PHYSICAL REVIEW B VOLUME 51, NUMBER 15 15 APRIL 1995-I

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Implications of Fumi's theorem for auxiliary particle methods

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(Received 27 December 1994)

Fumi's theorem in conjunction with some general theorems associated with auxiliary particle methods dictates the functional form of the on-shell auxiliary particle self-energy Σ for a certain class of impurity scattering problems. An explicit calculation which confirms the result is described and the implications for various approaches to the Kondo effect discussed.

During the past decade the author's auxiliary particle method[1] for highly correlated electron systems has achieved a considerable amount of popularity. However, many of the approximate schemes based upon this method are poorly controlled and in fact violate certain basic theorems which are special to this method. The purpose of this paper is to sketch the proof for a number of such theorems for a certain class of impurity scattering problems which includes most cases of the Kondo effect.

Fumi's theorem in conjunction with some of these general theorems dictates the functional form of the on-shell value Σ of the self-energy for the lowest energy pole of the auxiliary particle propagators. Most popular auxiliary particle methods including those based on the mean-field[2] and the no-crossing approximation[3] appear not consistent with these theorems.

Fumi's theorem[4] relates the ground-state energy of an impurity problem to the phase shifts. Consider for simplicity a one-dimensional problem in which conduction electrons with wave vector k have an unperturbed energy $\epsilon_k^0=ck$, c being the Fermi velocity. There are $\mathscr{N}$ sites in the system, the lattice spacing is a, and δ_k^m is the phase shift. Here m indicates spin and flavor, etc. The phase shift is defined such that the *energy* shift for this wave vector is $2c\delta_k^m/\mathscr{N}a$ and so the total shift in the ground-state energy is

$$\Delta E_0=\sum_{k,m} n_k\left(\frac{2c\,\delta_k^m}{\mathscr{N}a}\right), \tag{1a}$$

where n_k is the usual Fermi occupation factor. *However*, a statement that a problem reduces to an impurity scattering *in the low-energy limit* will have a somewhat weaker implication. Such an assertion would only imply that the scattering matrix is of the required form for low-energy excitations of the conduction electron sea. In turn it would only be possible to insist that the *change* δE_0 in the ground-state energy due to small changes δn_{km} in these low-energy conduction electron populations is determined by the phase shifts in this simple fashion, i.e., that

$$\delta E_0=\sum_{k,m} \delta n_{km}\left(\frac{2c\,\delta_k^m}{\mathscr{N}a}\right). \tag{1b}$$

It is to be expected that this weaker form of Fumi's theorem should apply to the Kondo problem. In what follows the strong and weak form of Fumi's theorem will be indicated, respectively, by the "a" and "b" versions of the relevant equations.

Because of the constraint that the total number of auxiliary particles Q is fixed strictly to unity the usual Feynman diagram rules are modified. Let $\mathscr{G}_n(i\nu)$ be defined to be the propagator for auxiliary particle labeled n determined by the *usual* Feynman prescription for the temperature-ordered quantity. A basic theorem[1] states that the ratio of the exact Z to the unperturbed conduction electron partition function Z_0 is given by

$$\frac{Z}{Z_0}=\sum_n (e^{\beta\lambda})\frac{1}{\beta}\sum_\nu \mathscr{G}_n(i\nu)\,. \tag{2}$$

Here $\beta=1/kT$ and the factor $(e^{\beta\lambda})$, involving λ the projection energy, is required since here the projection method is used to enforce the constraint $Q=1$. While this result is known its principal implications do not seem to be widely appreciated if at all.

Assume that the impurity ground state is nondegenerate. (This covers, e.g., all versions of the Kondo effect except the ferromagnetic problems and the overcompensated case when the field in energy units $h<kT$.) This statement implies, in the limit $T\rightarrow 0$,

$$\frac{Z}{Z_0}=e^{-\beta\Delta E_0}\,, \tag{3}$$

where ΔE_0 is the shift in ground-state energy for the limit $T\rightarrow 0$. This has important implications for the spectral densities $\mathrm{Im}\mathcal{G}_n(\omega+is)$ for the auxiliary particles.

