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FERMI LIQUID THEORY OF THE DEGENERATE ANDERSON MODEL (*)

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Résumé. — On généralise le modèle d'Anderson pour des orbitales dégénérées. On formule une théorie d'un liquide de Fermi à basse température en utilisant les identités de Ward ; les quantités physiques sont exprimées en fonction de cinq paramètres du liquide de Fermi. Le comportement d'un spin $\frac{1}{2}$ à basse température est obtenu exactement dans le cas limite du couplage s-d.

Abstract. — The Anderson model is generalized for degenerate orbitals. Fermi liquid theory is derived for low temperatures by using Ward identities and the physical quantities are expressed in terms of five Fermi liquid parameters. In the s-d limit the low temperature behaviour for spin $S = \frac{1}{2}$ is solved exactly.

1. Introduction. — Wilson's numerical solution [1] of the Kondo problem for spin $S = \frac{1}{2}$ s-d model exhibits very simple universal behaviour at low temperature with a single scaling parameter (Kondo temperature). In order to describe this behaviour Nozières [2] formulated a pseudo-phenomenological Fermi liquid theory in a very elegant simple manner. The assumptions of this theory were justified by Yamada [3] and Yosida in a serie of papers. Two years ago Yoshimori [4] developed a theory for the degenerate Anderson model which was based on Ward identities derived by Shiba [5]. The aim of the present letter is to generalize the Hamiltonian used by them and to discuss the changes due to this generalization in the observable quantities.

The quantities to be considered are : the change in the d-level population due to the shift of the d-level energy ε_d , which is expressed as the charge susceptibility χ_c , and the orbital and spin susceptibilities, χ_{orb} and χ_s which are respectively the responses due to changes in magnetic fields $H_m \sim m$ and $H_\sigma \sim \sigma$ acting on orbitals with azimuthal quantum number m and spin σ . These responses are finite at temperature $T = 0$. Furthermore, the additional heat capacity C_{imp} due to the impurity is proportional to T near $T = 0$, thus $C_{imp} = \gamma T$.

These quantities can be expressed in terms of dimensionless quantities (indicated by bars) by intro-

ducing the renormalized single d-level density of states ρ_d taken at the Fermi energy, thus

$$\frac{\bar{\chi}_c}{\chi_c} = \frac{\bar{\chi}_s \mu_B^2}{\chi_s} = \frac{\bar{\chi}_{orb} \mu_B^2}{\chi_{orb}} = 2(2l + 1) \rho_d \quad (1)$$

$$\gamma = \frac{\pi^2}{3} 2(2l + 1) \rho_d k_B \bar{\gamma} \quad (2)$$

where the orbital degeneracy is $(2l + 1)$ -fold and $l = 2$.

The most prevailing result of Yoshimori [4] is that the could express the Landau Fermi liquid parameters by measurable quantities ($\bar{\chi}_s$ and $\bar{\chi}_{orb}$) and then he derived the remarkable inequality

$$\frac{\bar{\chi}_s + \bar{\chi}_{orb}}{\bar{\gamma}} = \frac{\bar{\chi}_s + \bar{\chi}_{orb}}{(\bar{\chi}_c/10) + (3/14)(\bar{\chi}_s + (8/5)\bar{\chi}_{orb})} \leq \frac{14}{3} \quad (3)$$

where the upper bound is reached for half filled d-orbitals (electron-hole symmetry) in the s-d limit. For single orbital [1, 2] $\bar{\chi}_s/\bar{\gamma} \leq 2$ and $\bar{\chi}_{orb} = 0$. The relation (3) can be checked by experiment, but the data (see eq. in ref. [6]) are not conclusive. There is one more quantity to be considered, the impurity resistivity

$$R_{imp}(T) = R_0 \left(1 - \left(\frac{T}{\theta_R} \right)^2 \right) \quad (4)$$

where the parameter θ_R can be expressed by $\bar{\gamma}$ in the symmetric case.

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2. Hamiltonian. — Yoshimori [4] achieved these results by using the generalization of the Anderson Hamiltonian to degenerate orbitals given by Dworin and Narath [7]. This generalization is based on the assumption that an electron pair with quantum numbers $(m\sigma, m'\sigma')$ can scatter only in the states $(m\sigma, m'\sigma')$ or $(m\sigma', m'\sigma)$, thus the individual quantum numbers as m and σ are conserved in the scattering. In this Hamiltonian there are two coupling constants for electron-electron scattering (U, J). Considering the atomic limit, it is well known [8], that the Coulomb integrals for d-electron depend on three parameters, R^0, R^2, R^4 , and, furthermore, only the total azimuthal quantum number $M = m + m'$ is a conserving quantity. This point has also been made independently by Blandin and Nozières [9]. The explicit form of the correct Hamiltonian is not given here, because we make use only of the symmetry properties. It will be shown, however, that dropping the conservation for individual quantum number m results in essential changes in the conclusions (like eq. (3)).

