Comment on “ $\mathbb{Z}_2$ -slave-spin theory for strongly correlated fermions”

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The authors of Ref. 1 introduced a new slave-spin (SS) mean-field (MF) approach to the Hubbard model of strongly correlated electrons in terms of Ising spins and standard fermion operators by constructing an enlarged Hilbert space with both physical and unphysical states. The purpose of this construction is clear: this formulation involves a much smaller number of slave fields, compared with more standard slave particle frameworks. In this way, the complexity of the original model is reduced to a more readily tractable system of Ising spins in a transverse field coupled to free fermions. In this Comment, we show that the unphysical states are not properly excluded, and despite the claimed good agreement with previous results, the consistency of their MF theory is unjustified.

Reference 1 may be considered as an extension and an improvement of the formalism developed earlier in Ref. 2. It can also be thought of as a minimal formulation of previous slave-spin representations.³

The single-band Hubbard model is written in the form

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{U}{2} \sum_i (n_i - 1)^2. \quad (1)$$

The hopping amplitude is denoted by t_{ij} , and U is the on-site repulsion. The operator $c_{i\sigma}^{(\dagger)}$ creates an electron at site i with spin σ , and $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$.

The authors introduce auxiliary local pseudospin variables $\vec{I}_i = (I_i^x, I_i^y, I_i^z)$ with eigenstates $I_i^z |\pm\rangle_i = \pm \frac{1}{2} |\pm\rangle_i$. The physical electron operator is then represented as

$$c_{i\sigma}^{(\dagger)} = 2 I_i^x f_{i\sigma}^{(\dagger)}, \quad (2)$$

where $f_{i\sigma}^{(\dagger)}$ is an auxiliary fermion operator defined on the space spanned by the vectors $|0\rangle_i, |\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i$.⁴

The SS representation (2) expands the Hilbert space. The authors identify the on-site physical Hilbert space to be spanned by the states

$$\mathcal{H}_{\text{phys}} = \{ |+\rangle|0\rangle, |-\rangle|\uparrow\rangle, |-\rangle|\downarrow\rangle, |+\rangle|\uparrow\downarrow\rangle \}. \quad (3)$$

The unphysical states are then

$$\mathcal{H}_{\text{unphys}} = \{ |-\rangle|0\rangle, |+\rangle|\uparrow\rangle, |+\rangle|\downarrow\rangle, |-\rangle|\uparrow\downarrow\rangle \}. \quad (4)$$

To obtain a faithful representation of the original problem, the authors claim to single out the physical subspace by the local constraint $A_i := I_i^z + 1/2 - (n_i - 1)^2 = 0$. This equation justifies the substitution in (1),

$$\frac{U}{2} \sum_i (n_i - 1)^2 \rightarrow \frac{U}{2} \sum_i (I_i^z + 1/2), \quad (5)$$

which appears to be a necessary step to recover the transverse field Ising model representation.

The projection of the Hubbard model

$$H' = - \sum_{ij\sigma} t_{ij} I_i^x I_j^x f_{i\sigma}^\dagger f_{j\sigma} + \frac{U}{2} \sum_i \left(I_i^z + \frac{1}{2} \right) \quad (6)$$

onto the physical subspace is equivalent to the original model (1). Such a projection can be achieved explicitly by imposing the requirement $Q_i := A_i^2 = 1/2 + I_i^z [1 - 2(n_i - 1)^2] = 0$ for each lattice site. The projection operator Q_i commutes with Hamiltonian (1) and generates a U(1) local gauge symmetry which takes care of the redundancy of the decomposition (2). However, notice that the operator constraints $A_i = 0$ and $Q_i = 0$ are not equivalent to each other.⁷

The so far exact SS formulation is then treated at MF level by fully decoupling the SS and the auxiliary fermion operators in the form $H' \rightarrow H^{\text{MF}} = H_f + H_I$, where

$$H_f = - \sum_{ij\sigma} g_{ij} t_{ij} f_{i\sigma}^\dagger f_{j\sigma}, \quad (7)$$

$$H_I = - \sum_{ij} \chi_{ij} t_{ij} I_i^x I_j^x + \frac{U}{2} \sum_i I_i^z.$$

Here the hopping amplitude and the Ising exchange coupling are renormalized by the factors g_{ij} and χ_{ij} , respectively. These are to be determined through the self-consistency equations

$$g_{ij} = 4 \langle I_i^x I_j^x \rangle_{H_I}, \quad \chi_{ij} = 4 \sum_\sigma \langle (f_{i\sigma}^\dagger f_{j\sigma})_{H_f} + \text{c.c.} \rangle. \quad (8)$$

