# Resonant-level model in the Kondo problem

P. B. Vigman and A. M. Finkel'shteĭn

*L. D. Landau Institute of Theoretical Physics, USSR Academy of Sciences*
(Submitted 5 January 1978; resubmitted 21 March 1978)
Zh. Eksp. Teor. Fiz. **75**, 204–216 (July 1978)

We consider the *s–d* exchange model that describes electron scattering by a magnetic impurity in a metal. The investigation is based on a transition to an equivalent model that admits of formulating a perturbation theory that is regular at low temperatures. Wilson's relation, which connects the impurity parts of the susceptibility and of the heat capacity, is derived. This relation is generalized to include the case of unequal Lande factors of the impurity and of the electrons.

PACS numbers: 72.15.Qm

## 1. INTRODUCTION

In 1964, Kondo[1] noted that the second-order correction to the amplitude of the scattering of an electron by a magnetic impurity increases logarithmically as the temperature $T\to 0$. At sufficiently low temperatures perturbation theory therefore ceases to hold. Kondo investigated scattering in the so-called $s-d$ exchange model, whose Hamiltonian is

$$H_{sd}=\sum_{k,\sigma=+,-}\varepsilon_k a_{k\sigma}^+ a_{k\sigma}+J\sum_{k,k'} a_k^+\sigma a_{k'}\cdot\mathbf{S} \qquad (1)$$

(the impurity spin is $S=1/2$).

It was shown later[2,3] by summing the principal terms that when the exchange interaction sign corresponds to antiferromagnetism ($J>0$) the effective scattering amplitude increases with decreasing temperature and has a pole at the Kondo temperature:

$$T_K\sim\tau^{-1}e^{-1/J}, \qquad (2)$$

where $\tau^{-1}$ is a quantity of the order of the width of the conduction band.[1)] Despite considerable efforts, the low-temperature behavior of the $s-d$ model remained unknown until Anderson, Yuval, and Hamann[4] obtained a qualitative solution of the problem. This solution was based on the fact that at a definite value of the exchange-interaction constant $J=J_T (J_T\approx 0.97)$ the partition function of the $s-d$ model turns out to be equal to the partition function of a simple model that has an exact solution and a Hamiltonian[5]

$$H_T=\sum_k\varepsilon_k c_k^+ c_k+V\sum_k (c_k^+ d+d^+ c_k). \qquad (3)$$

Here $c_k^+$ are the operators for the production of free zero-spin fermions, and $d^+$ is the operator of fermion production on a local resonance level. The mixing term $V$ causes the local level to acquire a width $\Delta_0=\pi V^2$, which is the energy scale of the theory. Anderson *et al.*[4] assumed that the renormalized value of $J$ is equal to $J_T$. The low-temperature behavior of the $s-d$ model at small $J$ is therefore the same as for the model given by (3), but the energy scale $\Delta_0$ should be replaced by $T_K$. As a result, they obtained in Ref. 4 the correct statement that the susceptibility of the magnetic impurity in the metal, $\chi$, is finite at $T=0$ and its order of magnitude is

$$\chi\sim T_K^{-1}. \qquad (4)$$

The procedure used in Ref. 4, however, is not rigorous. It was assumed that the Hamiltonian (1) is not altered by the renormalization, but this not the actual case. None the less, the estimate (4) turned out to be correct. This became clear after Wilson[6,7] undertook a thorough investigation of the Kondo problem by using numerical methods. Besides calculating $\chi(T)$, Wilson obtained (also numerically) the relation

$$\lim_{T\to 0}\frac{3g^2\mu^2}{4\pi^2}\frac{C}{T\chi(g,g)}=\frac{1}{2}, \qquad (5)$$

where $C$ is the correction to the heat capacity due to the presence of the magnetic impurity, and $\chi(g,g)$ is the correction to the magnetic susceptibility when the Lande factors of the impurity are equal, $g_i=g_e=g$; $\mu$ is the Bohr magneton.

In the present paper we propose a model whose Hamiltonian is a natural generalization of expression (3):

$$H_{RL}=H_T+\frac{1}{4}U(d^+d-dd^+)\sum_{kk'}(c_k^+c_{k'}-c_{k'}c_k^+). \qquad (6)$$

This model will hereafter be called the resonant-level (RL) model. It will be shown that the partition functions of the RL and $s-d$ models coincides if $V$ is properly chosen and if

$$1-\frac{2}{\pi}\,\mathrm{arctg}\,\frac{\pi U}{2}=\sqrt{2}\left(1-\frac{2}{\pi}\,\mathrm{arctg}\,\frac{\pi J}{4}\right) \qquad (7)$$

(a particular case of this equivalence, corresponding to $U=0$, occurs at $J=J_T$). The equality of the partition function makes it possible to use the RL model for the study of the low-temperature properties of the model at small $J$.

The Hamiltonian (6) admits of an exact solution both at $V=0$ and at $U=0$. Perturbation theory in $V$ (as well as its equivalent, the perturbation theory in $J$ in the $s-d$ model) does not make it possible to investigate the low-temperature properties of the system. The reason is that the ground state of the zeroth approximation chosen in this manner is orthogonal to the true one. To study the low-temperature properties it is necessary to consider the perturbation-theory series in $U$. Each member of this series is regular as $T\to 0$. Therefore, even though small $J$ corresponds to $U\sim -0.48$, the choice of this zeroth approximation is preferable.