It is necessary to characterize these spectral densities. If the Hamiltonian $\mathcal{H}$ is bounded below, then so must the *zero-temperature* spectral density $\mathrm{Im}\mathcal{G}_n(\omega+is)$. For the limit $T\rightarrow 0$, the continuum of this spectrum *must* terminate at $\Delta E_0+\lambda$. In general the spectral density is comprised of three parts, i.e., the continuum (i) plus (ii) a pole at the end of this continuum and (iii) certain exponentially small continuum tails[5] that extend below the energy $\Delta E_0+\lambda$ and which are essential for the determination of the correct zero-temperature limit.

It is to be noted that, when dressed, every part of an auxiliary particle propagator which lies between any two adjacent vertices, including each part of a Dysonian self-energy, is of the form of a fully dressed auxiliary particle propagator with an argument which comprises an external frequency plus or minus a certain number of conduction electron energies. It follows, because of the projection $\lambda\rightarrow\infty$, that the pole of any such part of an auxiliary particle propagator generates a thermal factor of the form

$$\exp[-\beta(\Delta E_p+\lambda+\text{conduction electron energies})]\,, \tag{4}$$

where ΔE_p is the energy of some auxiliary particle pole. It is easily shown that the conduction electron energies can be absorbed into existing thermal factors by changes $n_k \leftrightarrow (1-n_k)$. If there are several energies ΔE_p such that $\Delta E_p-\Delta E_0<kT$, then

$$\frac{Z}{Z_0}=\sum_p c_p e^{-\beta\Delta E_p}\,, \tag{5}$$

where the c_p are difficult to determine net coefficients for the given exponential and which have well-defined limits $T\rightarrow 0$. Either, as $\mathcal{N}\rightarrow\infty$, with kT finite, this simplifies to $Z/Z_0=c_0e^{-\beta\Delta E_0}$, with $c_0=1$, or this contradicts the assumption that the impurity ground state is nondegenerate. It is totally inconsistent that there be a continuum of ΔE_p values *relevant* at low energies.

This constitutes the sketch of a proof for a theorem[6] which insists that the pole (ii) has sufficient strength in the thermodynamic limit that its contribution totally outweighs that of the continuum (i). This determines the on-shell form of Σ the self-energy for any auxiliary propagator which manifests this lowest pole, i.e.,

$$\Sigma=\Delta E_0=\sum_{k,m} n_k\left(\frac{2c\delta_k^m}{\mathcal{N}a}\right) \tag{6a}$$

or

$$\delta\Sigma=\delta E_0=\sum_{k,m} \delta n_{km}\left(\frac{2c\delta_k^m}{\mathcal{N}a}\right)\,. \tag{6b}$$

The phase shifts are determined by the conduction electron scattering matrix, i.e., the on-shell value of the auxiliary particle propagator is essentially determined once the conduction electron scattering matrix has been evaluated. A particular transparent formula involving the R matrix will be given below.

The physics and direct calculation[6] illustrate the existence of the dominant pole (ii). It has a strength

$$r_0=\left(\sum_n \frac{1}{1-\Sigma_n'}\right)\sim\left(\frac{1}{\mathcal{N}}\right)^{\Sigma_m\delta_m^2/\pi^2}\,, \tag{7}$$

where Σ_n' is the on-shell value of the self-energy *derivative* and where the sum runs over all auxiliary propagators (usually all of them) which exhibit this lowest pole. The δ_m ($\delta_m<\pi/2$) are the phase shifts *at the Fermi surface* for the conduction electron channel m. Physically this corresponds to the orthogonality catastrophe limited overlap between the noninteracting and interacting ground states. Poles associated with any continuum have strengths $\sim 1/\mathcal{N}$ at best and in comparison are negligible.

