New Fermionic Description of Quantum Spin Liquid State

A. M. Tsvelik[(a)]
Department of Physics, Princeton University, Princeton, New Jersey 08540
(Received 19 June 1992; revised manuscript received 20 August 1992)

A novel approach to $S = 1/2$ antiferromagnets with strong quantum fluctuations based on the representation of spin-1/2 operators as bilinear forms of real (Majorana) fermions is suggested. This representation does not contain unphysical states and thus does not require the imposition of constraints on the fermionic Hilbert space. This property allows one to construct a simple and effective mean field theory of the spin liquid state. As an example illustrating the basic properties of this state I consider a model of the Kondo lattice. It is shown that this model has a singlet ground state; elementary excitations have a spectral gap and are $S = 1$ real (Majorana) fermions.

PACS numbers: 75.10.Jm, 75.20.Ck

The traditional picture representing magnets as arrays of weakly interacting rigid rotors fails to describe systems with strong quantum fluctuations. Such fluctuations can be increased by a small value of spin, a frustrated interaction, or a large value of the rank of a spin group. An alternative point of view on strongly fluctuating systems has been gradually emerging from Anderson's original conjecture of a "spin liquid" state in two-dimensional $S = 1/2$ Heisenberg systems [1]. Later he used these ideas to explain unusual magnetic properties of the copper oxide superconductors [2] which have attracted much attention. Anderson's proposal for systems with strong fluctuations is to concentrate on bonds between spins rather than on spins themselves and thus define slow bond variables $\Delta(r,r')$ (usually called the RVB—resonating valence bond—order parameter). Thus according to this approach a theory of the spin liquid should be considered as a lattice gauge theory where spin waves are composite particles.

Current efforts to develop a gauge invariant theory of a spin liquid are based on the Wigner and Schwinger [3] representation of spin operators:

$$S^a = b^\dagger_\alpha \sigma^a_{\alpha,\beta} b_\beta \,, \tag{1}$$

$$b^\dagger_1 b_1 + b^\dagger_2 b_2 = 2S \,, \tag{2}$$

where σ^a are the Pauli matrices and $b^\dagger, b$ are either Bose or Fermi operators.

The above representation has a continuous gauge group U(1) (in other words the above bosons or fermions are charged particles). In a path integral representation of the corresponding models the Heisenberg exchange term is decoupled with an auxiliary field $\Delta(r,r')$ by the Hubbard-Stratonovich transformation and the constraint (2) is enforced by a local Lagrange multiplier field $\lambda(t,r)$. Then as usual in a mean field approach both auxiliary fields are treated as weakly fluctuating around their saddle point values. Naturally, the bosonic and fermionic representations lead to different mean field theories (Refs. [4,5] provide examples of the bosonic and Refs. [6–9] of the fermionic mean field theories). It is argued that this difference will be removed at small energies by the strongly fluctuating U(1) gauge field present in all these theories. The presence of this field reflects the fact that the obtained liquid of bosons or fermions is incompressible or, in other words, that their charge is fictitious. The most probable scenario is that the long-distance gauge force confines the Schwinger particles thus restoring the conventional spin wave picture. In this case instead of a spin liquid we would have a conventional magnet ordered or disordered. Thus the described approach fails to provide persuasive evidence for a spin liquid state.

In this Letter I describe another approach to the problem of spin liquids based on an unconstrained representation of the spin-1/2 operators which I use instead of the Schwinger-Wigner representation [1,2]. In this approach the spin-1/2 operators are represented as bilinear forms of real (Majorana) fermions. The fermions transform according to the adjoint representation of the SU(2) group (i.e., they have spin 1). This Majorana representation of spin has been used in quantum mechanics and in field theory [10].

As will be explained below in detail, the Majorana representation has two advantages. The first one is that it does not require any constraint. The other is that its gauge group is not U(1) as for the Schwinger-Wigner representation, but Z_2; i.e., the corresponding particles are chargeless. Since the gauge group is discrete, there are no long-distance gauge forces associated with the U(1) group and the chargeless Majorana particles remain unconfined if the spin liquid state is stable.

As an example of a model of a spin liquid I consider a model of the Kondo lattice. The Kondo lattice can be viewed as a magnet with interactions between spins being formed in an indirect way via a polarization of the conduction electron band (RKKY coupling). The conduction electrons not only provide the interaction, but also screen the local spins reducing their effective moments and thus making a disordered magnetic ground state preferable.

