

Fermi-liquid theory of the Korringa relations for the impurity-lattice relaxation of a pair of interacting Anderson impurities

P. Schlottmann

*Institut für Theoretische Physik, Freie Universität Berlin, 1000 Berlin 33, Arnimallee 3, Germany
and Institute for Theoretical Physics, University of California, Santa Barbara, California 93106*

(Received 22 September 1980)

We consider a pair of single-orbital Anderson impurities interacting with each other via a general two-body Hamiltonian. Using the Ward identities corresponding to the conservation of the total charge and the total spin, we derive the Korringa relations for the spin- and charge-lattice relaxation. The results are complementary to the Fermi-liquid relations for the specific heat, the charge, and spin susceptibilities derived previously. The results simplify in some special cases, i.e., two Kondo impurities, two nonmagnetic ions, a pair of mixed valence ions, the case of spinless impurities, and if the mean free path is much smaller than the distance between the impurities.

I. INTRODUCTION

The electronic structure of magnetic impurities embedded in a metallic host is usually appropriately described by the Anderson model.¹ At low temperatures isolated magnetic impurities are strongly coupled to the conduction band of the metal.² The system exhibits a universal behavior which is adequately described by a Fermi-liquid theory.³ The specific heat is proportional to the temperature, and the magnetic spin and orbital susceptibilities, as well as the charge susceptibility, are finite at zero temperature. Fermi-liquid theories have been successfully applied to obtain relations among these quantities to the single-orbital⁴ and the degenerate^{5,6} Anderson model and to the Kondo problem.³

The Fermi-liquid theory also provides a relation between the static susceptibilities and the dynamical response functions at low energies and zero temperature. These relations are known as the Korringa relations and have been derived by Yosida and Yamada⁷ for the nondegenerate Anderson impurity and extended by Shiba⁸ to the multiple-orbital impurity. If we assume that the dynamical susceptibilities have approximately a Lorentzian energy dependence, then the Korringa relations provide the corresponding relaxation times of the impurity, i.e., the time scale for the charge, spin, and orbital excitations.

The Fermi-liquid theory makes use of the conservation laws of the system. In the case of the degenerate Anderson impurity the total charge, spin, and orbital angular momentum are conserved. The conservation laws lead to Ward identities that relate the susceptibilities, the specific heat, and the zero-energy-invariant vertex parts. There are three such relations and $2l + 1$ invariant vertex couplings for the most general atomic interaction Hamiltonian,⁶ where

l is the individual orbital momentum of the localized electrons. If we restrict the interaction such that the individual quantum numbers m and σ are conserved in the scattering process of two electrons then the number of invariant vertex couplings can be reduced to 2.⁵

In a recent paper⁹ we considered the case of a pair of interacting Anderson impurities. The low-temperature and low-energy behavior of this system is also described by a Fermi-liquid theory. If we restrict ourselves to single-orbital impurities, the total charge and spin are conserved quantities of the system. They give rise to Ward identities that lead to relations of the specific heat and charge and spin susceptibilities. There are five invariant vertex couplings, but the problem simplifies in a number of special cases: (a) a system of spinless fermions, (b) the case of a short mean free path, (c) two interacting Kondo impurities, (d) two interacting nonmagnetic ions, and (e) the case of two mixed-valence ions.

The purpose of this paper is to derive the Korringa relations for the pair of Anderson impurities that relates the dynamical response functions at low energies and $T = 0$ to the static susceptibilities. They are derived using the same Ward identities that lead to the relations between the susceptibilities and the specific heat. The model is defined in Sec. II, where we state the Ward identities and the relations between the static quantities derived in Ref. 9. The ω -linear part of the dynamical correlation functions is obtained in Sec. III and it is expressed in terms of the static susceptibilities and Fermi-liquid parameters. In Sec. IV we discuss the results for the above-mentioned five special cases. We close the paper with a brief summary and conclusions.

The formulation of the problem is made in terms

of localized $4f$ electrons and extended $5d$ states in view of rare-earth ions. The two-impurity problem has been treated previously for the Kondo case by perturbational methods^{10,11} and ground-state calculations were performed by Sato and Nagaoka.¹² Within the framework of the Anderson model the papers by Alexander and Anderson,¹³ Casoli,¹⁴ Kim,¹⁵ and Yamada¹⁶ should be mentioned.

II. MODEL AND WARD IDENTITIES

In this section we define the model and summarize the results derived in Ref. 9.

We consider two interacting rare-earth ions, labeled by α and β , in a metallic matrix. The impurity $4f$ electrons interact with the $5d$ electrons of the metal through a hybridization term V

$$H_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}\sigma} d_{\vec{k}\sigma}^\dagger d_{\vec{k}\sigma} + \sum_{\sigma} (E_{\alpha\sigma} f_{\alpha\sigma}^\dagger f_{\alpha\sigma} + E_{\beta\sigma} f_{\beta\sigma}^\dagger f_{\beta\sigma}) + V \sum_{\vec{k}\sigma} (e^{i\vec{k}\cdot\vec{R}_\alpha} f_{\alpha\sigma}^\dagger d_{\vec{k}\sigma} + e^{i\vec{k}\cdot\vec{R}_\beta} f_{\beta\sigma}^\dagger d_{\vec{k}\sigma} + \text{H.c.}) , \quad (2.1)$$

$$\begin{bmatrix} i\omega - E_{\alpha\sigma} - V^2 F_\sigma(\omega, 0) & -V^2 F_\sigma(\omega, R) \\ -V^2 F_\sigma(\omega, R) & i\omega - E_{\beta\sigma} - V^2 F_\sigma(\omega, 0) \end{bmatrix} \hat{G}_{0\sigma}(\omega) = \hat{1} , \quad (2.3)$$