It is implied that there is a relationship between the contribution from (iii) the exponential tails and (ii) the pole. Since the pole makes a contribution $r_0e^{-\beta\Delta E_0}$ to Z/Z_0, and since the continuum contribution (i) is negligible, it follows as another theorem that the contribution from (ii) *must* be $(1-r_0)e^{-\beta\Delta E_0}$. This can be shown explicitly by a somewhat involved diagram identity.[6]

With some fair generality the reaction matrix R_m as a function of the energy ω can be written in the form

$$R_m(\omega)=\frac{1}{\dfrac{1}{v_m(\omega)}-S(\omega)}\,,\qquad S(\omega)=\frac{1}{\mathcal{N}}\sum_{k'}\frac{1}{\omega-\epsilon_{k'}^0}\,. \tag{8}$$

The exact eigenenergies are the values of $\omega\equiv\epsilon_k$ for which $(1/R_m)=0$. A new function

$$R_{km}(\omega)=\frac{1}{\dfrac{1}{v_m(\omega)}-S(\omega)}\,,\qquad S_k(\omega)=\frac{1}{\mathcal{N}}\sum_{k'\neq k}\frac{1}{\omega-\epsilon_{k'}^0}\,, \tag{9}$$

differs by having the sum restricted. It follows that

$$\frac{2c\,\delta_{nk}}{Na}=\epsilon_k-\epsilon_k^0=\frac{1}{\mathcal{N}}R_{km}(\epsilon_k)\,, \tag{10}$$

and so on-shell

$$\Sigma=\frac{1}{\mathcal{N}}\sum_{km} n_kR_{km}(\epsilon_k)\,, \tag{11a}$$

or

$$\delta\Sigma=\frac{1}{\mathcal{N}}\sum_{km} \delta n_{km}R_{km}(\epsilon_k)\,, \tag{11b}$$

a surprisingly simple and powerful result. This is the principal result reported here. A discussion of its implications follows.

The auxiliary particle version of the problem of conduction electrons scattering off a structureless impurity potential is the simplest on which these theorems might be tested. This

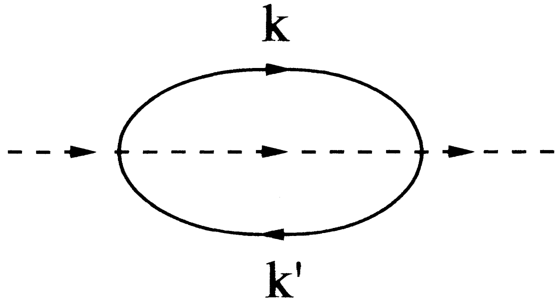

FIG. 1. The simplest $O(v^2)$ self-energy for the impurity scattering problem. This contains a logarithmic divergence and is the first such term in the degeneracy $N=1$ parquet series.

also represents a good test of the diagram summations techniques for the general Kondo, x-ray-edge, class of problems. The auxiliary particle formulation can be viewed as the degeneracy $N=1$ version of the Kondo problem which is equivalent to the x-ray-edge problem. Of course, the original problem is trivial to solve by standard single-body quantum mechanics. The only point of using the auxiliary particle method is as a test of the methodology and in particular to verify the applicability of Eqs. (11).

The Hamiltonian is

$$\mathscr{H}=\sum_k \epsilon_k^0 c_k^\dagger c_k+\lambda d^\dagger d+v\sum_{k,k'} c_k^\dagger c_{k'} d^\dagger d\,, \qquad (12)$$

where $\lambda\to\infty$ is the projection energy and where $d^\dagger$ is the creation operator for the auxiliary particle. By virtue of the constraint $Q=d^\dagger d=1$ this reduces to the impurity problem except for the additive constant λ.

