1-1-1988

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Brief Reports

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Alternative Feynman-diagram method for the general-spin Kondo problem

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(Received 20 February 1987)

We introduce a new method of replacing spin operators with pseudofermions. For a spin value S there are $2S$ pseudofermions each of which can have spin "up" or "down." In contrast to the standard Abrikosov method which has $2S+1$ inequivalent fermions, i.e., one for each S_z value, the present pairs are all equivalent. It follows that the general spin expression is obtained by multiplying the $S=\frac{1}{2}$ result by a certain combinational factor. This aids in the construction of rotationally invariant solutions for the general-spin Kondo problem for the case when $n \leq 2S$, where n is the number of conduction-electron scattering channels.

In this Brief Report I wish to introduce a new method for replacing spin operators by pseudofermions, as a step in the Feynman-diagram formulation of the Kondo and other spin problems.

The standard Abrikosov[1] projection method for general spin consists of using the following replacement for a spin operator $\hat{O}$.

$$\hat{O} \rightarrow \sum_{S,S'} d_S^{\dagger} \langle S | \hat{O} | S' \rangle d_{S'} \ , \tag{1}$$

where $|S'\rangle \equiv |J=S, J_z=S'\rangle$ denotes an eigenstate of J_z.

The alternative method uses a product of $S=\frac{1}{2}$ representations. This turns out to be more useful for the $n \leq 2S$ versions of the Kondo problem.[2] Here n is the number of conduction electron scattering channels and S the impurity (or ionic) spin value. There is one drawback with the method in that it is not really useful unless the zero temperature limit is taken. As was shown some years ago[3] the method *can* be adapted to finite temperatures but becomes excessively cumbersome.

Consider the direct product of $2S$ spin $S=\frac{1}{2}$ spaces. The standard decomposition of such a product is

$$(\otimes S^{1/2})^{2S} = S^S \oplus (2S \times S^{S-1}) \oplus \cdots \ , \tag{2}$$

where $S^{1/2}$ denotes a spin-$\frac{1}{2}$ spin space and, e.g., $(2S \times S^{S-1})$ indicates that there are $2S$ spin $J=S-1$ representations in the direct sum on the right-hand side.

The interaction in the Kondo problem is

$$-J\mathbf{S}\cdot\mathbf{s}(0) \ , \tag{3}$$

where $\mathbf{S}$ is the ionic spin and $\mathbf{s}(0)$ that of the conduction electrons at the origin. As with any relevant interaction, this has no matrix elements between the different manifolds on the right-hand side of Eq. (2). If the system is subject to a large enough magnetic field at zero temperature then only the lowest-energy state in the largest spin manifold on the right-hand side of Eq. (2) will be occupied, i.e., the state

$$|J=S, J_z=S\rangle \ . \tag{4}$$

Reducing the field will cause the interaction to become effective and mix the states of the $J=S$ spin space. Specifically for the Kondo effect, the ground state appropriate to spin S will be obtained if the initial field is such that

$$H \gg T_K \ ,$$

where T_K is the Kondo temperature, and if the limits are taken in the order

$$T \rightarrow 0 \quad \text{then} \quad H \rightarrow 0 \ .$$

As has been reported elsewhere[4] the spin $S=\frac{1}{2}$ Kondo model can be exactly solved diagrammatically using the magnetic field as the scaling variable. In that approach to the Kondo problem the above procedure is that used in the analytical derivation of the relevant renormalization-group equations.

There is some choice possible as to the method used to represent the spin operators in the direct product on the left-hand side of Eq. (2). In the original finite-temperature method[3] this was done using the so-called "drone boson" method (not to be confused with the so-called "slave boson" method for the Anderson model[5]). Although it is perhaps a matter of taste, and familiarity, I now prefer to use the regular $S=\frac{1}{2}$ Abrikosov method along with the projection technique. Specifically, Eq. (1) is used to represent the spin operators *associated with a given* $S=\frac{1}{2}$ *subspace on the left-hand side of Eq. (2),*

