Order parameters in the resonating-valence-bond model

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We show that the ambiguity in the fluxoid unit in the resonating-valence-bond model arises from the choice of an order parameter which violates a local gauge symmetry. We give an explicit example of a gauge-invariant order parameter, other than electron pairs, which possess a nontrivial topology depending upon the lattice.

I. INTRODUCTION

In Anderson's resonating-valence-bond (RVB) model for high-temperature superconductivity,[1-6] electrons residing on a square lattice of copper atoms are described by a superexchange Hamiltonian H. This may be thought of as having been derived from a single-band Hubbard model near half filling, in the limit of strong on-site repulsion U. In the postulated RVB state, the atoms are bonded to a neighbor by a singlet electron pair; in the modification of Kivelson, Rokshar, and Sethna (KRS), the bonded atoms are nearest neighbors.[6] The half-filled lattice is an insulator, but charge transport is possible when vacancies are present.

In mean-field treatment of the doped RVB state, superconductivity arises either by the Bose-Einstein condensation of the vacancies,[2] or by the pairing of fermionic excitations.[4] This has been taken to imply that the unit of magnetic-flux quantization is h/e in the former case, and $h/2e$ in the latter case.

This note shows that the origin of this apparent ambiguity is the failure of mean-field theory to respect a local gauge symmetry. This failure occurs in the assignment of charge to the slave bosons and fermions, which physically enforce the limit of large U, and in the subsequent approximations. This gauge symmetry applies even in the doped state, and should not be confused with the SU(2) symmetry which is present at half filling.[7] It is evident that the order parameter for superconductivity must be gauge invariant, and we give two examples of such an order parameter. A trivial example is the anomalous pair of electron operators, while a second nontrivial example corresponds to a topological boson, whose precise nature depends upon the lattice. In the case of a square lattice, this object corresponds to a hole attached to a string extending to infinity, or a pair of holes attached by a string.

II. CHARGE-ASSIGNMENT SYMMETRY

When the on-site Coulomb repulsion U is much larger than the effective intersite-hopping matrix element t, double occupancy of sites by electrons is effectively forbidden. An approximate way to proceed in this limit is to perform a canonical transformation to derive the superexchange Hamiltonian which acts on a subspace T of the real Hilbert space S, in which double occupancy is forbidden.[8] This awkward constraint can be achieved by representing the electron annihilation and creation operators with spin σ at site i ($c_{i\sigma}$ and $c_{i\sigma}^{\dagger}$, respectively) in terms of slave fields[9] e_i, d_i, and $s_{i\sigma}$:

$$c_{i\sigma}=e_i^{\dagger}s_{i\sigma}+\sigma d_i^{\dagger}s_{i-\sigma}\,. \tag{1}$$

Here e_i and d_i are boson fields and $s_{i\sigma}$ are fermion fields, which obey

$$Q_i\equiv e_i^{\dagger}e_i+d_i^{\dagger}d_i+\sum_{\sigma}s_{i\sigma}^{\dagger}s_{i\sigma}=1\;, \tag{2}$$

in order that the $c_{i\sigma}$ satisfy the usual anticommutation relations. The no-double-occupancy condition now becomes the simple condition $d_i=0$.

The slave-boson (SB) formalism introduces an ambiguity into the definition of a physical observable such as charge because, e.g., one can identify the operator

$$q_i(\alpha)=-(1-\alpha)e_i^{\dagger}e_i+\alpha\sum_{\sigma}s_{i\sigma}^{\dagger}s_{i\sigma}-\alpha \tag{3}$$

for any α to be the charge operator. Now the ambiguity occurs when one introduces approximation schemes which fail to treat the SB constraint exactly. For example, the authors of Refs. 2, 4, and 5 replace the constraint by adding a Lagrange multiplier λ_iQ_i to the Hamiltonian and then make a Hartree-Fock-type mean-field approximation. This, in effect replaces λ_i with a constant λ chosen such that $\langle Q_i\rangle=1$. The constraint $Q_i=1$ is thus only satisfied on average. It is at this point that results become dependent on the choice of the charge operator $q_i(\alpha)$. In particular, if α is chosen as zero then only the slave bosons carry charge and hence the conclusion by Zou and Anderson[2] and by Isawa, Maekawa, and Ebisawa[5] that the condensate consists of charge-e holes. If, on the other hand, α is chosen as one, then only the slave fermions carry charge which suggests that one has a charge-$2e$ condensate. Provided one treats the constraint $Q_i=1$ on every site exactly, however, all physical results should be independent of α.