To proceed, the authors replace the constraint $A_i = 0$ by its ground-state expectation value, ignoring completely the condition $Q_i = 0$. In the enlarged Hilbert space, the Q_i operator is a projection matrix, $Q_i |\mathcal{H}_{\text{phys}}\rangle_i = 0$, $Q_i |\mathcal{H}_{\text{unphys}}\rangle_i = |\mathcal{H}_{\text{unphys}}\rangle_i$. Because of this, the local MF constraint $\langle Q_i \rangle = 0$ still eliminates the unphysical states. In contrast, the same condition does not hold for the constraint expectation value $\langle A_i \rangle$ that can be nullified by the unphysical subspace as well. To see this, let us pick up a state

$$|\Phi\rangle = c_i^{(1)} |-\rangle_i |0\rangle_i + c_i^{(2)} |-\rangle_i |\uparrow\downarrow\rangle_i + c_i^{(3)} |+\rangle_i |\uparrow\rangle_i + c_i^{(4)} |+\rangle_i |\downarrow\rangle_i \in \mathcal{H}_{\text{unphys}},$$

where $|c_i^{(1)}|^2 + |c_i^{(2)}|^2 = |c_i^{(3)}|^2 + |c_i^{(4)}|^2$. It then follows that $\langle \Phi | A_i | \Phi \rangle = 0$. Consequently, the condition $\langle A_i \rangle = 0$ no longer discriminates between physical and unphysical states (as opposed to the requirement $\langle Q_i \rangle = 0$), and the resulting SS MF theory becomes inconsistent. The substitution (5) now implies that the uncontrolled unphysical degrees of freedom contribute to the theory as well.

The authors refer to their MF approach as a Z_2 gauge theory. They claim that the local Z_2 transformations, $f_i \rightarrow u_i f_i u_i = -f_i$, $I_i^x \rightarrow u_i I_i^x u_i = -I_i^x$, $u_i = 1 - 2Q_i$, respect the MF decomposition (7) and “in this sense, the mean-field ansatz breaks the U(1) gauge theory down to Z_2 .”¹ This statement may cause some confusion.⁸ It is of course legitimate to restrict the space of variational states to a subspace generated by the states related by the u_i transformations. However, this does not result in a Z_2 -invariant MF

theory: the gauge-related variational states still belong to the *different* Hamiltonians, H^{MF} and $u_i H^{\text{MF}} u_i \neq H^{\text{MF}}$. In fact, a Z_2 gauge-invariant MF theory only arises if one considers both functions χ_{ij} and g_{ij} as Hubbard-Stratanovich dynamical fields, $\chi_{ij} = \bar{\chi}_{ij} \sigma_{ij}$, $g_{ij} = \bar{g}_{ij} \sigma_{ij}$. Here $\bar{\chi}_{ij}$ and $\bar{g}_{ij}$ are precisely the solutions to the saddle point Eqs. (8), and $\sigma_{ij} = \pm 1$ is an Ising dynamical gauge field that takes care of the Z_2 gauge fluctuations beyond the saddle point approximation.

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⁴In the limit $U \gg t$, the physical electron operators admit representations in terms of the su(2) spins and spinful fermions.⁵ Within that approach, the underdoped Hubbard model reduces to the Kondo-Heisenberg problem.⁶

⁵T. C. Ribeiro and X.-G. Wen, *Phys. Rev. Lett.* **95**, 057001 (2005); A. Ferraz, E. Kochetov, and B. Uchoa, *ibid.* **98**, 069701 (2007).

⁶R. T. Pepino, A. Ferraz, and E. Kochetov, *Phys. Rev. B* **77**, 035130 (2008).

⁷The operator A_i does not commute with the Hamiltonian (1). The consistency of the constraint $A_i = 0$ with time evolution requires that $[A_i, H]_{\mathcal{H}_{\text{phys}}} = 0$. The consistency of this secondary constraint implies in turn that $Q_i = 0$. Therefore, the constraint $A_i = 0$ can be imposed self-consistently only if the requirement $Q_i = 0$ holds.

⁸To start with, there is a confusion with the very definition of gauge invariance. The authors claim that a Z_2 gauge invariant operator O obeys the condition $u_i O u_i = O$. Since $u_i^2 = 1$, this implies that $[O, Q_i] = 0$. In other words, the discrete Z_2 symmetry is automatically promoted back to the continuous U(1) local gauge symmetry generated by Q_i . In contrast, the conservation of a genuine Z_2 parity operator implies the conservation of a Z_2 charge modulo 2.