  

We derive below the Wilson relation (5) analytically by using the RL model. This relation can be generalized to the case when the $g$-factors of the electron and impurity are not equal ($g_e \neq g_i$):

$$\lim_{T\to 0}\frac{3}{4\pi^2}g_i^2\mu^2\frac{C}{T\chi(g_i,g_e)}$$
$$=\frac{1}{2}\left[\left(1-\frac{2}{\pi}\arctan\frac{J\pi}{\pi}\right)\bigg/\left(1-\frac{g_e}{g_i}\frac{2}{\pi}\arctan\frac{J\pi}{4}\right)\right]^2. \qquad (8)$$

## 2. EQUIVALENCE OF THE RL AND s-d MODELS

Following Anderson and Yuval,[8] we express the $s-d$ model Hamiltonian in the form

$$H=\sum_{k\sigma=\pm}\varepsilon_k a_{k\sigma}^+a_{k\sigma}+\frac{J_\parallel}{2}\sum_{kk'\sigma=\pm}\sigma a_{k\sigma}^+a_{k'\sigma}S^z+J_\perp\sum_{kk'}(a_{k+}^+a_{k-}S^-+a_{k-}^+a_{k+}S^+). \qquad (9)$$

The real situation corresponds to $J_\parallel = J_\perp = J$. It is convenient, however, to distinguish between the corresponding coefficients, since the Hamiltonian (9) is diagonal at $J_\perp = 0$ and it is possible to construct a perturbation theory in terms of $J_\perp$ (Ref. 8). The $s-d$ model partition function, regarded as a series in $J_\perp$, takes the form

$$Z_{s-d}=Z_0Z_1,$$

where $Z_0$ is the partition function at $J_\perp = 0$ and has no singularities connected with the Kondo problem; it will no longer be considered. On the other hand

$$Z_1=2\sum_{n=0}^{\infty}\left(\frac{J_\perp\cos^2\delta}{2\tau}\right)^{2n}\int_0^{\beta-\tau}d\tau_{2n}\ldots\int_0^{\tau_2-\tau}d\tau_1P_{2n}(\tau_1\ldots\tau_{2n}), \qquad (10)$$

where

$$P_{2n}=\exp\left\{2\left(1-\frac{2}{\pi}\delta\right)^2\sum_{\nu>\nu'}^{2n}(-1)^{\nu-\nu'}\ln\frac{\sin\pi T(\tau_\nu-\tau_{\nu'})}{\pi T\tau}\right\}, \qquad (11)$$

and $\delta = \tan^{-1}J_\parallel\pi/4$ is the phase shift of the scattering by the potential $J_\parallel/4$. The quantity $Z_1$ describes the thermodynamics of a one-dimensional classical gas of impermeable particles with alternating-sign charges.[9,10] The cutoff factor $\tau$ regularizes the theory when the distance between particles is small; $\tau^{-1}$ is a quantity of the order of the Fermi energy. To take into account the magnetic field, we add to the Hamiltonian (9) a term

$$-\mu\mathscr{H}\left(g_iS^z+\frac{1}{2}g_e\sum_{k\sigma=\pm}\sigma a_{k\sigma}^+a_{k\sigma}\right). \qquad (12)$$

The quantity $P_{2n}$ is multiplied in this case by the factor

$$\mathrm{ch}\left\{g_i\left(1-\frac{2}{\pi}\frac{g_e}{g_i}\delta(J)\right)\mu\mathscr{H}\left(\sum_{\nu=0}^{2n}(-1)^\nu\tau_\nu-\frac{\beta}{2}\right)\right\}. \qquad (13)$$

At $g_e = g_i = g$, the partition function of the $s-d$ model is a function of three arguments:

$$Z_1=z({}^1/{}_2J_\perp\cos^2\delta,\ q_{sd}^2,\ 2^{-1/2}g\mu\mathscr{H}q_{sd}), \qquad (14)$$

where

$$q_{sd}=2^{1/2}\left(1-\frac{2}{\pi}\delta(J)\right).$$

We proceed to consider the resonant-level model. We add to the Hamiltonian (6) the quantity

$$-\frac{1}{2}h_c\sum_k(c_k^+c_k-c_kc_k^+)-\frac{1}{2}h_d(d^+d-dd^+). \qquad (15)$$

The field $h_c$ alters the chemical potential of the fermions, and the field $h_d$ changes the position of the local level. We shall henceforth compare the heat capacity and susceptibility of the RL model relative to the field $h = h_c = h_d$ with the corresponding quantities in the $s-d$ model:

$$C_{RL}=-\frac{d}{dT}T^2\frac{d}{dT}\ln Z_{RL},\quad \chi_{RL}=-T\frac{d^2\ln Z_{RL}}{dh^2}.$$