Now this charge assignment freedom is not only important because of the demands it places on approximation schemes but also because it tells us something about the nature of the condensate. For example, a ground state $|\psi\rangle$ in which $\langle\psi|s_{i\sigma}s_{j-\sigma}|\psi\rangle\neq0$ would be aphysical in the sense that $q_i(\alpha)|\psi\rangle$ is α dependent for some i and charge becomes an ill-defined quantity. This can be seen as follows: from Eq. (4), $q_i(\alpha)|\psi\rangle$ is α independent only if

$(Q_i-1)|\psi\rangle=0$ for all sites i. This, in turn, implies that $\langle\psi|s_{i\sigma}s_{j-\sigma}|\psi\rangle=0$ since $s_{i\sigma}s_{j\sigma}$ decreases the "Q number" on both sites i and j by one unit and hence can only connect states whose Q_i and Q_j each differ by one unit.

An alternative and particularly direct way to look at this is that the slave-boson constraint $Q_i=1$ generates a local U(1) gauge symmetry and, therefore, any operator which transforms nontrivially under this gauge symmetry vanishes according to Elitzurs[10] theorem. In this way we see that neither e_i nor e_ie_j can acquire an expectation value. Furthermore, due to the local nature of the symmetry, off-diagonal long-range order cannot occur either. Of course, one need not appeal to the charge-assignment freedom to realize this consequence of the slave-boson constraint. Obviously there is no prohibition of the condensation of physical electrons since $c_{i\sigma}c_{j-\sigma}$ commutes with Q_i. It is also possible to construct operators which commute with the constraint, but which do not have any obvious relation to the physical electron operators. We give an example of such an operator below.

III. TOPOLOGICAL BOSON OPERATOR

The above arguments do not prohibit a condensate of an operator E_i which creates a single charge-e hole at site i. However such operators must be nonlocal. The topological solitons envisaged by KRS are examples of this, and are not to be identified with slave-boson operators e_i, which are strictly defined on a single site. A corollary of the nonlocal character of E_i is that its nature will depend on the lattice. To see these points explicitly, let us first construct a physically observable operator E_i on a triangular lattice, such that $E_i^\dagger E_i=e_i^\dagger e_i$, but which nevertheless commutes with Q_i. States created by $E_i^\dagger$ possess a well-defined charge.

We first write down the Euclidean action for a one-band Hubbard model in two dimensions in imaginary time τ. The starting point is the superexchange Hamiltonian

$$H=t\sum_{\langle i,j\rangle}c_{i\sigma}^\dagger c_{j\sigma}-2J\sum_{\langle i,j\rangle}b_{ij}^\dagger b_{ij}\ ,$$

where $b_{ij}=(c_{j\downarrow}c_{i\uparrow}-c_{j\uparrow}c_{i\downarrow})/\sqrt{2}$. Additional pair hopping terms arise if H is derived from the one-band Hubbard model using the canonical transformation method,[8] but these have not been included above, as they are not crucial to our main points here. In the slave-boson representation the corresponding Euclidean action $\int d\tau L$ involves a set of fields λ_i to implement the constraints $Q_i=1$ and a Hubbard Stratonovich field $\Delta_{ij}=A_{ij}\exp(-i\phi_{ij})$ introduced to decouple the four fermion interaction

$$L=\sum_i(s_{i\sigma}^\dagger\partial_\tau s_{i\sigma}+e_i^\dagger\partial_\tau e_i)+t\sum_{\langle i,j\rangle}e_ie_j^\dagger s_{i\sigma}^\dagger s_{j\sigma}+\sum_{i,j}J^{-1}|\Delta_{ij}|^2+\sum_{\langle i,j\rangle}[\Delta_{ij}^*(s_{j\downarrow}s_{i\uparrow}-s_{j\uparrow}s_{i\downarrow})+\text{c.c.}]+i\sum_i\lambda_i(s_{i\sigma}^\dagger s_{i\sigma}+e_i^\dagger e_i-1)\ . \tag{4}$$