I begin the discussion with a brief description of the Majorana fermions. Let us consider real lattice fermions $\eta_a(r)$ ($a = 1,2,3$; r labels lattice sites) with the following commutation relations:

$$[\eta_a(r), \eta_b(r')]_+ = \delta_{a,b}\delta_{r,r'} \ . \quad (3)$$

In mathematics the algebra (3) is called the Clifford algebra. For the particular case of a single site lattice η_a coincide with the spin-1/2 matrices. In general the commutation relations (3) can be obtained from a quantization of the following Lagrangian:

$$L_0 = \frac{1}{2}\sum_r \eta_a(r,t)\partial_\tau\eta_a(r,t) \ . \quad (4)$$

It is easy to check that the following representation reproduces the commutation relations of the spin operators:

$$S^a(r) = -\tfrac{1}{2}i\epsilon_{abc}\eta_b(r)\eta_c(r) \ . \quad (5)$$

It follows from (3) that $\mathbf{S}^2 = 3/4$. The representation (5) is reducible, however; it contains too many states. It can be shown that for a lattice with an even number of sites $N = 2M$ the dimensionality of the Majorana Hilbert space is equal to $2^{3N/2}$; $2^{N/2}$ times larger than the dimensionality of the spin space. Nevertheless, all states are physical; the representation just replicates states with the right value of $\mathbf{S}^2$ many times. This replication can be understood as a gauge symmetry of the representation (5). Namely, the expression for spin operators is invariant with respect to the local Z_2 transformation of the Majorana fermions:

$$\eta_a(r) \to (-1)^{q(r)}\eta_a(r) \quad (6)$$

$[q(r) = 0, 1]$.

The Majorana representation of spins is going to work well in the magnetic systems with disordered ground states. For such systems it is possible that low-lying excitations are represented by the Majorana fermions themselves and thus the situation can be described by some simple RVB-type mean field theory.

As an example of such a theory I consider a three-dimensional two-channel Kondo lattice model with the following Hamiltonian:

$$H = \sum_{n,\alpha,\mathbf{k}} \epsilon(\mathbf{k})a^\dagger_{n\alpha}(\mathbf{k})a_{n\alpha}(\mathbf{k}) + \sum_r Ja^\dagger_{n\alpha}(r)\sigma_{\alpha\beta}a_{n\beta}(r)\mathbf{S}(r') \ , \quad (7)$$

where $n = 1,2$, σ^a are the Pauli matrices, and I require the total particle-hole symmetry $\epsilon(\mathbf{k}) = -\epsilon(-\mathbf{k})$.

The model (7) is chosen as a toy model to demonstrate properties of the spin liquid state. It turns out that due to the special symmetry properties of this model the charge degrees of freedom decouple completely thus making the integration over the conduction electrons easier. Namely, one can prove that as far as only the spin degrees of freedom are concerned the above model is equivalent to the Kondo lattice with Majorana conduction band:

$$H = \sum_{a=1,2,3;\mathbf{k}} \epsilon(\mathbf{k})\chi_a(-\mathbf{k})\chi_a(\mathbf{k}) + iJ\sum_r \epsilon_{abc}\chi_b(r)\chi_c(r)S^a(r) \ . \quad (8)$$

The band Majorana fermions are neutral and satisfy the following commutation relations:

$$[\chi_a(\mathbf{k}), \chi_b(\mathbf{p})]_+ = \delta_{ab}\delta(\mathbf{k}+\mathbf{p}) \ . \quad (9)$$

Their Green's function is given by

$$\langle\langle\chi(-\omega_n,-\mathbf{k})\chi(\omega_n,\mathbf{k})\rangle\rangle = \frac{1}{i\omega_n - \epsilon(\mathbf{k})} \ . \quad (10)$$

Thus it coincides with the conventional Green's function, but since the Majorana fermions are real it does not contain an arrow. The diagrammatic expansion for spin-spin correlation functions contains only correlation functions of the spin density operators $\sigma^a(r) = a^\dagger_{n\alpha}(r)\sigma^a_{\alpha\beta}a_{n\beta}(r)$ and it is easy to see that all correlation functions of the original spin density operators coincide with the correlation functions of the operators $\sigma^a(r) = -i\epsilon_{abc}\chi_b(r)\chi_c(r)$. Indeed, the Feynman diagrams in both representations are proportional to each other because the Majorana fermions have the same Green's functions as the conventional ones; the exact equality is achieved due to the identity of the numerical factors:

$$2\,\mathrm{Tr}[\sigma^{a_1}\cdots\sigma^{a_n}] = (-i)^n\,\mathrm{Tr}[\epsilon^{a_1}\cdots\epsilon^{a_n}] \ , \quad (11)$$

$$(\epsilon^a)_{bc} = \epsilon_{abc} \ ,$$

where the factor 2 comes from summation over the flavor indices of the conventional fermions.

When the transformation to the effective Hamiltonian (8) is done all irrelevant charge degrees of freedom of the conduction band are decoupled (it will not happen so easily in the Kondo lattice problem with conventional conduction bands where electrons do not carry additional flavors [11]). With the Hamiltonian written in the form (8) it is easy to recognize what the order parameter is. Representing the local spins as in Eq. (5) I decouple the interaction as follows:

$$J\sum_{a\neq b}(\chi_a\eta_a)(\chi_b\eta_b) \sim \Delta(\chi_a\eta_a) \ ,$$
$$\Delta(r) = \frac{2i}{3}J\sum_a\langle[\chi_a(r)\eta_a(r)]\rangle. \quad (12)$$