As shown in the Appendix, the partition function $Z_{\rm RL}$ of the RL model, regarded as the perturbation-theory series in $V$, takes at $h = h_c = h_d$ the form

$$Z_{RL}=z(V\cos\delta^*\tau^{1/2},\ q_{RL}^2,\ hq_{RL}). \qquad (16)$$

Here

$$\delta^*=\mathrm{arctg}\frac{\pi U}{2},\quad q_{RL}=1-\frac{2}{\pi}\delta^*,$$

and $z$ is the same function, of three arguments, as in the right-hand side of (14). We note that $q_{sd}^2(\delta J)$ has, compared with $q_{\rm RL}^2(\delta^*(U))$, an extra coefficient 2. The point is that in the case of the $s-d$ model (formula (11) $P_{2n}$ is made up of a product of two identical factors corresponding to electrons with different spin projections.

Thus, at

$$q_{RL}=q_{sd},\quad V\cos\delta^*\tau^{1/2}={}^1/{}_2J_\perp\cos^2\delta,\quad h=2^{-1/2}g\mu\mathscr{H} \qquad (17)$$

the partition functions of the two models coincide. Hence

$$C_{sd}=C_{RL},\quad \chi_{sd}={}^1/{}_2(g\mu)^2\chi_{RL}. \qquad (18)$$

It will be shown below that in the resonant-level model, in the low-temperature limit, the following relation holds:

$$C_{RL}/T\chi_{RL}=\pi^2/3. \qquad (19)$$

Consequently, in the $s-d$ model,

$$\frac{(g\mu)^2C_{sd}}{T\chi_{sd}(g,g)}=\frac{2\pi^2}{3}. \qquad (20)$$

It follows from (13) that the metal susceptibility due to the presence of the magnetic impurity depends on the Lande factors of the electrons and of the impurity in the following manner:

$$\chi_{s-d}(g_i,g_e)=\left\{\left[1-\frac{g_e}{g_i}\frac{2}{\pi}\delta(J)\right]\bigg/\left[1-\frac{2}{\pi}\delta(J)\right]\right\}^2\chi_{sd}(g_i,g_i). \qquad (21)$$

This enables us to generalize the ratios (20) to the case of unequal Lande factors (formula (8)).

## 3. ZEROTH APPROXIMATION

In this section we derive relation (19) at $U = 0$, and introduce the symbols that will be needed hereafter.

At $U=0$ the RL-model Hamiltonian is

$$H_{RL}^0=\sum_k \varepsilon_k c_k^+c_k+V\sum_k (c_k^+d+d^+c_k)$$
$$-\frac{1}{2}h_c\sum_k (c_k^+c_k-c_kc_k^+)-\frac{1}{2}h_d(d^+d-dd^+). \quad (22)$$

We introduce the free temperature Green's functions of the local level and of the fermions situated in the fields $h$:

$$\mathcal{D}(t-t')=-\langle Td(t)d^+(t')\rangle,\quad \mathcal{D}(\omega)=1/(i\omega+h_d), \quad (23)$$
$$\mathcal{F}_k(\omega)=1/(i\omega-\xi_k+h_c), \quad (24)$$

where $\xi_k$ is the free-fermion energy reckoned from the Fermi surface. Since we are investigating an interaction with a local level, the thermodynamics is determined only by Green's functions with equal spatial arguments:

$$\mathcal{F}(\omega,h_c)=\sum_k \mathcal{F}_k(\omega)=-i\pi\,\mathrm{sign}\,\omega\cdot\theta(\Lambda-|\omega+h_c|), \quad (25)$$

where

$$\theta(x)=\begin{cases}1, & x>0,\\ 0, & x<0,\end{cases}$$

and $\Lambda$ is a quantity of the order of the width of the fermion band. To describe the model (22) it is convenient to introduce the following two-row matrix:

$$G^{-1}=\begin{pmatrix} i\omega+h_d & V\\ V & \mathcal{F}^{-1}\end{pmatrix}. \quad (26)$$

It is the inverse of the matrix of the Green's functions with equal spatial arguments

$$G(\omega,h)=\begin{pmatrix} G^{dd} & G^{dc}\\ G^{cd} & G^{cc}\end{pmatrix}=\mathrm{Det}\,G\begin{pmatrix}\mathcal{F}^{-1} & -V\\ -V & i\omega+h_d\end{pmatrix}. \quad (27)$$

The change of the free energy of the fermion gas due to the presence of the resonant level at $U=0$ is

$$\delta F^0=-T\sum_n 2\int_0^1 d\lambda\, VG_\lambda^{cd}(\omega_n), \quad (28)$$

where $\omega_n=(2n+1)\pi T$, and $G_\lambda^{cd}$ is an element of the matrix (27), but with $V$ replaced by $\lambda V$. Thus, the part of the free energy connected with the resonant level is equal to

$$F^0=-T\sum_n [\ln \mathrm{Det}\,G^{-1}(\omega_n)-\ln\mathcal{F}^{-1}]. \quad (29)$$

From this we get at low temperatures

$$C_{RL}^0=-\frac{\pi}{3}T\frac{d}{d\omega}\mathrm{Im}\ln\mathrm{Det}\,G_R^{-1}\Big|_{\omega,h=0}=\frac{\pi^2}{3}\frac{T}{\pi\Delta_0},$$
$$\chi_{RL}^0=-\frac{1}{\pi}\frac{d}{dh}\mathrm{Im}\ln\mathrm{Det}\,G_R^{-1}\Big|_{\omega,h=0}=\frac{1}{\pi\Delta_0}, \quad (30)$$

where $G_R$ is a matrix of retarded Green's functions. Thus, relation (19) is satisfied in zeroth order of perturbation theory. We note that the change of the free energy turns out to be independent of the field $h_c$. This takes place only at $U=0$.

