is really in the charge sector, we have carried out several numerical and analytic investigations. First, we have verified that the “order” probed by the singlet insertion is not that of the spin degrees of freedom by conducting a finite temperature study of the singlet insertion-singlet deletion correlation function for the XY model. In that case, the mapping of the model onto free fermions allows us to study large systems sizes at finite temperatures to examine how the spin and $Z_2$ orders are degraded. Some results from Monte Carlo are shown in Fig. 1. It is clear that the order is not degraded by finite temperature in the same way as the more conventional spin correlations are.

![FIG. 1. Zero and finite temperature results for the singlet insertion/deletion correlator and the more conventional two point function of $s_x$. Results are for a one dimensional XY model of 100 sites with periodic boundary conditions (PBC). Inset: results for correlators for a fixed separation of 25 sites as a function of temperature, $T$.](image)

Apparently, the identification of the singlet insertion with a $c$ number in the spin model does not hold rigorously and the singlet-correlation/singlet-deletion correlator is affected by the finite temperature in the spin model, lacking ODLRO at high and probably all finite temperature. Nonetheless, the degradation is enormously less severe than that occurring for other, typical spin correlation functions. For example, at $T = 0.15J$, $(s^x s^x)$ decays exponentially with a correlation length of $\sim 4.0$ lattice spacings, while $(O^1 O)$ decays by well less than a factor of 2 over a separation of 50 sites! It is not even clear from results at this temperature that the ODLRO has been destroyed. We attribute this difference in behavior from conventional spin correlators as the result of the fact that the XY model, viewed as a model with an Mott-Hubbard ordered charge sector, has an infinitely large charge gap. Thus the charge order, as probed by our singlet insertion, is unaffected by finite temperature, which rapidly destroys all of the usual spin order; the singlet insertion/deletion correlator is only indirectly connected with the charge sector order and it appears that only if the spin degrees of freedom are effectively at zero temperature does it exhibit ODLRO, so its correlator does decay at finite temperatures, but extremely slowly.

Having shown that our order is almost not degraded for separations and temperatures where spin order is totally lacking, it remains to show that it is sensitive to charge ordering of the Mott-Hubbard type. First, it is possible to show that, for free, $SU(2)$, spin $\frac{1}{2}$ fermions at half filling, the operator which adds two adjacent, occupied sites with spins in a singlet configuration does not have ODLRO. Rather, the correlation function decays algebraically like $x^{-1}$ (or, for $SU(N)$ generalizations, like $x^{-\frac{1}{N}}$ for $N$ inserted sites in an $SU(N)$ singlet). We have shown this both numerically and analytically [12], and therefore know that free fermion systems, which should not show Mott-Hubbard order, do not show ODLRO as probed by the singlet insertion operator.

![FIG. 2. Singlet insertion/deletion correlators for $SU(2)$ and $SU(3)$ Hubbard models of various sizes (PBC). Insertion and deletion were separated by half the system size, $L$.](image)

Conversely, if we consider the large $U$ limit of the one dimensional Hubbard model at half filling, then the singlet insertion operator clearly does display long range
order. This can be seen from the Ogata-Shiba factorized wavefunction [13] which has a charge wavefunction given by that of spinless fermions and a spin part given by the groundstate of the Heisenberg model with the “sites” defined as the positions of the spinless fermions. At half filling, there is a fermion on every site and the charge part is trivial, a property unchanged by inserting or deleting singly occupied sites. For this reason the singlet insertion correlations, are identical those of the Heisenberg model and have ODLRO, as we have previously established [1]. For finite U, the Lieb-Wu solution [1] shows there is a charge gap for arbitrarily small U and thus one expects Mott-Hubbard order for any positive U, but with a magnitude vanishing as $U \rightarrow 0$. This is consistent with our numerical results (Fig. 3) for the behavior of the singlet insertion/deletion correlator.

In contrast, for the simplest SU(3) generalization of the Hubbard model, a finite critical interaction strength, $U_c$, should be required to induce a metal-insulator transition [4]. Our numerical results for this model are consistent with the absence of ODLRO for SU(3) singlet insertion for $U < U_c \sim 2t$, and the presence of ODLRO for SU(3) singlet insertion for larger values of $U$.

We can also make contact between our singlet insertion operator and the bosonization picture of the one dimensional Mott-Hubbard transition; in the large operator and the bosonization picture of the one dimensional SU

$U \rightarrow 0$ via a Kosterlitz-Thouless transition. This further supports the singlet insertion operator acting as an order parameter for the one dimensional Mott-Hubbard transition and we feel confident that our operator is an effective probe of the Mott-Hubbard transition in one dimension.