The form of the d-electron Green's function is

$$G_{m\sigma}(\omega) = \frac{1}{i\omega - \varepsilon_d + H_m + H_\sigma - \Sigma_{m\sigma}(\omega) + i\Delta \text{sg}(\omega)} \quad (5)$$

where Σ is the self-energy and Δ is the width due to s-d mixing. The physical quantities can be expressed in terms of the derivatives of the self-energy using Luttinger's relations [4]

$$\tilde{\chi}_c = 1 - \left. \frac{\partial \Sigma}{\partial \varepsilon_d} \right|_{\omega=0}, \quad \tilde{\chi}_s = 1 - \sum_{\sigma\sigma'} \sigma\sigma' \left. \frac{\partial \Sigma_\sigma}{\partial H_{\sigma'}} \right|_{\omega=0}$$

and

$$\tilde{\chi}_{\text{orb}} = \frac{l(l+1)}{3} - \sum_{mm'} mm' \left. \frac{\partial \Sigma_m}{\partial H_{m'}} \right|_{\omega=0} \quad (6)$$

furthermore

$$\tilde{\gamma} = 1 - \left. \frac{\partial \Sigma}{\partial \omega} \right|_{\omega=0} \quad (7)$$

3. Ward identities. — The Ward identities are a consequence of conservation laws. The conserving quantities are : the number of electrons, the Z-components of the total spin and of the total angular momentum. Following Shiba's work [5] the following three Ward identities can be derived

$$\frac{\partial \Sigma_{m\sigma}(\omega)}{\partial i\omega} = \frac{\delta G}{2\pi i} \sum_{m'\sigma'} \Gamma_{m\sigma m'\sigma'}(\omega, 0) + \frac{\partial \Sigma_{m\sigma}(\omega)}{\partial \varepsilon_d} \quad (8)$$

$$\sigma \frac{\partial \Sigma_{m\sigma}(\omega)}{\partial i\omega} = \frac{\delta G}{2\pi i} \sum_{m'\sigma'} \sigma' \Gamma_{m\sigma m'\sigma'}(\omega, 0) + \sum_{\sigma'} \sigma' \frac{\partial \Sigma_{m\sigma}(\omega)}{\partial H_{\sigma'}} \quad (9)$$

$$m \frac{\partial \Sigma_{m\sigma}(\omega)}{\partial i\omega} = \frac{\delta G}{2\pi i} \sum_{m'\sigma'} m' \Gamma_{m\sigma m'\sigma'}(\omega, 0) + \sum_{m'} m' \frac{\partial \Sigma_{m\sigma}}{\partial H_{m'}} \quad (10)$$

where only the diagonal part of the four-legs d-electron vertex occurs $\Gamma_{m\sigma m'\sigma'}(\omega, 0) = \Gamma_{m\sigma m'\sigma' m\sigma}(\omega, 0, 0, \omega)$ and $\delta G = G(0^+) - G(0^-)$. E.g. eq. (10) is obtained by comparing the following two Ward identities

$$\frac{\partial \Sigma_{m\sigma}(\omega)}{\partial H_{m'}} = -\frac{1}{2\pi} \int d\omega_1 \sum_{\sigma'} \Gamma_{m\sigma m'\sigma'}(\omega\omega_1) G^2(\omega_1) \quad (11)$$

and

$$m \frac{\partial \Sigma_{m\sigma}(\omega)}{i\omega} = \frac{\delta G}{2\pi i} \sum_{m'\sigma'} m' \Gamma_{m\sigma m'\sigma'}(\omega, 0) - \frac{1}{2\pi} \int d\omega_1 \sum_{m'\sigma'} m' \Gamma_{m\sigma m'\sigma'}(\omega, \omega_1) G^2(\omega_1). \quad (12)$$

The last equation is different from the one used by Yoshimori [4], because of a different conservation law. It is obtained in the following way. The energy variable ω is changed to $\omega + m\delta\omega$ for any internal line of quantum number m in the self-energy diagram and then the derivative is taken with respect to $\delta\omega$.