It will be shown below that relation (19) is satisfied in all orders in $U$.

## 4. HEAT CAPACITY

In the presence of interaction, the Green's function takes the form

$$\mathcal{G}^{-1}=G^{-1}-\Sigma, \quad (31)$$

where the self-energy part $\Sigma$ is a $2\times 2$ matrix.

To find the heat capacity it is convenient to use for the free energy an expression in the form proposed by Luttinger and Ward[11,12]

$$F=-T\sum_n \mathrm{Sp}\{\ln\mathcal{G}^{-1}+\mathcal{G}\Sigma\}+F'\{\mathcal{G}\}, \quad (32)$$

where $F'\{\mathcal{G}\}$ is a functional whose variational derivative with respect to $\mathcal{G}$ is equal to $\Sigma$. The free energy in this form is a functional that is stationary in $\mathcal{G}$. Just as in the Fermi-liquid theory, this property enables us to express the heat capacity at low temperatures in terms of the Green's function:

$$C_{RL}=-\frac{\pi}{3}T\frac{d}{d\omega}\mathrm{Im}\,\mathrm{Sp}\ln\mathcal{G}_R^{-1}(0)=-\frac{\pi}{3}T\frac{d}{d\omega}\mathrm{Im}\ln\mathrm{Det}\,\mathcal{G}_R^{-1}(0), \quad (33)$$

where

$$\mathrm{Det}\,\mathcal{G}^{-1}=(\mathcal{F}^{-1}-\Sigma^{cc})(i\omega-\Sigma^{dd})-(V-\Sigma^{cd})^2. \quad (34)$$

Expression (33) can be substantially simplified by determining the properties of the matrix $\Sigma$ at small $\omega$. We note for this purpose that at $h=0$ the functions $G^{dd}$ and $G^{cc}$ are odd, and the function $G^{cd}$ is even. In addition, on the imaginary axis of the $\omega$ plane the functions $G^{dd}$ and $G^{cc}$ are imaginary and $G^{cd}$ is real. Similar properties are possessed also by the matrix $\Sigma$. In fact, any diagram $\Sigma$ contains an odd number of lines. Furthermore, the diagrams $\Sigma^{cd}$ must of necessity contain an odd number of $G^{cd}$ lines, while $\Sigma^{dd}$ and $\Sigma^{cc}$ must contain an even number of such lines. Therefore the function $\Sigma^{cd}$ is even and real on the imaginary axis, while the functions $\Sigma^{dd}$ and $\Sigma^{cc}$ are odd and imaginary. It follows therefore that on the real axis, at small $\omega$, we have

$$\Sigma^{cd}(\omega)=\alpha_0+\alpha_1 i\omega\,\mathrm{sign}\,\omega+\alpha_2\omega^2+\ldots,$$
$$\Sigma^{dd},\ \Sigma^{cc}(\omega)=i\beta_0\,\mathrm{sign}\,\omega+\beta_1\omega+\beta_2 i\omega^2\,\mathrm{sign}\,\omega+\ldots. \quad (35)$$

The function $G^{dd}$ is the only $G$-matrix element whose derivative is singular at small $\omega$:

$$\frac{d}{di\omega}G^{dd}(\omega)=-(G^{dd}(\omega))^2+\frac{2}{\Delta_0}\delta(\omega). \quad (36)$$

Therefore the non-analytic terms of the type $\omega^n$ sign $\omega$ in the series (35) can stem only from diagrams that have sections consisting of $n+1$ $G^{dd}$ lines. Since any section must contain at least three lines, non-analytic terms appear only at $n\geqslant 2$. This means that

$$\Sigma^{dd}(0)=\Sigma^{cc}(0)=\frac{d}{d\omega}\Sigma^{cd}(0)=0, \quad (37)$$

while the quantities $\Sigma^{cd}(0)$ and

$$Z_\omega-1=-\frac{d}{d\omega}\Sigma_R^{dd}(0)$$

are real.

These properties suffice to be able to express (33) in the form

$$\frac{C_{RL}}{T}=\frac{\pi^2}{3}\frac{Z_\omega}{\pi\Delta}, \tag{38}$$

where

$$\Delta=\pi(V-\Sigma^{cd}(0))^2. \tag{39}$$

Thus, the contribution of the magnetic impurity to the heat capacity of the metal at low temperatures is proportional to $T$ in all orders of perturbation theory in $U$.