What does this picture imply for the Mott-Hubbard transition in higher dimensions? First, note that the singlet insertion operator reveals the presence of a broken $Z_2$, spatial symmetry. Such a broken symmetry doubles the unit cell and might be expected to lead, for a half-filled system, to a filled band and a gap to all excitations; however, if the broken symmetry involves only the charge degrees of freedom, then the result is an anti-ferromagnetic insulator rather than a band insulator, which would have gapped spin degrees of freedom. This behavior is reminiscent of the formation a spin density wave (SDW) insulator, however, in that case the “order parameter” transfers real electrons across the Fermi surface and therefore couples to both spin and charge degrees of freedom. Further, the low lying spin degrees of freedom of the SDW are Goldstone bosons resulting from the broken SU(2) symmetry and therefore the spin-density wave picture can not apply in one spatial dimension or in two dimensions at any finite temperature [7]. The breaking of a discrete symmetry, such as $Z_2$, is allowed in one dimension at $T = 0$ and causes the Mott-Hubbard transition. Such a breaking is also allowed at finite temperature in two or more dimensions. This suggests that higher dimensional Mott-Hubbard transitions in pure Hubbard models may well be finite temperature transitions at which a $Z_2$ symmetry breaks in the charge sector, leaving a low energy effective theory containing only magnetic degrees of freedom. This contrasts sharply with the conventional wisdom on the Mott-Hubbard transition which follows the line of argument that, if the only order parameter for the Mott-Hubbard transition is the conductance, then no true, finite temperature distinction exists between metal and insulator [13]. This argument fails if one is prepared to admit the possibility of the breaking of a $Z_2$ symmetry only in the charge sector. Based on our one dimensional result that the Mott-Hubbard transition does admit a pure charge order parameter which breaks a discrete symmetry, we feel that this proposal should be seriously considered.

Interestingly, two organic conductors, (TMTTF)$_2$SbF$_6$ and (TMTTF)$_2$ReO$_4$ [10] exhibit abrupt changes in their charge properties consistent with finite temperature metal-insulator transitions, and, moreover, these transitions are unaccompanied by any detectable magnetic, structural or charge density wave transitions. Existing explanations for the transition between metallic and insulating behavior in similar materials [17] are based on a finite temperature crossover that can not account for such sharp “transitions”, thus it appears very natural to interpret this behavior as finite temperature Mott-Hubbard transitions of the type we are proposing.

To test whether the exotic sort of ordering we are proposing actually occurs requires a suitable probe for Mott-Hubbard order beyond one dimension. In this case, the singlet insertion operator we have used is no longer appropriate, however, it can be generalized into a useful probe. Consider the two dimensional case of a Hubbard model of size $L_x \times L_y$:

$$H_{2D Hubb} = \sum_{x,y,\sigma,\nu} t_\parallel c_{\sigma,x,y}^{\dagger} c_{\sigma,x,y} + t_\perp c_{\sigma,x,y+\nu}^{\dagger} c_{\sigma,x,y} + U \sum_{x,y} n_{\uparrow,x,y} n_{\downarrow,x,y}$$

(2)

where we identify $x = L_x + 1$ with $x = 1$, with $L_x$ an even integer, and $y = L_y + 1$ with $y = 1$. Now, we define a multi-singlet insertion operator which inserts $L_y$ singlet pairs, all at fixed $x$, and study the dependence on $L_x$ of the expectation value of this operator acting at $x = 0$ and
the conjugate removal operator acting at \( x = \frac{L}{2} \). If the system has completely anisotropic hopping \((t_\perp = 0)\) so that each of the \( L_y \) chains is independent then, at zero temperature and for positive \( U \), this expectation value behaves like the \( L_y \)th power of the one dimensional singlet insertion correlator. For large \( L_x \) and odd \( L_y \), this depends on \( L_x \) only as \((-1)^{\frac{L_y}{2}}\), reflecting the underlying one-dimensional Mott-Hubbard order. Now imagine that we turn on some finite interchain hopping, \( t_\perp \), with \( U \gg t_\parallel \) and \( U \gg t_\perp \). We can use the multi-singlet insertion operator to see if the Mott-Hubbard order persists at finite \( t_\perp \).