Using Ward identities (8)-(10) the quantities given by (6) and (7) can be expressed in terms of $\Gamma_{m\sigma m'\sigma'}(0, 0)$ and $\partial \Sigma(0)/\partial \omega$, and, then eliminating $\partial \Sigma/\partial \omega$ by $\tilde{\chi}_c$ one obtains

$$\tilde{\gamma} = \tilde{\chi}_c - \frac{1}{2(2l+1)} \sum_{m\sigma} \tilde{\Gamma}_{m\sigma m'\sigma'}(0, 0) \quad (13)$$

$$\tilde{\chi}_s = \tilde{\chi}_c - \frac{1}{2(2l+1)} \sum_{m\sigma} \frac{1}{2} (\sigma - \sigma')^2 \tilde{\Gamma}_{m\sigma m'\sigma'}(0, 0) \quad (14)$$

$$\tilde{\chi}_{\text{orb}} = \frac{l(l+1)}{3} \tilde{\chi}_c - \frac{1}{2(2l+1)} \sum_{m\sigma} \frac{1}{2} (m - m')^2 \times \times \tilde{\Gamma}_{m\sigma m'\sigma'}(0, 0) \quad (15)$$

where $\tilde{\Gamma} = \rho_d \Gamma(\delta G = 2\pi i \rho_d)$. According to Fermi liquid theory everything is expressed by the diagonal part of the vertex.

The expression for the resistivity is somewhat more complicated. According to Yoshimori, the resistivity at low temperature can be expressed by $\partial \Sigma/\partial \omega$ and $\partial^2 \Sigma/\partial \omega^2$ taken at $\omega = 0, T = 0$. $\partial \Sigma/\partial \omega$ is real and given by $\tilde{\gamma}$, see (7). Further simplification occurs, if the electron-hole symmetrical case is studied, where $\partial^2 \Sigma/\partial \omega^2$ is pure imaginary. Thus

$$R_{\text{imp}} = R_0 \left(1 - \frac{\pi^2 T^2}{3 \Delta^2} (\tilde{\gamma}^2 + 2I) \right) \quad (16)$$

where $I = \frac{\Delta}{i} \{ \partial^2 \Sigma/(\partial i\omega)^2 \}_{\omega=0}$. This quantity can be obtained by considering three excitations in the intermediate state. A straightforward consideration gives, that

$$I = \frac{1}{2(2l+1)} \times \times \frac{1}{2} \sum_{\substack{mm'm'' \\ \sigma\sigma'\sigma''}} |\tilde{\Gamma}_{m'\sigma', m''\sigma'', m'+m''-m, \sigma'+\sigma''-\sigma, m\sigma}(0, 0, 0, 0)|^2 \quad (17)$$

where the off-diagonal vertex elements occur as well. The asymmetric case can be treated in a similar way, but $\text{Re} \{ \partial^2 \Sigma / (\partial \omega)^2 \}_{\omega=0}$ appears, which is a new parameter [4].

4. Group theory. — In order to reduce the number of parameters the rotational invariance must be used in real and spin space. Thus, the four-legs vertex can be expressed in terms of the couplings $\Gamma_f^{(S)}$ which depend on the total spin S and angular momentum J associated with the two incoming lines. Thus, an arbitrary matrix element of the vertex can be written as

$$\tilde{\Gamma}_{m_1 \sigma_1, m_2 \sigma_2, m_3 \sigma_3, m_4 \sigma_4} = \sum_J \sum_S C_{m_1 m_2 J M} C_{m_3 m_4 J M} C_{\sigma_1 \sigma_2 S S_Z} C_{\sigma_3 \sigma_4 S S_Z} \tilde{\Gamma}_J^{(S)} \quad (18)$$

where C 's are the Clebsch-Gordan coefficients and $S_Z = \frac{1}{2}(\sigma_1 + \sigma_2)$. As the electrons obey Fermi statistics, thus for singlet ($S = 0$) $J = 0, 2, 4$ and for triplet ($S = 1$) $J = 1, 3$, all together there are five independent parameters. Inserting (18) in the expressions of the physical quantities and using the orthogonality relations for cases (13), (14), (15) and carrying out direct calculation for eq. (17) one gets

$$\tilde{\chi}_{\text{orb}} = \frac{l(l+1)}{3} \tilde{\chi}_c + \frac{1}{2(2l+1)} \sum_{J=0}^4 A_J (3 \Gamma_J^{(1)} + \Gamma_J^{(0)}) \quad (19)$$

$$\tilde{\chi}_s = \tilde{\chi}_c + \frac{1}{(2l+1)} \sum_{J=0}^4 (2J+1) (\Gamma_J^{(1)} + \Gamma_J^{(0)}) \quad (20)$$

$$\tilde{\gamma} = \tilde{\chi}_c + \frac{1}{2(2l+1)} \sum_{J=0}^4 (2J+1) (3 \Gamma_J^{(1)} + \Gamma_J^{(0)}) \quad (21)$$

$$I = \frac{1}{2(2l+1)} \frac{1}{2} \sum_{J=0}^4 (2J+1) (3 \Gamma_J^{(1)^2} + \Gamma_J^{(0)^2}) \quad (22)$$

where $A_0 = 4$, $A_1 = 11$, $A_2 = 15$, $A_3 = 14$ and $A_4 = 6$. Note that in contrast to Yoshimori's theory, we have five parameters

$$(\Gamma_0^{(1)} = \Gamma_2^{(1)} = \Gamma_4^{(1)} = \Gamma_1^{(0)} = \Gamma_3^{(0)} = 0)$$

instead of $\tilde{\Gamma}_c$ and $\tilde{\Gamma}_e$.