## 5. SUSCEPTIBILITY

We proceed now to the study of the susceptibility. The change in the number of particles in fields $h_d=h_c=h$, due to the presence of the resonant level, consists of two parts:

$$-\frac{dF}{dh}=T\sum_n \mathscr{G}^{dd}(\omega_n)+\sum_k (n_k-n_k^0) \tag{40}$$

($d/dh$ denotes the sum of the partial derivatives with respect to $h_d$ and $h_c$). The second term describes the change of the number of fermions. Since the interaction with the local level is a contact interaction, $n_k-n_k^0$ can be represented in the form

$$T\sum_n \mathscr{F}_k(\omega_n)t(\omega_n)\mathscr{F}_k(\omega_n),$$

where the amplitude $t$ does not depend on $k$ and can be expressed in terms of the function $\mathscr{G}^{cc}$:

$$t(\omega)=(\mathscr{G}^{cc}-\mathscr{F})\mathscr{F}^{-2}. \tag{41}$$

We note that, in contrast to the Anderson model,[13] the last term in (40) is not equal to zero and the "compensation theorem" does not hold here.

Taking (41) into account, we can represent the change in the number of particles in the form

$$-\frac{dF}{dh}=T\sum_n \mathrm{Sp}\left\{\frac{d}{di\omega_n}\ln\mathscr{G}^{-1}(\omega_n)+\mathscr{G}\frac{d}{di\omega_n}\Sigma(\omega_n)\right\}. \tag{42}$$

Just as in Fermi-liquid theory,[12] the second term vanishes as $T\to 0$. Changing from summation over the frequencies to integration, we get

$$-\frac{dF}{dh}=-\frac{1}{\pi}\,\mathrm{Im\,Sp}\ln\mathscr{G}_R^{-1}(0) \tag{43}$$

and consequently

$$\chi_{RL}=-\frac{1}{\pi}\frac{d}{dh}\,\mathrm{Im}\ln\mathrm{Det}\,\mathscr{G}_R^{-1}. \tag{44}$$

Just as in the derivation of the formula for the heat capacity, it is easy to show that $d\Sigma^{dd}(0)/dh$ is real and $d\Sigma^{cd}/dh$ is odd in $\omega$. Since the terms that are not analytic in $\omega$ appear only in the higher-order derivatives with respect to $\omega$, it follows that $d\Sigma^{cd}(0)/dh=0$. Bearing these properties in mind, we get for $\chi_{RL}$

$$\chi_{RL}=Z_h/\pi\Delta, \tag{45}$$

where

$$Z_h=1-\frac{d}{dh}\Sigma^{dd}(0).$$

We note that the susceptibility of the magnetic impurity is finite in each order of perturbation theory.

## 6. PROOF OF WILSON'S RELATION

To prove relation (19) it remains to show that

$$\left(\frac{d}{d\omega}-\frac{d}{dh}\right)\Sigma^{dd}(0)=0. \tag{46}$$

Before we proceed to the general proof, we make the following remark. The only element of the matrix $G^{-1}$ independent of $h_c$ is $(G^{-1})^{cc}=\mathscr{F}^{-1}$, and the field $h_c$ is contained in the function $\mathscr{F}$ only in the cutoff factor $\theta(\Lambda-|\omega+h_c|)$. At small $\omega$ the functions $G$ do not depend on $h_c$. However, as shown in the Appendix, allowance for the field $h_c$ multiplies the susceptibility of the RL model by the quantity $(1-2\delta^*/\pi)$.[2] The reason is that the diagrams in which the lines $G^{cc}$ form a closed contour diverage linearly at large $\omega$. When such diagrams are calculated, inclusion of the factor $\theta(\Lambda-|\omega+h_c|)$ in (25) is essential.[2] We shall illustrate this circumstance using as an example first-order perturbation theory:

$$\Sigma_1^{dd}(\omega)=-iU\int G^{cc}(\omega')\frac{d\omega'}{2\pi}, \tag{47}$$

where

$$G^{cc}(\omega)=\theta(\Lambda-|\omega+h_c|)\tilde{G}(\omega),$$

and $G$ does not depend on $h_c$:

$$\tilde{G}=-i\pi\frac{(\omega+h_d)\,\mathrm{sign}\,\omega}{\omega+h_d+i\Delta_0\,\mathrm{sign}\,\omega}. \tag{48}$$

Using the fact that $(d/d\omega-\partial/\partial h_d)\tilde{G}=0$ at $h_x=0$, we get

$$\frac{\partial\Sigma_1^{dd}}{\partial h_d}=-i\frac{U}{2\pi}(\tilde{G}(\Lambda)-\tilde{G}(-\Lambda)).$$

Next, differentiating $\Sigma_1^{dd}$ with respect to $h_c$, we have

$$\frac{\partial\Sigma_1^{dd}}{\partial h_c}=i\frac{U}{2\pi}(\tilde{G}(\Lambda)-\tilde{G}(-\Lambda))=U.$$

Thus, in contrast to zeroth-order perturbation theory, the contribution of the field $h_c$ to the susceptibility becomes essential even in first order. Allowance for this contribution leads to $(d/dh)\Sigma_1^{dd}=0$. Since $\Sigma_1^{dd}$ does not depend on $\omega$, we verify that relation (46) is satisfied in first order.