where

$$F_\sigma(\omega, R) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{R}}}{i\omega - \epsilon_{\vec{k}\sigma}} \quad (2.4)$$

and $\vec{R} = \vec{R}_\alpha - \vec{R}_\beta$. The one-particle self-energy is defined by

$$\left[\hat{G}_{0\sigma}^{-1}(\omega) - \hat{\Sigma}_\sigma(\omega) \right] \hat{G}_\sigma(\omega) = \hat{1} \quad (2.5)$$

and the discontinuity of $\hat{G}_\alpha(\omega)$ at the Fermi energy is denoted by

$$\rho_{ll'\sigma} = -\frac{1}{\pi} \text{Im} G_{ll'\sigma}(+i0) , \quad (2.6)$$

where l and l' are indices denoting the ions α and β .

The T -linear coefficient γ of the specific heat and the spin and charge susceptibilities can be expressed in terms of derivatives of the f -electron self-energy.

$$\sum_{l\sigma'} \frac{\partial \Sigma_{ij\sigma}(\omega)}{\partial E_{l\sigma'}} = \sum_{ll'\sigma'} \int \frac{dx}{2\pi} \Gamma_{ll'j}(\omega\sigma, x\sigma'; x\sigma', \omega\sigma) G_{ll''\sigma'}(x) G_{l'l'\sigma'}(x) , \quad (2.10)$$

$$\sum_{l\sigma'} \sigma' \frac{\partial \Sigma_{ij\sigma}(\omega)}{\partial B_{l\sigma'}} = - \sum_{ll'\sigma'} \sigma' \int \frac{dx}{2\pi} \Gamma_{ll'j}(\omega\sigma, x\sigma'; x\sigma', \omega\sigma) G_{ll''\sigma'}(x) G_{l'l'\sigma'}(x) . \quad (2.11)$$

Making use of similar relations for the derivatives with respect to ω , we obtained the following relations between

where $f_{\alpha\sigma}^\dagger$ is the creation operator of a f electron at the site α with spin σ and $d_{\vec{k}\sigma}^\dagger$ is the creation operator of a conduction electron with momentum \vec{k} and spin σ . Our results are not affected by the inclusion of a hopping integral for the f electrons between the α and β sites.

Since we make use only of the symmetry properties of the interaction Hamiltonian, its explicit form is not given here. It is assumed that (a) it only involves f -electron operators, (b) it conserves the total number of f electrons, (c) it conserves the total spin of the system, and (d) it preserves the spin-rotational invariance. These interactions involve direct and exchange Coulomb integrals, as well as indirect interactions via the conduction electrons [Ruderman Kittel Kasuya Yosida (RKKY)] or phonons.

It is useful to define the one-particle Green's function

$$\hat{G}_\sigma(\omega) = \begin{bmatrix} \langle \langle f_{\alpha\sigma}; f_{\alpha\sigma}^\dagger \rangle \rangle_{i\omega} & \langle \langle f_{\alpha\sigma}; f_{\beta\sigma}^\dagger \rangle \rangle_{i\omega} \\ \langle \langle f_{\beta\sigma}; f_{\alpha\sigma}^\dagger \rangle \rangle_{i\omega} & \langle \langle f_{\beta\sigma}; f_{\beta\sigma}^\dagger \rangle \rangle_{i\omega} \end{bmatrix} , \quad (2.2)$$

which evaluated in the noninteracting system yields

These relations are⁹

$$\tilde{\gamma} = \sum_{\sigma} \text{Tr} \left[\hat{\rho}_\sigma - \hat{\rho}_\sigma \frac{\partial \hat{\Sigma}_\sigma(\omega)}{\partial i\omega} \Big|_{\omega=0+} \right] , \quad (2.7)$$

$$\chi_c = \sum_{\sigma} \text{Tr} \left[\hat{\rho}_\sigma + \hat{\rho}_\sigma \sum_{l\sigma'} \frac{\partial \hat{\Sigma}_\sigma(+i0)}{\partial E_{l\sigma'}} \right] , \quad (2.8)$$

$$\chi_s = \sum_{\sigma} \text{Tr} \left[\hat{\rho}_\sigma + \sigma \hat{\rho}_\sigma \sum_{l\sigma'} \sigma' \frac{\partial \hat{\Sigma}_\sigma(+i0)}{\partial B_{l\sigma'}} \right] , \quad (2.9)$$

where $\tilde{\gamma}$ is defined as

$$\gamma = \frac{1}{3} \pi^2 \tilde{\gamma} .$$

The charge and spin conservation laws of the system lead to the following Ward relations linking the derivatives of the self-energy to the antisymmetrized vertex functions⁹

$\tilde{\gamma}$, χ_c , and χ_s

$$\tilde{\gamma} = - \sum_{ijl'\sigma\sigma'} \rho_{ij\sigma} \rho_{ll'\sigma'} \Gamma_{ll'j} (0\sigma, 0\sigma'; 0\sigma', 0\sigma) + \chi_c \quad (2.12)$$

$$\tilde{\gamma} = - \sum_{ijl'\sigma\sigma'} \sigma\sigma' \rho_{ij\sigma} \rho_{ll'\sigma'} \Gamma_{ll'j} (0\sigma, 0\sigma'; 0\sigma', 0\sigma) + \chi_s \quad (2.13)$$

Notice that according to the Fermi-liquid theory the relations (2.12) and (2.13) only involve diagonal matrix elements of the vertex function.