This Hamiltonian is that for the x-ray absorption problem in which the $d^\dagger$ particle plays the role of the deep hole. The trivial impurity scattering problem has been turned into a problem which took a considerable number of years[4] and a great amount of ingenuity[7] to solve. The point to be made is that such an x-ray problem occurs in *any* problem in which auxiliary particles have been introduced. Even if in some limit a problem reduces to simple impurity scattering, as do many versions of the Kondo problem, then there will still remain an implicit x-ray-edge problem which must be dealt with. If the associated singularities do not occur then the basic approximations of the theory are inadequate. Even if the constraint is enforced in a different fashion the orthogonality catastrophe behind the x-ray-edge problem must still occur. If, say, in the auxiliary particle propagator it is the d operator which acts first at $t=0$, this necessarily destroys the single auxiliary particle which existed in the true ground state on which this operator acts. During the time which follows, until the operator $d^\dagger$ operates at time t, the system is one of nonscattering conduction electrons since the $d^\dagger d$ factor in the interaction is zero. The lowest-energy pole of this propagator will involve the overlap between the ground states appropriate to $t>0$ and $t<0$ and hence involves an orthogonality catastrophe. The infrared catastrophe is evident from the $O(v^2)$ self-energy shown in Fig. 1 which is approximately

$$\omega(\rho v)^2\ln(\omega/D) \qquad (13)$$

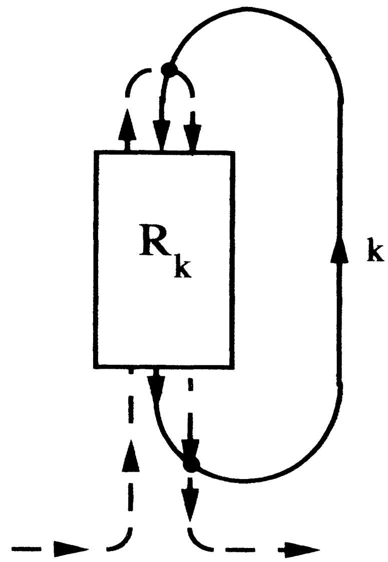

FIG. 2. Form of the self-energy after certain mathematical manipulations. The conduction electron line k is considered to be a pseudoexternal line, i.e., the sum on the internal frequency corresponding to this line is to be performed last [giving the n_k in Eq. (11)] and a partial fraction expansion sequence is performed in such an order that horizontal cuts across the diagram, ignoring the pseudoexternal line, determine the energy denominators (which no longer contain the true external frequency but rather the pseudoexternal quantity). It is a result that the diagrams, other than those of the general structure shown, and which do not have this k line leaving from the bottom of the diagram, cancel in pairs.

and contains the telltale logarithmic singularity. In fact the $N=1$ version of the parquet series exists. *None* of the popular approximation schemes gives the exact result, $\Sigma=\Sigma_k n_k \delta_k$. The author has devised a scheme in which the self-energy is pictured as being derived from the scattering matrix as illustrated in Fig. 2. One conduction electron line, the one which eventually becomes the n_k, is treated as a pseudoexternal line. Using this technique it is possible to show the existence of the massive cancellation of diagrams needed to reduce the diagrams to Eq. (11). The details will be presented elsewhere.[6] Also obtained in a rather direct fashion is the x-ray-edge result, i.e., the appropriate version of Eq. (7).

The no-crossing approximation is a popular scheme[3] for making a partial sum of the parquet series for the Kondo effect within the Anderson model. (It has been claimed recently[8] that it is exact for the overcompensated Kondo model for a certain large degeneracy limit which will *not* be dealt with here.) Denote $\mathscr{G}_p(i\nu)$ and $\mathscr{D}(i\nu)$ as the propagators which correspond, respectively, to the singly occupied orbital with $p=1,\ldots,N$ and the unoccupied orbital. Since in the Kondo limit the propagator $\mathscr{D}(i\nu)$ plays the role of a vector boson, it would be expected that the simple pole of interest for the ground-state properties *must* occur in $\mathscr{G}_p(\omega+is)$ and *possibly* in $\mathscr{D}(\omega+is)$. The self-energy for the former quantity, on-shell ($\omega=\Delta E_0$), is of the form

$$v^2\sum_k (1-n_k)\mathscr{D}(\Delta E_0-\epsilon_k)\,, \qquad (14)$$

which is consistent with Eq. (11b). However, $\mathscr{D}(\Delta E_0 - \epsilon_k)$ is *not* even a good approximation for either the relevant conduction scattering matrix or the phase shifts. The full scattering matrix R is given by a certain complicated convolution of the $\mathscr{D}$ and $\mathscr{S}$ propagators, the details of which can be found in Ref. 3.