To obtain the proof in the general case we proceed as in the derivation of the Ward identity. We write $\Sigma^{dd}(\omega)$ in such a way that each line depends on the input frequency $\omega$. Differentiating all lines with respect to the frequency and the fields $h$, we obtain the identity

$$\left(\frac{d}{d\omega}-\frac{d}{dh}\right)\Sigma^{dd}(\omega)=\int\Gamma_{\alpha\beta}^{dd}(\omega,\omega')\hat{\delta}\mathscr{G}^{\alpha\beta}(\omega')\frac{d\omega'}{2\pi}. \tag{49}$$

The action of the operator $\hat{\delta}$ on the Green's functions $\mathscr{G}^{\alpha\beta}$ denotes differentiation $(d/d\omega-d/dh)$ of only the lines that join irreducible self-energy parts in $\mathcal{G}^{\alpha\beta}$. Thus, when the operator $\hat{\delta}$ is applied to the function

$$\mathcal{G}^{-1}=(G^{-1}-\Sigma)^{-1}$$

the self-energy part $\Sigma$ is not differentiated.

The following formulas are then valid:

$$\hat{\delta}\mathcal{G}^{cc}=\left(1+\frac{(V-\Sigma^{cd})^2}{\mathcal{F}^{-1}-\Sigma^{cc}}\mathcal{G}^{dd}\right)^2\hat{\delta}(\mathcal{F}^{-1}-\Sigma^{cc})^{-1}, \tag{50}$$

$$\hat{\delta}\mathcal{G}^{cd}=\left(1+\frac{(V-\Sigma^{cd})^2}{\mathcal{F}^{-1}-\Sigma^{cc}}\mathcal{G}^{dd}\right)\hat{\delta}(\mathcal{F}^{-1}-\Sigma^{cc})^{-1}, \tag{51}$$

$$\hat{\delta}\mathcal{G}^{dd}=(V-\Sigma^{cd})^2(\mathcal{G}^{dd})^2\hat{\delta}(\mathcal{F}^{-1}-\Sigma^{cc})^{-1}, \tag{52}$$

where

$$\hat{\delta}(\mathcal{F}^{-1}-\Sigma^{cc})^{-1}=(1-\mathcal{F}\Sigma^{cc})^2\left(\frac{d}{d\omega}-\frac{\partial}{\partial h_c}\right)\mathcal{F}.$$

We note next that

$$\left(\frac{d}{d\omega}-\frac{\partial}{\partial h_c}\right)\mathcal{F}=-2i\pi\delta(\omega).$$

Since

$$\left(1+\frac{(V-\Sigma^{cd})^2}{\mathcal{F}^{-1}-\Sigma^{cc}}\mathcal{G}^{dd}\right)\Big|_{\omega,h=0}=0,$$

we see that $\mathcal{G}^{dd}$ is the only function that yields a nonzero result when acted upon by the operator $\hat{\delta}$ at small $h$:

$$\hat{\delta}\mathcal{G}^{dd}|_{h=0}=\frac{2i}{\Delta}\delta(\omega). \tag{53}$$

The identity (49) thus reduces to

$$\left(\frac{d}{d\omega}-\frac{d}{dh}\right)\Sigma^{dd}(\omega)'\Big|_{h=0}=\frac{2i}{\Delta}\Gamma_{dd}^{dd}(\omega,0), \tag{54}$$

where $\Gamma_{dd}^{dd}(\omega,0)$ is an antisymmetrized vertex whose all four external lines are $G^{dd}$. If the entering frequency is zero, then by virtue of the antisymmetry we have

$$\Gamma_{dd}^{dd}(0,0)=0. \tag{55}$$

In other words, each diagram $\Sigma^{dd}$ corresponds to another diagram such that after the corresponding lines $G^{dd}$ are differentiated their contributions cancel out if the entering frequency is equal to zero. (An example of two such diagrams is shown in Fig. 1.) The cause of this circumstance is that the particles have no spin in the model under consideration.

We have thus proved (46). According to (38) and (45) this means that in the RL model we have $C/T\chi=\pi^2/3$. As shown in Sec. 2, this follows that the Wilson relation holds in the $s-d$ model.

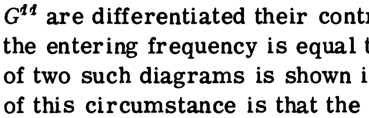

FIG. 1.

## 7. CONCLUSION

The use of the resonant-level model to study the low-temperature properties of a magnetic impurity in a metal has made it possible to construct a perturbation theory that is regular at low temperatures. In each order in $U$, the heat capacity is proportional to the temperature, the susceptibility is finite, and Wilson's relation (5) holds. The obtained behavior of the heat capacity and of the susceptibility agrees with Wilson's calculations at small $J>0$.