III. KORRINGA RELATIONS

In order to derive the Korringa relations for the charge and spin susceptibilities we have to calculate the corresponding low-frequency response functions

$$\delta_{\sigma\sigma'} \int \frac{d\omega'}{2\pi} G_{ij\sigma}(\omega + \omega') G_{ji\sigma}(\omega') + \sum_{l_1 l_2 l_3 l_4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} G_{il_1\sigma}(\omega + \omega_1) G_{l_2 i\sigma}(\omega_1) \Gamma_{l_1 l_4 l_3 l_2}(\omega + \omega_1\sigma, \omega_2\sigma'; \omega_2 + \omega\sigma', \omega_1\sigma) \times G_{l_3 j\sigma'}(\omega_2 + \omega) G_{j l_4 \sigma'}(\omega_2) \quad (3.2)$$

In order to obtain the $|\omega|$ -linear contribution we differentiate Eq. (3.2) with respect to ω at $\omega = 0$. Following Shiba⁸ we divide the result into three contributions that arise from the first diagram, the differentiation of the two propagators carrying energy ω in the second diagram and the differentiation of the vertex function.

(1) The contribution of the first diagram is given by

$$i\omega \int \frac{d\omega'}{2\pi} \frac{dG_{ij\sigma}(\omega')}{d\omega'} G_{ji\sigma}(\omega') \quad (3.3)$$

$$i\omega \sum_{l_1 l_2 l_3 l_4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \left[- \sum_l G_{il\sigma}(\omega_1) G_{ll_1\sigma}(\omega_1) - 2\pi \rho_{il_1\sigma} \delta(\omega_1) \right] G_{l_2 i\sigma}(\omega_1) \times \Gamma_{l_1 l_4 l_3 l_2}(\omega_1\sigma, \omega_2\sigma'; \omega_2\sigma', \omega_1\sigma) G_{l_3 j\sigma'}(\omega_2) G_{j l_4 \sigma'}(\omega_2) \quad (3.6)$$

The first term in the large parentheses vanishes because of the symmetry of the integral and we obtain

$$-|\omega|\pi \sum_{l_1 l_2 l_3 l_4} \rho_{l_1\sigma} \rho_{l_2 i\sigma} \int \frac{d\omega_2}{2\pi} \Gamma_{l_1 l_4 l_3 l_2}(0\sigma, \omega_2\sigma'; \omega_2\sigma', 0\sigma) G_{l_3 j\sigma'}(\omega_2) G_{j l_4 \sigma'}(\omega_2) \quad (3.7)$$

Similarly the differentiation of $G_{l_3 j\sigma'}(\omega_2 + \omega)$ yields

$$-|\omega|\pi \sum_{l_1 l_2 l_3 l_4} \rho_{l_3 j\sigma'} \rho_{j l_4 \sigma'} \int \frac{d\omega_1}{2\pi} \Gamma_{l_1 l_4 l_3 l_2}(\omega_1\sigma, 0\sigma'; 0\sigma', \omega_1\sigma) G_{il_1\sigma}(\omega_1) G_{l_2 i\sigma}(\omega_1) \quad (3.8)$$

(3) The differentiation of the vertex function is divided into two steps. We separate the vertex into two

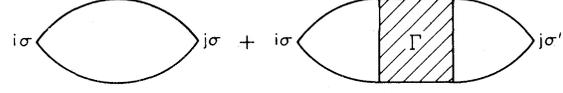


FIG. 1. Diagrammatic representation of the correlation function $\langle\langle n_{i\sigma}; n_{j\sigma'} \rangle\rangle_{i\omega}$.

at zero temperature. Since the static quantities are finite the dynamical correlations decrease linearly with $|\omega|$ for small imaginary frequencies. We consider the correlation function

$$\langle\langle f_{i\sigma}^\dagger f_{i\sigma}; f_{j\sigma'}^\dagger f_{j\sigma'} \rangle\rangle_{i\omega} \quad (3.1)$$

and calculate its $|\omega|$ -linear contribution for $\omega \rightarrow 0$.

The correlation (3.1) is diagrammatically represented in Fig. 1 and its analytical expression is given by

Substituting the relation

$$\frac{dG_{ij\sigma}(\omega)}{d\omega} = - \sum_l G_{il\sigma}(\omega) G_{lj\sigma}(\omega) - 2\pi \rho_{ij\sigma} \delta(\omega) \quad (3.4)$$

where $\rho_{ij\sigma}$ is defined by Eq. (2.6), into expression (3.3) we obtain

$$-|\omega|\pi \rho_{ij\sigma} \rho_{ji\sigma} \quad (3.5)$$

The first term of (3.4) does not contribute because of the symmetry of the integral.

(2) The differentiation of $G_{il_1\sigma}(\omega_1 + \omega)$ in the second diagram leads to

many-leg vertices joined by $2n$ propagators as shown in Fig. 2. This splitting of the vertex function is absolutely arbitrary. Following Shiba⁸ we first show that the only vertex partitions that contribute to the $|\omega|$ -linear part of (3.1) are those with $n = 1$, i.e., two propagators joining the vertices. The second step consists in evaluating this contribution.