As a first step in this direction, we considered multi-singlet insertion for coupled spin chains; the low energy theory for the two dimensional Hubbard model at sufficiently large \( U \) should be that of the Heisenberg model:

\[
H = \sum_{x,y} J_{\|} \vec{S}(x,y) \vec{S}(x+1,y) + J_\perp \vec{S}(x,y) \vec{S}(x,y+1)
\]

with \( J_{\|} \sim \frac{t^2}{U} \) and \( J_\perp \sim \frac{t^2}{U} \). The interchain spin couplings are relevant operators \([15]\) and could destroy the singlet insertion order; however, recall that our order parameter acted as a \( c \)-number in the spin sector. In this case, the usual arguments about perturbed conformal field theories imply that its behavior should show no infrared divergences caused by the relevant interchain couplings \([14]\). Therefore the behavior of our multi-singlet insertion operator should be be qualitatively the same as the isolated chains case: \( \propto (-1)^{\frac{L_y}{2}} \). If so, the two dimensional Heisenberg model, and, by inference, presumably the two dimensional Hubbard model in the Mott insulating phase, possess hidden, broken \( Z_2 \) symmetries. We have numerically studied the behavior of the multi-singlet insertion correlator for two and three leg spin chains with the results depicted in Fig. 3.

As can be seen from the figure, the relevance of the interchain coupling does not lead to any strong change in behavior in the multi-singlet insertion operator. For the three leg case a broken \( Z_2 \) appears to persist; this suggests that such a discrete symmetry breaking may be present in the two dimensional Hubbard model and under its Mott-Hubbard transition. In the future, we hope that it may be possible to use the multi-singlet insertion to resolve the question of the existence of a finite temperature \( Z_2 \) breaking in this model and we are currently exploring this possibility.

In summary, we have proposed and given evidence in support of the proposal that an operator which inserts a pair of singly occupied sites in a singlet spin configuration into a one dimensional Hubbard model acts as an order parameter for the Mott-Hubbard transition. The transition occurs in this language because of the breaking of a spatial \( Z_2 \) symmetry in the charge sector of the model, doubling the charge unit cell and causing an insulator. A natural conjecture based on this picture is that a similar Mott-Hubbard transition can occur in higher dimensions, involving the breaking of a charge sector \( Z_2 \) symmetry, possibly at finite temperature. In support of this, we have given some numerical evidence for a broken \( Z_2 \) for the two dimensional Heisenberg model and identified two experimental systems whose behavior is suggestive of the proposed, new kind of ordering.

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\[\text{FIG. 3. Results of multi-singlet insertion/deletion correlator for two and three leg spin ladders (PBC, and } J_{\text{out of chain}} = 2J_{\text{in chain}}). \text{ Three leg ladder shows alternation, and both two and three leg ladders appear to have ODLRO for } O \text{ with the magnitude of } (\langle O^\dagger O \rangle \text{) only slightly reduced from that of uncoupled chains. Contrast this with the dramatic effects of the interchain coupling on } \langle s^x s^x \rangle, \text{ which, for example, switches from algebraic to exponential decay for the two leg ladder.}\]

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The behavior of our operator is very similar to that of the Girvin-MacDonald-Read order parameter on the sphere (S. Girvin and A. MacDonald, Phys. Rev. Lett. 58, 1252 (1987); N. Read, Phys. Rev. Lett. 62, 86 (1989)); both operators exhibit “hidden” ODLRO in that they connect states which live in somewhat different Hilbert spaces, but their correlation functions are well defined and do not decay to zero for infinite separation. Additionally, both are “local” in the same sense [4].

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This is in contrast to any of the conventional types of spin chain ordering or even the exotic “topological orders” (see K. Rommelse and M. den Nijs, Phys. Rev. Lett 59, 2578 (1987); M. den Nijs and K. Rommelse Phys. Rev. B40, 4709 (1989); S. M. Girvin and D. P. Arovas, Phys. Scr. T27, 156 (1988)). In all of those cases, the order parameter can be understood as a non-trivial operator in some Luttinger liquid description which acquires an expectation value when the Luttinger liquid state is perturbed by a relevant operator. The sole exception is that ferromagnetic state which is reached via a first order level crossing transition; however, even in that case, the relevant order parameter does map onto a non-trivial operator in the adjacent, Luttinger liquid phase.

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We thank C. S. Stafford for calling our attention to this property of the $SU(3)$ Hubbard model, which results because the Umklapp processes, which can lead to the opening of the charge sector gap, are irrelevant for weakly interacting, $SU(3)$ fermions.

Naturally, if the metal-insulator transition is tied to some more conventional transition, then the order parameter for that transition can be used. See also Ref. [4] where a first order, finite temperature metal-insulator transition was found.

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In fact, the robustness of the order to relevant interchain spin couplings provides another argument in support of the proposal that our singlet insertion/deletion is probing a charge sector order.