The resonant-level model obviates the need of the renormalization, proposed by Anderson, Yuval, and Hamann, at the point $J=J_T$. This procedure is not rigorous, since the Hamiltonian (1) is not reproduced upon renormalization. Therefore, when the scale $\tau=\tau_T$ at which $J$ becomes equal to $J_T$ is reached, the system is no longer described by the Hamiltonian (3). Neglecting the last circumstance, the Wilson relation can be obtained by the method proposed in Ref. 4. To this end it is necessary to know the ratio of the factors $g_i$ and $g_e$ at which the susceptibility is a universal quantity, i.e., a function of one argument:

$$\chi_{sd}=\frac{1}{T}f\left(\frac{T}{T_K}\right).$$

It is seen even from the series of the principal logarithmic terms of the expansion of the susceptibility in the interaction constant that the susceptibility can be universal only at $g_i=g_e$. Wilson has shown by numerical means that the susceptibility $\chi_{sd}(g,g)$ and the heat capacity $C$ are indeed universal. This means that at $T=0$ the ratio $C/T\chi_{sd}(g,g)$ does not depend on $J$. Using (21), we write this ratio in the form

$$\frac{C}{T\chi_{sd}(g,g)}=\frac{C}{T\left(1-\frac{2}{\pi}\delta(J)\right)^2\chi_{sd}(g,0;\tau,T)} \tag{56}$$

and subject it to renormalization. When the scale $\tau=\tau_T$ at which $(1-2\pi^{-1}\delta(J_T))^2=\frac{1}{2}$ is reached, the heat capacity $C$ and the susceptibility $\chi_{sd}(g,0)$ can be easily calculated: they coincide at this point with corresponding values of the RL model at $U=0$. Their ratio is therefore equal to $\pi^2T/3(g\mu)$.[2] Substituting this value in (56), we obtain Wilson's relation.

We note that the susceptibility $\chi_{sd}(g,0)$ is not a universal quantity and therefore its ratio to the heat capacity depends on $J$:

$$\frac{(g\mu)^2C}{T\chi_{sd}(g,0)}=\frac{2\pi^2}{3}\left(1-\frac{2}{\pi}\delta(J)\right)^2; \tag{57}$$

if $J$ is small, this ratio is close to $2\pi^2/3$. However, if we calculate it at $J=J_T$, the answer is half as much. This is apparently the cause of the erroneous opinion[6] that the theory of Anderson, Yuval, and Hamman yields $\pi^2/3$ for the ratio $(g\mu)^2C/T\chi_{sd}$.

Relation (5) was obtained phenomenologically by Nozieres,[14] who combined Wilson's qualitative results with Fermi-liquid considerations. In addition, Yamada[15] obtained this relation in a study of perturbation theory in Anderson's model in the limit of large Coulomb repulsion, which corresponds to $J\to 0$.

In our study of the thermodynamics of the $s-d$ model we did not consider the potential scattering of the electrons by the impurities. It can be shown that allowance for this interaction does not alter the result of (5). We note that there are grounds for assuming that the result remains in force also if the magnetic field differs from zero.

In conclusion, the authors thank A. I. Larkin and D. E. Khmel'nitskiĭ for useful discussions of the results.

## APPENDIX

We consider the perturbation-theory in $V$ for the partition function of the RL model:

$$Z_{RL}=2\sum_{n=0}^{\infty}V^{2n}\int_0^\beta d\tau_{2n}\ldots\int_0^{\tau_2}d\tau_1\langle 0|\exp[-H^-(\beta-\tau_{2n})]c^+d \times\exp[-H^+(\tau_{2n}-\tau_{2n-1})]\ldots d^+c\exp[-H^-\tau_1]|0\rangle, \quad (A.1)$$

where

$$H^\pm=\sum_k\varepsilon_k c_k^+c_k\pm\frac{U}{4}\sum_{k,k'}(c_k^+c_{k'}-c_{k'}c_k^+)\mp\frac{h_d}{2}-\frac{h_c}{2}\sum_k(c_k^+c_k-c_kc_k^+). \quad (A.2)$$

The operators $d^+$ and $d$ change $H^-$ to $H^+$ in succession and vice versa. The local-level potential acting on the fermions then changes instantaneously from $-U/2$ to $+U/2$. A similar situation arises in the $s-d$ model when the partition function is expanded in powers of $J_\perp$, where Anderson and Yuval[8] used a method used to determine the singularities in the absorption (or emission) spectrum of an x-ray photon in a metal.[16] Using this method, let us find the correlator that determines the second order of the expansion of $Z_{RL}$ in terms of $V$:

$$F_2(t,t')=\langle 0|e^{iH^-t}c^+de^{-iH^+(t-t')}d^+ce^{-iH^-t'}|0\rangle. \quad (A.3)$$

We note that Nozieres and De Dominicis[16] calculated analogous quantities for the case when the localized potential was switched on (or off) in the interval $(t,t')$. The function $F_2$ differs from these quantities in that here we consider the case of switching a localized potential.