(i) The diagram with the partitioned vertex, as shown in Fig. 2, yields

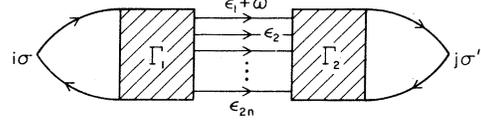


FIG. 2. Schematic partition of the vertex function of Fig. 1. The two vertices, Γ_1 and Γ_2 , have $2n + 2$ legs. Only one incoming and one outgoing line of each vertex carries the external energy ω .

$$\begin{aligned}
 i\omega \sum_{l_1 l_2 l_3 l_4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} G_{il_1\sigma}(\omega_1) G_{l_2j\sigma}(\omega_1) G_{l_3j\sigma'}(\omega_2) G_{jl_4\sigma'}(\omega_2) \\
 \times \sum_{m_1 n_1 \sigma_1} \delta\left(\sum \sigma_i\right) \int \frac{d\epsilon_1}{2\pi} \cdots \int \frac{d\epsilon_{2n}}{2\pi} \\
 \times \frac{dG_{m_1 n_1 \sigma_1}(\epsilon_1)}{d\epsilon_1} G_{m_2 n_2 \sigma_2}(\epsilon_2) \cdots G_{m_{2n} n_{2n} \sigma_{2n}}(\epsilon_{2n}) \\
 \times \Gamma_1[-\omega_1 l_1 \sigma, \omega_1 l_2 \sigma | \epsilon_1 m_1 \sigma_1, \dots, \epsilon_{2n} m_{2n} \sigma_{2n}] \\
 \times \Gamma_2[\omega_2 l_3 \sigma', -\omega_2 l_4 \sigma' | -\epsilon_1 n_1 \sigma_1, \dots, -\epsilon_{2n} n_{2n} \sigma_{2n}] 2\pi \delta\left(\sum \epsilon_i\right). \quad (3.9)
 \end{aligned}$$

We substitute the derivative using Eq. (3.4). The contribution due to the first term of Eq. (3.4) vanishes by symmetry of the integral. The derivative $dG/d(\epsilon_1)$ has then essentially been replaced by $\delta(\epsilon_1)$. Since there are $2n - 1$ propagators left, the contribution vanishes by symmetry, unless $n = 1$. In this case the discontinuities of $G_{m_1 n_1 \sigma_1}(\epsilon_1)$ and $G_{m_2 n_2 \sigma_2}(\epsilon_2)$ are superimposed and lead to a nonzero contribution.

(ii) For $n = 1$ the many-leg vertices Γ_1 and Γ_2 are just the four-leg vertex. We have then

$$\begin{aligned}
 -|\omega|\pi \sum_{l_1 l_2 l_3 l_4} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} G_{il_1\sigma}(\omega_1) G_{l_2j\sigma}(\omega_1) G_{l_3j\sigma'}(\omega_2) G_{jl_4\sigma'}(\omega_2) \\
 \times \sum_{m_1 m_2 n_1 n_2 \sigma''} \rho_{m_1 n_1 \sigma''} \rho_{m_2 n_2 \sigma''} \Gamma_{l_1 m_2, m_1 l_2}(\omega_1 \sigma, 0\sigma''; 0\sigma'', \omega_1 \sigma) \Gamma_{l_4 n_1, n_2 l_3}(\omega_2 \sigma', 0\sigma''; 0\sigma'', \omega_2 \sigma') \quad (3.10)
 \end{aligned}$$

that rewritten in a more convenient form yields

$$\begin{aligned}
 -|\omega|\pi \sum_{m_1 m_2 n_1 n_2 \sigma''} \rho_{m_1 n_1 \sigma''} \rho_{m_2 n_2 \sigma''} \sum_{l_1 l_2} \int \frac{d\omega_1}{2\pi} \Gamma_{l_1 m_2, m_1 l_2}(\omega_1 \sigma, 0\sigma''; 0\sigma'', \omega_1 \sigma) G_{il_1\sigma}(\omega_1) G_{l_2j\sigma}(\omega_1) \\
 \times \sum_{l_3 l_4} \int \frac{d\omega_2}{2\pi} \Gamma_{l_4 n_1, n_2 l_3}(\omega_2 \sigma', 0\sigma''; 0\sigma'', \omega_2 \sigma') G_{jl_4\sigma'}(\omega_2) G_{l_3j\sigma'}(\omega_2). \quad (3.11)
 \end{aligned}$$

The $|\omega|$ -linear contribution to Eq. (3.1) is then obtained by summing expressions (3.5), (3.7), (3.8), and (3.11). The charge susceptibility is obtained by summing (3.1) over i, j, σ, σ' . It is convenient to introduce a matrix

$$A_{l_1 l_2 \sigma} = \sum_{j l_3 l_4 \sigma'} \int \frac{d\omega}{2\pi} \Gamma_{l_1 l_4 l_3 l_2}(0\sigma, \omega \sigma'; \omega \sigma', 0\sigma) G_{l_3 j \sigma'}(\omega) G_{j l_4 \sigma'}(\omega) = \sum_{l \sigma'} \frac{\partial \Sigma_{l_1 l_2 \sigma}(+i0)}{\partial E_{l \sigma'}} \quad (3.12)$$

such that the static susceptibility is given by

$$\chi_c = \sum_{\sigma} \text{Tr}(\hat{\rho}_{\sigma} + \hat{\rho}_{\sigma} \hat{A}_{\sigma}) = \text{Tr} \hat{\chi}_c \quad (3.13)$$

and the $|\omega|$ -linear part of $\chi_c(\omega)$ by

$$-|\omega| \pi \sum_{\sigma} \text{Sp}(\hat{\rho}_{\sigma} + \hat{\rho}_{\sigma} \hat{A}_{\sigma})^2 = -|\omega| \frac{\pi}{2} \text{Tr} \hat{\chi}_c^2 \quad (3.14)$$

Equation (3.13) is the definition of a matrix charge susceptibility. The Korringa relation for the charge relaxation finally becomes for real energies

$$\lim_{\omega \rightarrow 0} \text{Im} \frac{\chi_c(\omega)}{\omega} = \frac{\pi}{2} \text{Tr} \hat{\chi}_c^2 \quad (3.15)$$

The main difference with Shiba's⁸ result for a single impurity is that the one-particle Green's function, Eq. (2.2), is not diagonal for a pair of impurities, since an f electron at one ion can submerge in the conduction band and emerge as an f electron at the other ion. This makes it necessary to handle with matrices instead of scalars.