i.e.,

$$S_r^+ \rightarrow d_{r\uparrow}^\dagger d_{r\downarrow},\ S_r^- \rightarrow d_{r\downarrow}^\dagger d_{r\uparrow}\ ,$$

and

$$S_r^z \rightarrow \tfrac{1}{2}(d_{r\uparrow}^\dagger d_{r\uparrow} - d_{r\downarrow}^\dagger d_{r\downarrow})\ , \tag{5}$$

where r, which has $2S$ values, is the subspace label. The physical subspace for *each* of the product $S=\frac{1}{2}$ spaces has only one-half the states of the associated pseudofermion space. The unphysical states with two pseudofermions are removed by Abrikosov's projection technique. Technically this is not necessary since all three of the spin operators give zero when they act on the pseudovacuum *and* the offending doubly occupied state. However, the projection reduces the number of diagrams and so is used as a convenience. It involves adding a term, for each subspace,

$$\mathcal{H}_{r\lambda} = \lambda(d_{r\uparrow}^\dagger d_{r\uparrow} + d_{r\downarrow}^\dagger d_{r\downarrow})\ , \tag{6}$$

to the Hamiltonian and taking the limit $\lambda \rightarrow \infty$, before either of the limits following Eq. (4) is taken.

In a departure from previous work,[4] because they are easier to computer generate, I denote the pseudopropagators by dashed lines and the conduction electrons by solid straight lines. To begin with it is necessary to use a label r for each dashed line to denote which of the $2S$ spin-$\frac{1}{2}$ spaces it belongs in.

Because of the Abrikosov projection a diagram with more than one loop is proportional to $e^{-\beta m\lambda}$ where m is the number of loops. As compared with the usual $S=\frac{1}{2}$ technique, a new complication arises because a given diagram with m loops corresponds to several classes of diagrams depending upon the number N of subspace labels involved. Clearly the maximum number of such labels is $2S$ but in general a diagram will have less than this maximum number. In principle, because there is a term corresponding to Eq. (6) in the Hamiltonian for each subspace, it might be expected that there is a projection factor $e^{\beta 2S\lambda}$ independent of the number of spin labels involved in a diagram, i.e., independent of N. However, in applying Wick's theorem to the string of operators associated with a diagram with N labels, it is observed that the pseudovacuum gives the dominant contribution to the trace for subspaces which *do not* occur in the diagram and hence the net compensating factor is $e^{\beta N\lambda}$. It follows that no given spin subspace can have more than a single loop.

Consider specifically the diagram illustrated in Fig. 1(a); it has only a single ionic loop, and it must be that $m=1$ and $N=1$. This diagram is multiplied by $2Se^{\beta\lambda}$, where the factor of $2S$ corresponds to the number of possible values for the subspace label r. A diagram such as Fig. 1(b) has two loops; therefore, $m=2$ and there is an apparent choice of $N=1$ or 2. However, with $N=1$ there would be two loops with the same spin-space label and so such diagrams are projected out in the $\lambda \rightarrow \infty$ limit. When $N=2$ the first subspace label ranges over the $2S$ possible values; however, the second label cannot repeat the first and has only $2S-1$ values. There is now a prefactor of $2S(2S-1)e^{\beta 2\lambda} = 4S(S-\frac{1}{2})e^{\beta 2\lambda}$. Clearly no diagram can have a total of more than $2S$ ionic loops.

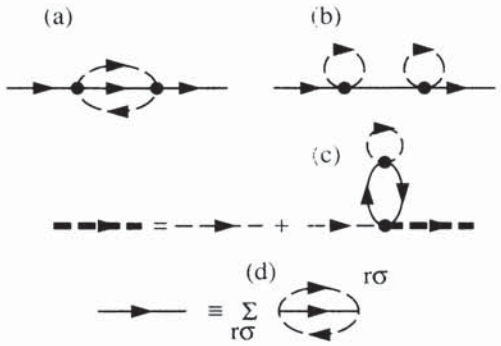

FIG. 1. (a) A conduction-electron scattering diagram with a single ionic loop. (b) A diagram with two loops. (c) Dyson's equation implies irreducible self-energy parts, with an associated bare propagator, form a geometric series. (d) Using the closure trick causes an ionic loop associated with each of the product spin-$\frac{1}{2}$ spaces to begin and end at the extreme ends of the conduction-electron propagator.