In this approach the order parameter weakly fluctuates around its saddle point value and the Majorana fermions are elementary excitations. Their Green's functions are equal to

$$G(\omega_n, \mathbf{k}) = \langle\langle \eta_a(-\omega, -\mathbf{k})\eta_a(\omega, \mathbf{k})\rangle\rangle = \frac{i\omega_n - \epsilon(\mathbf{k})}{i\omega_n[i\omega_n - \epsilon(\mathbf{k})] - \Delta^2}$$

$$D(\omega, \mathbf{k}) = \langle\langle \chi_a(\omega, -\mathbf{k})\chi_a(\omega, \mathbf{k})\rangle\rangle = \frac{i\omega_n}{i\omega_n[i\omega_n - \epsilon(\mathbf{k})] - \Delta^2}. \quad (13)$$

Their poles give the following threefold degenerate spectrum:

$$E(\mathbf{k}) = \frac{\epsilon(\mathbf{k})}{2} \pm [\tfrac{1}{4}\epsilon(\mathbf{k})^2 + \Delta_0^2]^{1/2}\ , \quad (14)$$

where Δ_0 is a saddle point value of the order parameter. This spectrum has an indirect gap, $T_K = 2\Delta_0^2/D$.

The spin susceptibility in the mean field approximation is equal to

$$\chi(\Omega, \mathbf{q}) = \frac{T}{2}\sum_n \int \frac{dk^3}{(2\pi)^3} G(\Omega - \omega, \mathbf{q} - \mathbf{k})G(\omega, \mathbf{k})\ . \quad (15)$$

It is strongly enchanced around the reciprocal lattice vector $\mathbf{Q}$:

$$\chi(\Omega = 0, \mathbf{Q}) = \int_{-D}^{D} d\epsilon\, \rho(\epsilon) \frac{(\epsilon^2 + 4\Delta_0^2)^{1/2} + \epsilon}{(\epsilon^2 + 4\Delta_0^2)^{1/2} - \epsilon} \frac{1}{(\epsilon^2 + 4\Delta_0^2)^{1/2}} \sim \frac{1}{T_K}. \quad (16)$$

The main contribution to the imaginary part at low frequencies comes from the region close to the zone boundary: $\epsilon \sim D$. I assume that in this region $\epsilon(k) = D - k^2/2m$. Then the imaginary part of the magnetic susceptibility at positive frequencies is given by

$$\mathrm{Im}\chi^{(R)}(\Omega, \mathbf{Q} - \delta\mathbf{q}) = \frac{2(ma^2 D)^{3/2}}{\pi^2 T_K} \left[\frac{\Omega}{T_K} - [1 + (\delta\mathbf{q})^2/16mD]\right]^{1/2} \quad (17)$$

(a is a lattice constant).

$\mathrm{Im}\chi(\Omega)$ has a threshold-type square root singularity which reveals the composite nature of the spin excitations.

Fluctuations of the order parameter are collective excitations. Integrating over the fermions I get the following Ginzburg-Landau-type effective action:

$$A = \rho(0) \int d\tau\, d^3x \left[\frac{3}{2}\Delta^2 \ln\left(\frac{\Delta}{\Delta_0}\right)^2 + \frac{1}{2\Delta_0^2}[(\partial_\tau \Delta)^2 + v^2(\boldsymbol{\partial}\Delta)^2]\right] \quad (18)$$

where $\rho(0)$ is the conduction band density of states on the Fermi level and v is of order of the Fermi velocity.

The fluctuations of Δ have a gap as expected and are not likely to provide significant corrections to the mean field picture.

Thus we can say that the above Kondo lattice model demonstrates two properties qualitatively predicted for the spin liquid state [1,2]: Its elementary excitations are fermions and there is no coherent propagation of spin waves.

I am grateful to P. W. Anderson and P. Coleman for intensive and valuable discussions and to P. B. Wiegmann for sending me his preprint. This work was supported by the National Science Grant Foundation, through Grants No. DMR 91-96212 and No. DMR-8518163 and AFOSR Grant No. 87-0392.

(a) Present address: Department of Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, England.

[1] P. W. Anderson, Mat. Res. Bull. **8**, 153 (1973).
[2] P. W. Anderson, Science **235**, 1196 (1987).
[3] J. Schwinger, U.S. Atomic Energy Commission Report No. NYO-3071, 1952 (unpublished); E. Wigner (private communication).
[4] D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988); Phys. Rev. Lett. **61**, 617 (1988).
[5] P. Chandra, P. Coleman, and A. I. Larkin, J. Phys. Condens. Matter **2**, 7933 (1990).
[6] D. Khvestchnko and P. B. Wiegmann, Mod. Phys. Lett. **3**, 1383 (1989); **4**, 17 (1990).
[7] P. B. Wiegmann (unpublished).
[8] X.-G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11 413 (1989).
[9] R. B. Laughlin and Z. Zou, Phys. Rev. B **41**, 664 (1989).
[10] J. L. Martin, Proc. R. Soc. London A **251**, 536 (1959); R. Casalbuoni, Nuovo Cimento **33A**, 389 (1976); F. A. Berezin and M. S. Marinov, Ann. Phys. (N.Y.) **104**, 336 (1977).
[11] P. Coleman, F. Miranda, and A. M. Tsvelik (to be published).