Similarly we define for the spin susceptibility

$$\chi_s(\omega) = \sum_{ij\sigma\sigma'} \sigma\sigma' \langle \langle f_{i\sigma}^{\dagger} f_{i\sigma}; f_{j\sigma'}^{\dagger} f_{j\sigma'} \rangle \rangle_{i\omega} \quad (3.16)$$

the matrices \hat{B}_{σ} and $\hat{\chi}_s$

$$\begin{aligned} B_{i_1 i_2 \sigma} &= \sum_{j_3 j_4 \sigma'} \sigma' \int \frac{d\omega}{2\pi} \Gamma_{i_1 i_4 j_3 i_2}(0\sigma, \omega\sigma'; \omega\sigma', 0\sigma) \\ &\quad \times G_{i_3 j_4 \sigma'}(\omega) G_{j_4 i_4 \sigma'}(\omega) \\ &= \sum_{i\sigma'} \sigma' \frac{\partial \Sigma_{i_1 i_2 \sigma} (+i0)}{\partial B_{i\sigma'}} \end{aligned} \quad (3.17)$$

$$\hat{\chi}_s = \sum_{\sigma} (\hat{\rho}_{\sigma} + \sigma \hat{\rho}_{\sigma} \hat{B}_{\sigma}) \quad (3.18)$$

such that

$$\chi_s = \text{Tr} \hat{\chi}_s \quad (3.19)$$

and the $|\omega|$ -linear part of χ_s is given by

$$-|\omega| \frac{\pi}{2} \text{Tr} \hat{\chi}_s^2 \quad (3.20)$$

For a real energy variable ω we finally have the Korringa relation for spin relaxation

$$\lim_{\omega \rightarrow 0} \text{Im} \frac{\chi_s(\omega)}{\omega} = \frac{\pi}{2} \text{Tr} \hat{\chi}_s^2 \quad (3.21)$$

The two matrices \hat{A} and \hat{B} are not independent, but related by the zero-energy vertex functions. From Eqs. (3.7) and (3.8) of Ref. 9 we obtain

$$\begin{aligned} A_{i_1 i_2 \sigma} &= \sigma B_{i_1 i_2 \sigma} + \sum_{i_3 i_4 \sigma'} (1 - \sigma\sigma') \rho_{i_3 i_4 \sigma'} \\ &\quad \times \Gamma_{i_1 i_4 i_3 i_2}(0\sigma, 0\sigma'; 0\sigma', 0\sigma) \end{aligned} \quad (3.22)$$

The general relations, Eqs. (3.15) and (3.21), simplify in a number of special cases which are discussed in Sec. IV.

IV. DISCUSSION OF SPECIAL CASES

In order to discuss the results we specify the interactions of our model. There are five possible invariants for the antisymmetrized zero-energy vertex which are compatible with the spin-rotational invariance. The most general single-site interaction has the form

$$U(n_{\alpha\uparrow} n_{\alpha\downarrow} + n_{\beta\uparrow} n_{\beta\downarrow}) \quad (4.1)$$

where $n_{i\sigma}$ are the f -electron number operators. There are two two-site interactions that preserve the number of electrons at each site (a Coulomb and an exchange term)

$$-J \vec{S}_i \cdot \vec{S}_j + W(n_{\alpha\uparrow} + n_{\alpha\downarrow})(n_{\beta\uparrow} + n_{\beta\downarrow}) \quad (4.2)$$

where \vec{S}_i is the f spin at the site i . Finally there are two interactions in which one and two electrons, respectively, jump from one ion to the other:

$$t \sum_{\sigma} (f_{\alpha\sigma}^{\dagger} f_{\beta\sigma} + f_{\beta\sigma}^{\dagger} f_{\alpha\sigma})(n_{\alpha-\sigma} + n_{\beta-\sigma}) \quad (4.3)$$

and

$$K(f_{\alpha\uparrow}^{\dagger} f_{\alpha\downarrow}^{\dagger} f_{\beta\downarrow} f_{\beta\uparrow} + \text{H.c.}) \quad (4.4)$$

These five interaction forms have been discussed already in Ref. 9.

We consider the following special cases, for which we already discussed the static properties in our previous paper.⁹

A. Case of spinless fermions

Here only the interactions W has a meaning and we can build up bonding and antibonding states of our diatomic molecule. The Green's function is then diagonal and the expressions like Ward identities, etc., are similar to those of an isolated Anderson impurity. The only difference is that the two spin orientations have different resonance widths, corresponding to the bonding and antibonding states, $\rho_b \neq \rho_a$.

The charge susceptibility χ_c can be written

$$\chi_c = \chi_{\text{even}} + \chi_{\text{odd}} \quad (4.5)$$

where χ_{even} (χ_{odd}) contains all even- (odd-) order diagrams in W of χ_c . We have then that

$$\chi_{\text{even}} = \tilde{\gamma}, \quad \chi_{\text{odd}} = -\rho_a \rho_b \Gamma_{abba}(\omega_i = 0) \quad (4.6)$$

and that $\chi_c/\tilde{\gamma}$ is a monotonically decreasing function of W which varies from zero (for $W \rightarrow +\infty$) to 1

(for $W \rightarrow -\infty$) and takes the value 1 for $W = 0$.