Within the mean-field approximation for the Kondo effect,[2] the Bose operator $b^\dagger$ is replaced by a c number. In this scheme the spectral density of $\mathscr{S}_p(\omega)$ is unbounded below. One might try to excuse this fault by insisting that the end of the continuum is an energy which lies beyond the limits of this low-energy approximation. However, this would be inconsistent since it is precisely the end of the continuum which corresponds to the low-energy excitations. It is claimed that the approximation is exact in the limit $N \rightarrow \infty$. The constraint is written $Q = qN$ and the limit $q = 1/N$ is to be taken at the end. In the relevant limit it is implied that $q \rightarrow 0$ whence the renormalized width of the impurity (Kondo) resonance goes to zero. The energy ξ of this limiting pole might be expected to satisfy Eq. (11). Indeed, to within an unimportant shift in energy E_f^*, the result

$$-\xi = v^2 \sum_k n_k G_k^0(\xi) - E_f^* \tag{15}$$

and is of the correct structure. However, $v^2 G_k^0(\xi)$ is the bare conduction electron propagator and not the scattering matrix or phase shift.

Finally, the nature of the ground state essentially dictates the form of the on-shell self-energy. For example, for the compensated Kondo ground state, the ground-state energy is of the form

$$\Delta E_0 = \text{const} + \frac{1}{2} \frac{h^2}{2\pi T_0} + \cdots , \tag{16}$$

where $2\pi T_0$ is the strong coupling energy scale. It follows[6] that

$$\Sigma_{S_z} = \text{const} + S_z h + \frac{1}{2} \frac{h^2}{2\pi T_0} + \cdots , \tag{17}$$

where now $S_z h$ is required to cancel the explicit similar energy which occurs in the auxiliary particle propagator labeled S_z. The phase shifts at the Fermi level have equal but opposite values of $\pm \pi/2$. The signs depend upon which component of the singlet is projected out by a given propagator. A detailed discussion will be given elsewhere.[6]

When $h > kT$ the overcompensated Kondo effect also has a singlet ground state. The magnetization $m \sim h^{2/n}$, the mh term in the ground-state energy $\sim h^{1+2/n}$, and so

$$\Sigma_{S_z} = \text{const} + S_z h + \text{const} \times T_0 \left(\frac{h}{T_0} \right)^{1+2/n} + \cdots , \tag{18}$$

$S_z h$ is still needed since otherwise the linear term would dominate the magnetic energy. If there are n conduction electron channels one deduces that the phase shift is $\pi/2n$ for each channel. This implies a finite value of the effective interaction and *might* imply a finite fixed point in agreement with the analysis of Nozières and Blandin.[9]

The author thanks H. Beck, P. Wolfle, K. Matho, A. E. Ruckenstein, and P. Nozières for helpful conversations.

[1] S. E. Barnes, Adv. Phys. **30**, 801 (1981); J. Phys. **39**, C6-828 (1978); J. Phys. F **6**, 1375 (1976); **7**, 2637 (1977); *Magnetic Resonance and Related Phenomena. Proceedings of the XIX Congress Ampere*, edited by H. Brunner, K. H. Hausser, and D. Schweitzer (Groupement Ampere, Heidelberg, 1976).

[2] P. Coleman, Phys. Rev. B **28**, 5255 (1983).

[3] See the review N. E. Bickers, Rev. Mod. Phys. **59**, 845 (1987).

[4] See G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1981).

[5] Such tails are accounted for in the work of Ref. 1, but see also E. Müller-Hartmann, Z. Phys. B **57**, 281 (1984).

[6] S. E. Barnes (unpublished); Phys. Rev. Lett. **55**, 2192 (1985); Phys. Rev. B **33**, 3209 (1986).

[7] P. Nozières and C. T. deDominics, Phys. Rev. **178**, 1097 (1969).

[8] D. L. Cox and A. E. Ruckenstein, Phys. Rev. Lett. **71**, 1613 (1993).

[9] P. Nozières and A. Blandin, J. Phys. (Paris) **41**, 193 (1980).