5. The symmetrical case in the s-d limit ($S = \frac{5}{2}$). — This is the limit, where electron-hole symmetry holds, and the couplings are very large compared with Δ , thus a well defined spin is formed at the impurity. The total spin is $S = \frac{5}{2}$ and the orbital momentum is zero, thus $\tilde{\chi}_{\text{orb}} = 0$. The number of independent constants can be reduced in three steps.

(i) If one extra electron is added to the d-level then the energy of that state is very large compared to the case where there are five electrons on the d-orbitals.

The life time is very short for these states. Thus, if two electron is scattered on the impurity described by the vertex $\Gamma_f^{(S)}$, then one find not more than one extra electron or hole in the intermediate state of the scattering at the same time, and when the extra electron or hole leaves the impurity into the conduction band, then the impurity must be left in its state characterized by $S = \frac{5}{2}$ and $J = 0$. It means, that only the vertex elements diagonal in quantum number m are different from zero. This is satisfied only if

$$\Gamma_1^{(1)} = \Gamma_3^{(1)} = \Gamma^t \quad (23)$$

and

$$\Gamma_0^{(0)} = \Gamma_2^{(0)} = \Gamma_4^{(0)} = \Gamma^s \quad (24)$$

thus there are two parameters, Γ^t for triplet and Γ^s for singlet.

(ii) Using the assumption, that $\tilde{\chi}_{\text{orb}} = 0$, one obtains

$$3 \Gamma^t + \Gamma^s = 0. \quad (25)$$

(iii) And also

$$\tilde{\chi}_c = 0. \quad (26)$$

The assumptions (ii) and (iii) are the consequence of the fact that in this limit the d-levels are far from the Fermi level.

Thus in the symmetric s-d limit there is only one free parameter e.g. Γ^s , which scales the problem, and, therefore it is inversely proportional to the Kondo temperature; $\Gamma^s \sim T_K^{-1}$. Inserting these results (23)-(26) into eqs. (19)-(22) and using (16) one obtains in that limit

$$\frac{\tilde{\chi}_s}{\tilde{\gamma}} = \frac{14}{3} \quad \text{or} \quad \frac{\chi_s}{\gamma} = \frac{14}{\pi^2} \quad (27)$$

and

$$R_{\text{imp}}(T) = R_0 \left(1 - \frac{\pi^2 T^2}{\Delta^2} \left(\frac{5\tilde{\gamma}}{3} \right)^2 \right) \quad (28)$$

or $\theta_R \gamma = 2$ in eq. (4). These results are not very far from the experimental data even for the asymmetric cases (see table I in ref. [6]).

These results agrees with those obtained by Yoshimori [4] for the s-d limit. That is due to the fact that in the s-d limit the vertex does not contain off-diagonal elements with respect to the quantum number m , if $\omega = 0$ and $T = 0$ is considered. It is a special feature of the s-d limit and does not hold generally as is assumed in Yoshimori's theory [4]. Thus the generalized form of the Anderson model suggested by Dworin and Narath [7] holds only as an effective Hamiltonian for the Fermi liquid theory in the limit where assumption (i) is fulfilled. (For comparison the parameters of ref. [7] are expressed by $\Gamma^{(0)}$ and $\Gamma^{(1)}$ as $u = \frac{1}{4}(\Gamma^s + \Gamma^t)$ and $J = \frac{1}{4}(\Gamma^s - \Gamma^t)$).

6. **Conclusion.** — In the general case the low temperature behaviour given by (19)-(22) and by (16) is determined by five parameters

$$(\Gamma_0^{(0)}, \Gamma_1^{(1)}, \Gamma_2^{(0)}, \Gamma_3^{(1)}, \Gamma_4^{(0)}) .$$

A complete solution of the problem would be required to connect these parameters with the five parameters of the original bare Hamiltonian as ε_d , Δ and three Coulomb integrals R^0, R^2, R^4 . The problem simplifies only in the s-d limit as is discussed. In the general case even the signs of the parameters are not known. The main difference between the results of Yoshimori's theory [4] based on a restricted Hamiltonian [7] and

of those presented here is that no upper bound like eq. (3) can be obtained. (e.g. $(\tilde{\chi}_{orb} + \tilde{\chi}_s)/\tilde{\gamma} = 6$ if only $\Gamma_0^{(0)}$ is different from zero, and this value is not an upper limit if negative coupling are considered as well). The conclusions given above are in complete agreement with the recent work by Blandin and Nozières [9] who came to similar conclusions by generalizing Nozières [2] Fermi liquid theory to the degenerate case.

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