Similarly the conservation of the bonding and antibonding states leads to an additional Ward identity which is associated with the charge-flip (from one site to the other) susceptibility⁹

$$\chi_{CF} = - \langle \langle (n_a - n_b); (n_a - n_b) \rangle \rangle_{\omega=0} = \chi_{\text{even}} - \chi_{\text{odd}} . \quad (4.7)$$

Consequently the ratio $\chi_{CF}/\tilde{\gamma}$ is a monotonically increasing function of W which varies from zero (for $W \rightarrow -\infty$) to 2 (for $W \rightarrow +\infty$) and also takes the value 1 for $W = 0$.

There exist three partial susceptibilities

$$- \langle \langle n_a; n_b \rangle \rangle_{\omega=0} = - \langle \langle n_b; n_a \rangle \rangle_{\omega=0} = \frac{1}{2} \chi_{\text{odd}} = \rho_a \int \frac{d\omega}{2\pi} \Gamma_{ab}(0, \omega) G_b^2(\omega) = \rho_b \int \frac{d\omega}{2\pi} \Gamma_{ba}(0, \omega) G_a^2(\omega) , \quad (4.8a)$$

$$- \langle \langle n_a; n_a \rangle \rangle_{\omega=0} = \rho_b \left[1 + \int \frac{d\omega}{2\pi} \Gamma_{aa}(0, \omega) G_a^2(\omega) \right] , \quad (4.8b)$$

$$- \langle \langle n_b; n_b \rangle \rangle_{\omega=0} = \rho_b \left[1 + \int \frac{d\omega}{2\pi} \Gamma_{bb}(0, \omega) G_b^2(\omega) \right] , \quad (4.8c)$$

and

$$\chi_{\text{even}} = - \langle \langle n_a; n_a \rangle \rangle_{\omega=0} - \langle \langle n_b; n_b \rangle \rangle_{\omega=0} . \quad (4.8d)$$

In this way we obtain that the relaxation time for charge excitation, T_{1c} , is given by

$$T_{1c} = \frac{\pi}{2} [(\langle \langle n_a; n_a + n_b \rangle \rangle_{\omega=0})^2 + (\langle \langle n_b; n_a + n_b \rangle \rangle_{\omega=0})^2] / \chi_c \quad (4.9)$$

and similarly the relaxation time for charge-flip excitations, T_{1CF} , is given by

$$T_{1CF} = \frac{\pi}{2} [(\langle \langle n_a; n_a - n_b \rangle \rangle_{\omega=0})^2 + (\langle \langle n_b; n_a - n_b \rangle \rangle_{\omega=0})^2] / \chi_{CF} . \quad (4.10)$$

For this simple model we have expressed five quantities in terms of the three partial susceptibilities.

If there is no direct hopping between the impurities the bonding and antibonding states resonate at the same energy. Their linewidths oscillate with the distance between the impurities and the amplitude of the oscillation decreases with the distance R . For large $k_F R$ the bonding and antibonding states have the same width, such that we have two isolated (or weakly interacting) impurities. If $k_F R \rightarrow 0$ the resonance width of the bonding state tends to zero. Hence if $E = 0$ both states are equally populated, but if $E < 0$ (> 0) the bonding state is empty (filled).

B. Case of $F(\omega, R) \approx 0$ for $R \neq 0$

This assumption means that an f electron at the α site cannot reach the β site and vice versa, e.g., because of a short mean free path, $\lambda \ll R$. Only interactions involving only number operators can survive in this case,⁹ i.e., $J = I = K = 0$. This simplified model is related to the one-impurity Anderson model with twofold orbital degeneracy but no spin exchange. The number of f electrons are conserved at each site, yielding a further Ward identity. The specific-heat coefficient, the charge, the spin, and the "orbital" susceptibilities are related by

$$\begin{aligned} \tilde{\gamma} &= \chi_s + \rho^2 \Gamma_U = \chi_c - \rho^2 (\Gamma_U + \Gamma_W) \\ &= \chi_0 - \rho^2 (\Gamma_U - \Gamma_W) , \end{aligned} \quad (4.11)$$

There are three relaxation times, corresponding to the charge, spin, and "orbital" (impurity-impurity) susceptibilities. Since the Green's-function matrix is diagonal, also the matrices $\hat{\chi}_c$, $\hat{\chi}_s$ and similarly $\hat{\chi}_0$ are diagonal and we obtain in a straightforward manner

$$T_{1c} = \frac{\pi}{4} \chi_c , \quad (4.12a)$$

$$T_{1s} = \frac{\pi}{4} \chi_s , \quad (4.12b)$$

$$T_{1\sigma} = \frac{\pi}{4} \chi_0 . \quad (4.12c)$$

In this case we have expressed seven physical quantities in terms of three Fermi-liquid parameters.

If the two ions are very distant, the W interaction is not relevant and we recover the case of two isolated Anderson impurities. In this case there remain two independent Fermi-liquid parameters that correspond to the χ_{even} and χ_{odd} of Yamada.⁴

C. Case of two Kondo impurities

We assume electron-hole symmetry and a large repulsive U interaction, such that each ion has one and only one f electron. In this case we neglect I , K , and W . The charge susceptibility vanishes and we have⁹

$$\tilde{\gamma} = -\rho_{\alpha\alpha}^2 \Gamma_U - \rho_{\alpha\beta}^2 \Gamma_J \quad (4.13a)$$

$$= \chi_s + \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_J \quad (4.13b)$$

or
$$\chi_s = 2\tilde{\gamma} \quad (4.14)$$

in analogy to noninteracting impurities.