The "$2S$ loop rule" implies that there can be no Dysonian self-energy for the pseudofermion lines which contain a dashed loop. Consider Dyson's equation illustrated in Fig. 1(c). If this is iterated, each diagram has a different counting prefactor and, in addition, there can be no more than $2S$ inclusions. Clearly Fig. 1(c), which implies a geometric series, makes no sense. This fact can be viewed upon as reflecting the spin algebra or, more physically, that the restricted number of loops carry the spin's "memory" of previous scattering events.

Also, because of the $2S$ loop rule, it follows that the linked cluster theorem does not work. More specifically it must be recognized that the usual result that the vacuum polarization diagram cancels against the explicit partition function in the denominator of the expression for a propagator also no longer works. As with the usual Abrikosov method each diagram must be divided explicitly by the exact partition function. However, now because $2S$ loops *are* allowed, a diagram with m loops can be multiplied by a vacuum polarization diagram with no more than $2S-m$ dashed loops.

There are various "tricks" which can be used to aid with the complications outlined in the previous paragraphs and to facilitate the calculation of the exact partition function. These are based on what might be called the "closure trick." The decomposition of unity can be written as

$$1 = (d_{r\uparrow}^\dagger d_{r\uparrow} + d_{r\downarrow}^\dagger d_{r\downarrow})\ , \tag{7}$$

where again r is the spin-space label. This factor of unity can be inserted, at will, at any vertex in a Feynman diagram. For example, it might be usefully inserted at the beginning and end of a conduction electron line, as illustrated in Fig. 1(d). This eliminates some vacuum polarization diagrams and, with a little experience, makes the scattering diagrams easier to evaluate.

The partition function can be evaluated by taking the expectation value of Eq. (7). By the usual prescription

the expectation value $\langle d_{r\uparrow}^{\dagger} d_{r\uparrow} \rangle$ is obtained by performing the imaginary frequency sum on the corresponding pseudofermion propagator. This implies

$$\frac{Z}{Z_0} = \frac{1}{\beta} \sum_{\omega_n} [D_{r\uparrow}(i\omega_n) + D_{r\downarrow}(i\omega_n)] \ , \tag{8}$$

where here $D_{r\sigma}(i\omega_n)$, $\sigma = \uparrow$ or $\downarrow$, denotes the sum of all pseudo-propagator diagrams *without* including the explicit factor of one over the partition function. When there is no broken symmetry the pseudofermions are each equivalent and hence any spin-space label can be used in this relationship. However, this symmetry *is* broken for the Kondo problem when the number of channels n is less than S and Eq. (8) must be reexamined. This is beyond the scope of the present report.

In conclusion, I have devised a new Abrikosov method for the general spin Kondo problem which permits results to be obtained by simply multiplying the $S = \frac{1}{2}$ diagrams by a suitable factor. This aids in the construction of rotationally invariant solutions to the Kondo, and possibly other spin problems, since the pseudofermions are not associated with states corresponding to a particular axis of quantization as they are in the usual general spin Abrikosov method. The application of this method to the solution of the multichannel Kondo problem will appear in a separate publication.[2]

[1] A. A. Abrikosov, Physica **2**, 5 (1965).
[2] S. E. Barnes (unpublished).
[3] S. E. Barnes, J. Phys. C **5**, L178 (1972).
[4] S. E. Barnes, Phys. Rev. Lett. **55**, 2192 (1985); Phys. Rev. B **33**, 3209 (1986).
[5] S. E. Barnes, Adv. Phys. **30**, 801 (1981); J. Phys. (Paris) Colloq. **39**, C6-828 (1978); J. Phys. F **6**, 1375 (1976); **7**, 2637 (1977); in *Proceedings of the Nineteenth Congress Ampere, Heidelberg, 1976,* edited by H. Brunner, K. H. Hausser, and D. Schweitzer (North-Holland, Amsterdam, 1977), p. 303.