Following Ref. 16, we represent $F_2$ in the form

$$F_2(t-t')=-iL(t'-t)\exp[C(t-t')+ih_d(t-t')]. \quad (A.4)$$

Here $e^c$ is the contribution from the closed loops, and

$$L(t'-t)=\lim_{\substack{x\to t'\\ x'\to t}}\varphi_\lambda(x,x';\ t,t'), \quad (A.5)$$

where $\varphi_\lambda(x,x';t,t')$ is the Green's function of a fermion located in a potential $\lambda U$ in the interval $(t',t)$, and in a potential $-U/2$ at all other instants of time. The function $\varphi_\lambda$ satisfies the Dyson equation

$$\varphi_\lambda(x,x';\ t,t')=G_{-1/2}(x-x')+U\left(\lambda+\frac{1}{2}\right)\int_{t'}^{t}G_{-1/2}(x-x'')\varphi_\lambda(x'',x;\ t,t')dx'', \quad (A.6)$$

where $G_{-1/2}$ is the Green's function of the fermions situated in the field of the static potential $-U/2$. Its Fourier transform is

$$G_{-1/2}(\omega)=\frac{\mathcal{F}(\omega)}{1+{}^1/_2U\mathcal{F}(\omega)}. \quad (A.7)$$

The solution of (A.6) yields

$$\varphi_\lambda(x,x';\ t,t')=G_\lambda(x-x')\left[\frac{(x'-t')(t-x)}{(x-t')(t-x')}\right]^{\alpha/\pi}, \quad (A.8)$$

where

$$\operatorname{tg}\alpha=\frac{\pi U(\lambda+{}^1/_2)}{1-{}^1/_2\lambda\pi^2U}.$$

We thus obtain at $\lambda=\frac{1}{2}$

$$L(t)=\cos^2\delta^\cdot\frac{1}{t}\left(\frac{t}{\tau}\right)^{4\delta^\cdot/\pi},\quad \operatorname{tg}\delta^\cdot=\frac{1}{2}\pi U. \quad (A.9)$$

The quantity $C$ can be obtained from the function $\varphi$:

$$\frac{\partial C(t-t')}{\partial\lambda}=-U\int_{t'}^{t}\lim_{x\to x'}\varphi_\lambda(x,x';,t,t')dx. \quad (A.10)$$

Taking (A.8) into account, we get

$$C(t)=-\int_{-1/2}^{1/2}\frac{2U\alpha(\lambda)d\lambda}{1+\pi^2U^2\lambda^2}\ln\frac{t}{\tau}-ih_ct\int_{-1/2}^{1/2}\frac{U\,d\lambda}{1+U^2\pi^2\lambda^2}. \quad (A.11)$$

As a result we get for the function $F_2$

$$F_2(t)=\frac{\cos^2\delta^\cdot}{i\tau}\left(\frac{t}{\tau}\right)^{-(1-2\pi^{-1}\delta^\cdot)^2}\exp\left(ih_dt-i\frac{2\delta^\cdot}{\pi}h_ct\right). \quad (A.12)$$

Just as in the derivation of formulas (10) and (11) for the $s-d$ model,[8,9] formula (A.12) is generalized in the next higher orders of perturbation theory in $V$ at $T\neq 0$ as follows:

$$F_{2n}(\tau_1\ldots\tau_{2n})=\tau^{-n}\exp\left\{\left(1-\frac{2}{\pi}\delta^\cdot\right)^2\sum_{\nu>\nu'}^{2n}\ln\frac{\sin T(\tau_\nu-\tau_{\nu'})}{\pi T\tau}(-1)^{\nu+\nu'} +\left(h_d-\frac{2}{\pi}\delta^\cdot h_c\right)\left(\sum_\nu^{2n}(-1)^\nu\tau_\nu-\beta/2\right)\right\}\cos^{2n}\delta^\cdot. \quad (A.13)$$

The partition function of the RL model is therefore

$$Z_{RL}=z\left(V\cos\delta^\cdot,\ \left(1-\frac{2}{\pi}\delta^\cdot\right),\ h_d-\frac{2}{\pi}\delta^\cdot h_c\right). \quad (A.14)$$


[1] I. Kondo, Prog. Theor. Phys. **32**, 37 (1964).
[2] A. A. Abrikosov, Physics (N. Y.) **2**, 21 (1965).
[3] H. Suhl, Phys. Rev. **138**, A515 (1965).
[4] P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B **1**, 4664 (1970).
[5] G. Toulouse, C. R. Acad. Sci. **268**, 1200 (1969).
[6] K. Wilson, Proc. Nobel Symp. XXIV, 1973, p. 68.
[7] K. Wilson, Rev. Mod. Phys. **47**, 773 (1975).
[8] P. W. Anderson and G. Yuval, Phys. Rev. Lett. **23**, 89 (1969).
[9] G. Yuval and P. W. Anderson, Phys. Rev. B **1**, 1522 (1970).
[10] K.-D. Schotte, Z. Phys. **230**, 99 (1970).
[11] I. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960).
[12] I. M. Luttinger, Phys. Rev. **119**, 1153 (1960).
[13] P. W. Anderson, Phys. Rev. **124**, 41 (1961).
[14] P. Nozieres, J. Low Temp. Phys. **17**, 31 (1974).
[15] K. Yamada, Prog. Theor. Phys. **53**, 970 (1975).
[16] P. Nozieres and C. T. De Dominicis, Phys. Rev. **178**, 1067 (1969).


Translated by J. G. Adashko