Since the static and dynamic charge susceptibilities vanish it follows that:

$$A_{\alpha\alpha\sigma} = A_{\beta\beta\sigma} = -1, \quad A_{\alpha\beta\sigma} = A_{\beta\alpha\sigma} = 0 \quad (4.15)$$

Using the relation (3.22) we have that

$$\begin{aligned} \sigma B_{\alpha\alpha\sigma} &= \sigma B_{\beta\beta\sigma} = -1 - \frac{1}{2} \rho_{\alpha\alpha} \Gamma_U, \\ \sigma B_{\alpha\beta\sigma} &= \sigma B_{\beta\alpha\sigma} = -\frac{1}{2} \rho_{\alpha\beta} \Gamma_J, \end{aligned} \quad (4.16)$$

such that the matrix $\hat{\chi}_s$ is given by

$$\hat{\chi}_s = - \begin{pmatrix} \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_J & \rho_{\alpha\alpha} \rho_{\alpha\beta} (\Gamma_U + \Gamma_J) \\ \rho_{\alpha\alpha} \rho_{\alpha\beta} (\Gamma_U + \Gamma_J) & \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_J \end{pmatrix} \quad (4.17)$$

Taking trace over $\hat{\chi}_s$ we recover χ_s as given by Eq. (4.13). Using (3.21) we finally arrive at

$$T_{1s} \chi_s = \frac{\pi}{4} \chi_s^2 + \pi \rho_{\alpha\alpha}^2 \rho_{\alpha\beta}^2 (\Gamma_U + \Gamma_J)^2 \quad (4.18)$$

This relation does not provide new information, since the second term on the right-hand side involves a new Fermi-liquid parameter.

The case of bare exchange coupling $J=0$ and second-order perturbation in $F(\omega, R)$ has been analyzed in more detail by Yamada.¹⁶ Here we have that only Γ_U remains and the matrix $\hat{\chi}_s$ reduces to

$$\hat{\chi}_s = - \rho_{\alpha\alpha} \Gamma_U \begin{pmatrix} \rho_{\alpha\alpha} & \rho_{\alpha\beta} \\ \rho_{\alpha\beta} & \rho_{\alpha\alpha} \end{pmatrix} \quad (4.19)$$

The static susceptibility is given by $\chi_s = -2\rho_{\alpha\alpha}^2 \Gamma_U$ and the relation (4.14) remains valid. Expanding $\rho_{\alpha\alpha}$ in powers of $F_\sigma(R)$,

$$\rho_{\alpha\alpha} = \rho_{\alpha\alpha}^{\text{imp}} + \rho_{\alpha\alpha}^{\text{cx}}, \quad (4.20)$$

where $\rho_{\alpha\alpha}^{\text{imp}}$ is the single-site contribution and $\rho_{\alpha\alpha}^{\text{cx}}$ is second order in $F_\sigma(R)$, we can separate the local impurity susceptibility from the correlation between the impurities

$$\chi_s^{\text{imp}} = -2(\rho_{\alpha\alpha}^{\text{imp}})^2 \Gamma_U, \quad \chi_s^{\text{cx}} = -4\rho_{\alpha\alpha}^{\text{imp}} \rho_{\alpha\alpha}^{\text{cx}} \Gamma_U \quad (4.21)$$

The relaxation time is then given by

$$T_{1s} = \frac{\pi}{4} \chi_s \left[1 + \left(\frac{\rho_{\alpha\beta}}{\rho_{\alpha\alpha}} \right)^2 \right]$$

D. Case of two nonmagnetic ions

We assume electron-hole symmetry and a large attractive U interaction such that each ion has either two or zero f electrons. We can neglect Γ_J , Γ_t , and Γ_W because of electron-hole symmetry. We have that $\chi_s = 0$, such that

$$\tilde{\gamma} = \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_K = \chi_c - \rho_{\alpha\alpha}^2 \Gamma_U - \rho_{\alpha\beta}^2 \Gamma_K \quad (4.22)$$

and

$$\chi_c = 2\tilde{\gamma}, \quad \chi_s = 0 \quad (4.23)$$

Since the static and dynamic spin susceptibilities vanish we obtain

$$\sigma B_{\alpha\alpha\sigma} = \sigma B_{\beta\beta\sigma} = -1, \quad \sigma B_{\alpha\beta\sigma} = \sigma B_{\beta\alpha\sigma} = 0 \quad (4.24)$$

and

$$\begin{aligned} A_{\alpha\alpha\sigma} &= A_{\beta\beta\sigma} = -1 + \frac{1}{2} \rho_{\alpha\alpha} \Gamma_U, \\ A_{\alpha\beta\sigma} &= A_{\beta\alpha\sigma} = \frac{1}{2} \rho_{\alpha\beta} \Gamma_K. \end{aligned} \quad (4.25)$$

The matrix $\hat{\chi}_c$ is then given by

$$\chi_c = \begin{pmatrix} \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_K & \rho_{\alpha\alpha} \rho_{\alpha\beta} (\Gamma_U + \Gamma_K) \\ \rho_{\alpha\alpha} \rho_{\alpha\beta} (\Gamma_U + \Gamma_K) & \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\beta}^2 \Gamma_K \end{pmatrix} \quad (4.26)$$

and

$$T_{1c} \chi_c = \frac{\pi}{4} \chi_c^2 + \pi \rho_{\alpha\alpha}^2 \rho_{\alpha\beta}^2 (\Gamma_U + \Gamma_K)^2 \quad (4.27)$$

The situation is similar to the case of two Kondo impurities where the second term on the right-hand side involves a new Fermi-liquid parameter.