Now consider sites i, j, and k forming a plaquette on a triangular lattice, and define

$$E_i=e_i\exp\left[\frac{i}{2}(\phi_{ij}-\phi_{jk}+\phi_{ki})\right]. \tag{5}$$

By construction $E_i^\dagger E_i=e_i^\dagger e_i$. The action is invariant under the local gauge transformations

$$U=\exp\left[i\sum_j Q_j\theta_j+\sum_{ij}(\theta_i+\theta_j)\frac{\partial}{\partial\phi_{ij}}\right],$$

for real θ_i. The fields e_i and ϕ_{ij} transform in the following way:

$$e_i\to Ue_iU^{-1}=e_ie^{-i\theta},\quad \phi_{ij}\to U\phi_{ij}U^{-1}=\phi_{ij}+\theta_i+\theta_j\ .$$

Thus $E_i\to UE_iU^{-1}=E_i$, showing that E_i is a physical operator since it is gauge invariant.

On a square lattice this rephasing is much more difficult since the cancellation of aphysical phases requires an odd number of bonds around a plaquette. However, even this does not prohibit the construction of physical holon operators. Indeed in Anderson's basic picture, one creates a holon by first destroying an electron and then moving the spin defect to infinity. Thus we see how the spin degrees of freedom are affected nonlocally. This suggests that E_i should be constructed by rephasing e_i using the phases of an infinite number of bonds. Say

$$E_i=e_i\exp\left[\frac{i}{2}(\phi_{ij}-\phi_{jk}+\phi_{kl}-\phi_{ln}+\cdots)\right], \tag{6}$$

where $\langle ij\rangle$, $\langle jk\rangle$, $\langle kl\rangle$ is a string of bonds to infinity. We see that E_i defined in Eq. (7) would create a string similar to that of a Dirac monopole.

Note that the fluxoid quantum in the superconducting state is different for these two cases. On the triangular lattice the boson operator given by Eq. (6) has a well-defined physical charge of e (since only bonds in a finite region are affected). A condensate of this boson would thus have an hc/e fluxoid. On the other hand, it is not so easy to define the charge of the boson operator on the square lattice given in Eq. (6) because of the infinite string. One possibility would be to end the string on another boson, thus giving boson pairs with physical charge $2e$ and hence an $hc/2e$ fluxoid. A similar argument has been given in Ref. 11.

To summarize, we have shown that because of the slave-boson constraint neither slave bosons or slave fermions can be assigned physical charge, nor can the bosons or fermion pairs condense. Operators which may condense include physical operators such as electron pairs as well as operators which are not so easily expressed in terms of electron creation and destruction operators, i.e., the topological bosons. The no-condensation theorem, in our opinion, does not provide a serious obstacle to Anderson's picture, since according to Anderson, a holon creation operator is the product of an electron annihilation operator followed by a Gutzwiller projection operator, i.e., an infinite product of physical operators. It does, however, suggest that slave-boson operators are unrelated to the elementary excitations of RVB theory.

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[1]P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987); P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987); P. W. Anderson (unpublished).

[2]Z. Zou and P. W. Anderson, Phys. Rev. B **37**, 627 (1988).

[3]P. W. Anderson and Z. Zou, Phys. Rev. Lett. **60**, 132 (1988).

[4]A. Ruckenstein, P. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).

[5]Y. Isawa, S. Maekawa, and H. Ebisawa, Physica B **148**, 391 (1987).

[6]S. Kivelson, D. Rokshar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987).

[7]E. Dagotto, E. Fradkin, and M. Moreo, Phys. Rev. B **38**, 2926 (1988).

[8]J. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985); C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987).

[9]S. E. Barnes, J. Phys. F **6**, 1375 (1976); S. E. Barnes, *ibid.* **7**, 2631 (1977); P. Coleman, Phys. Rev. B **29**, 3035 (1984).

[10]S. Elitzur, Phys. Rev. D **52**, 3978 (1975).

[11]S. Kivelson, D. Rokshar, and J. Sethna, Europhys. Lett. **6**, 353 (1988).