Setting the bare coupling K equal to zero and expanding in second order in $F(\omega, R)$ we obtain

$$\begin{aligned} \chi_c^{\text{imp}} &= -2(\rho_{\alpha\alpha}^{\text{imp}})^2 \Gamma_U, \quad \chi_c^{\text{cx}} = -4\rho_{\alpha\alpha}^{\text{imp}} \rho_{\alpha\alpha}^{\text{cx}} \Gamma_U, \\ T_{1c} &= \frac{\pi}{4} \chi_c \left[1 + \left(\frac{\rho_{\alpha\beta}}{\rho_{\alpha\alpha}} \right)^2 \right] \end{aligned} \quad (4.28)$$

The behavior of the charge susceptibility for the nonmagnetic impurities is similar to that of the spin susceptibility in the Kondo case.

E. Case of two mixed-valence ions

We assume that the ionic states with zero and one f electron have similar energies, whereas a large energy is required to localize a second electron at one site. We neglect Γ_K and also Γ_W can be disregarded if the zero and single occupancy states are quasidegenerate. We have then⁹

$$\begin{aligned} \tilde{\gamma} &= \chi_c - \rho_{\alpha\alpha}^2 \Gamma_U - \rho_{\alpha\alpha} \rho_{\alpha\beta} \Gamma_t - \rho_{\alpha\beta}^2 \Gamma_J \\ &\doteq \chi_s + \rho_{\alpha\alpha}^2 \Gamma_U + \rho_{\alpha\alpha} \rho_{\alpha\beta} \Gamma_t + \rho_{\alpha\beta}^2 \Gamma_J \end{aligned} \quad (4.29)$$

and

$$\chi_s + \chi_c = 2\tilde{\gamma} \quad (4.30)$$

Using Eq. (3.22) we obtain that

$$A_{\alpha\alpha\sigma} = \sigma B_{\alpha\alpha\sigma} + \frac{1}{4} (2\rho_{\alpha\alpha} \Gamma_U + \rho_{\alpha\beta} \Gamma_t) \quad (4.31a)$$

$$A_{\alpha\beta\sigma} = \sigma B_{\alpha\beta\sigma} + \frac{1}{4} (\rho_{\alpha\alpha} \Gamma_t + 2\rho_{\alpha\beta} \Gamma_J) \quad (4.31b)$$

With (4.31) we directly recover the relation for

$\chi_c - \chi_s$ of Eq. (4.29). The charge and spin-relaxation times are given by

$$T_{1c}\chi_c = \frac{\pi}{4}\chi_c^2 + \pi[\rho_{\alpha\beta}(1 + A_{\alpha\alpha}) + \rho_{\alpha\alpha}A_{\alpha\beta}]^2, \quad (4.32)$$

$$T_{1s}\chi_s = \frac{\pi}{4}\chi_s^2 + \pi[\rho_{\alpha\beta}(1 + \sigma B_{\alpha\alpha\sigma}) + \rho_{\alpha\alpha}\sigma B_{\alpha\beta\sigma}]^2. \quad (4.33)$$

The second terms on the right-hand side of both of these relations involve new Fermi-liquid parameters.

V. CONCLUSIONS

In a previous paper we obtained rigorous relations between the specific heat and the charge and spin susceptibilities for two interacting magnetic Anderson impurities. We have extended this calculation deriving the Korringa relations for the dynamical susceptibilities. The Korringa relation connects the ω -linear part of the dynamical response function, i.e., the relaxation time of the corresponding excitations, to the Fermi-liquid parameters.

These relations depend in general on the $A_{\mu'\sigma}$ and on five independent zero-energy vertex functions.

Under special assumptions the number of Fermi-liquid parameters can be reduced and the expressions simplify. For the two physically relevant cases, the pair of Kondo impurities and two interacting mixed valence ions, the relaxation times include new Fermi-liquid parameters. The Korringa relations in this way do not yield new relations among measurable quantities. It is seen that the relaxation time of the two-impurity molecule is always larger than that of a single impurity. This can be explained as follows. A charge leaving one impurity contributes to the impurity relaxation but not necessarily to the relaxation of the molecule, since the electron may emerge at the other impurity. A similar argument holds for spin-flip excitations. This difference is, for instance, explicitly given by the second terms on the right-hand side of Eqs. (4.18), (4.27), (4.32), and (4.33).

ACKNOWLEDGMENTS

The author would like to acknowledge the Deutsche Forschungsgemeinschaft (Germany) for a travel grant. The Institute for Theoretical Physics, University of California, Santa Barbara, is supported by the NSF through Grant No. PHY77-27084.

¹P. W. Anderson, Phys. Rev. 124, 41 (1961).

²K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).

³P. Nozières, J. Low Temp. Phys. 17, 31 (1974).

⁴K. Yamada, Prog. Theor. Phys. 53, 970 (1975).

⁵A. Yoshimori, Prog. Theor. Phys. 55, 67 (1976).

⁶L. Mihály and A. Zawadowski, J. Phys. Lett. (Paris) 39, L483 (1978).

⁷K. Yosida and K. Yamada, Prog. Theor. Phys. 53, 1286 (1975).

⁸H. Shiba, Prog. Theor. Phys. 54, 967 (1975).

⁹P. Schlottmann, Phys. Rev. B 21, 1084 (1980).

¹⁰M. T. Beal-Monod, Phys. Rev. 178, 874 (1969).

¹¹K. Sato and Y. Nagaoka, Prog. Theor. Phys. 47, 348 (1972).

¹²K. Sato and Y. Nagaoka, Prog. Theor. Phys. 50, 37 (1973); 53, 366 (1975).

¹³S. Alexander and P. W. Anderson, Phys. Rev. 133, A1594 (1964).

¹⁴B. Caroli, J. Phys. Chem. Solids 28, 1427 (1967).

¹⁵D. J. Kim, Phys. Rev. B 1, 3725 (1970).

¹⁶K. Yamada, Prog. Theor. Phys. 62, 901 (1979).