

Exact solution of the degenerate Anderson model

P. B. Vigman, E. I. Ogievetskii, and A. M. Tsvelik

L. D. Landau Institute of Theoretical Physics, Academy of Sciences of the USSR

(Submitted 3 May 1983)

Pis'ma Zh. Eksp. Teor. Fiz. **37**, No. 12, 580–583 (20 June 1983)

Analytic expressions are derived for the magnetic susceptibility and the valence of Ce and Yb impurities in a mixed-valence state at $T = 0$ from an exact solution of the Anderson model derived by the Bethe method.

PACS numbers: 75.10.Hk, 75.30.Cr, 75.20.Hr

1. The $(4f^{1/2}F_{5/2})$ and $(4f^0{}^1S_0)$ states of the Ce^{+3} ion in a metal are greatly hybridized. Mixed-valence states are customarily studied in the degenerate Anderson model¹ with

$$\mathcal{H} = \sum_{k,j} v_F (k - k_F) C_{kj}^+ C_{kj} + V \sum_{k,j} (C_{kj}^+ X_{0j} + \text{h. c.}) + \epsilon_f \sum_{j=1}^n X_{jj}. \quad (1)$$

Here ϵ_f is the energy level of a singly filled shell, which has a total angular momentum $J = 5/2$ for Ce or $J = 7/2$ for Yb; the operator C_{kj}^+ creates a conduction electron in a state with a total angular momentum J and angular-momentum projection j ; and the projection operator X_{0j} projects the shell from the $|J_j\rangle$ state onto the $|0\rangle$ state, in which the shell is not filled. The operators X_{ab} satisfy the algebra $X_{ab}X_{cd} = \delta_{bc}X_{ad}$.

The universal properties of Hamiltonian (1) are well known^{2,3}: All physical quantities depend on the renormalized energy level

$$\epsilon_f^* = \epsilon_f + (n-1) \frac{\Gamma}{\pi} \ln D^{(+)} / \Gamma,$$

where $D^{(+)}$ is the top of the conduction band, $\Gamma = \pi\rho(\epsilon_f)V^2$ is the width of the resonant level, and $n = 2J + 1$ is the degree of degeneracy of the level ϵ_f .

In this letter we report exact results for the magnetic susceptibility and the valence (i.e., the average number of electrons in the impurity shell):

$$\chi = \frac{\pi(n^2 - 1)}{12n\Gamma} \left\{ \frac{(en)^{\frac{n-1}{n}}}{n\Gamma(1 + \frac{1}{n})} e^{\pi \epsilon_f^*/n\Gamma} + \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{1-i\omega} \Gamma(1+i\omega) \right.$$

$$\times \left. \left(\frac{-i\omega+0}{e} \right)^{-i\omega(n-1)/n} \frac{1}{\Gamma(1+i\omega/n)} \exp \left[-i\omega \left(\frac{\pi \epsilon_f^*}{n\Gamma} - \frac{\ln n}{n} \right) - \frac{\pi|\omega|}{n} \right] \right\}, \quad (2)$$

$$n_f = 1 - \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega+i0} \frac{\Gamma(1+i\omega)}{\Gamma(1 + \frac{i\omega}{n})} e^{-\pi|\omega|/n} \left(\frac{-i\omega+0}{e} \right)^{-i\omega \frac{(n-1)}{n}}$$

$$\times \exp \left[-i\omega \left(\epsilon_f^* \pi / n\Gamma - \frac{1}{n} \ln n \right) \right]. \quad (3)$$

These expressions describe a smooth transition from a state with a localized angular momentum ($n_f = 1$) to a state with a mixed valence ($|\epsilon_f^*| \sim \Gamma$) and can be used for a quantitative description of the experimental results of Ref. 4.

2. Hamiltonian (1) is completely integrable. Using the Bethe method, which is described with reference to the Anderson model in Ref. 5, we can easily derive the spectrum of Hamiltonian (1) (Ref. 6). States which transform in accordance with an irreducible representation of the $SU(n)$ group, $S \equiv [N - m^{(1)}, m^{(1)}, -m^{(2)}, \dots, m^{(n-1)}]$ are characterized by momenta $\{k_j, \lambda_{\alpha_1}^{(1)}, \dots, \lambda_{\alpha_{n-1}}^{(n-1)}\}$, which are quantized in accordance with

$$\exp(i k_j L) \frac{(k_j - \epsilon_f - i\Gamma)}{k_j - \epsilon_f + i\Gamma} = \prod_{\alpha=1}^{m^{(1)}} \frac{\frac{k_j}{2\Gamma} - \lambda_{\alpha}^{(1)} - \frac{i}{2}}{\frac{k_j}{2\Gamma} - \lambda_{\alpha}^{(1)} + \frac{i}{2}}. \quad (4)$$

$$\prod_{\tau=\pm 1} \prod_{\beta=1}^{m^{(j+\tau)}} \left(\frac{\lambda_{\alpha}^{(j)} - \lambda_{\beta}^{(j+\tau)} + i/2}{\lambda_{\alpha}^{(j)} - \lambda_{\beta}^{(j+\tau)} - i/2} \right) = \prod_{\beta=1}^{m^{(j)}} \left(\frac{\lambda_{\alpha}^{(j)} - \lambda_{\beta}^{(j)} + i}{\lambda_{\alpha}^{(j)} - \lambda_{\beta}^{(j)} - i} \right). \quad (5)$$

The energy of the state is $E = \sum_i^N k_j; \lambda_j^{(0)} = k_j/2\Gamma; m^{(0)} = N$ is the number of electrons in the band with angular momentum J ; and $m^{(j)} = \sum_{j+1}^n n_k$, where n_k is the partial number of electrons with projection k .

3. In the ground state in the S representation the momenta k_j and $\lambda_{\alpha}^{(j)}$ form bound states or "complexes":

$$\lambda_{(p-1)r_j+p-2}^{(j)} + p r_j + p - 1 - q = \lambda_{r_j+p-1}^{(j+1)} + i \left(\frac{p+1}{2} - q \right); \quad q = 1, \dots, p,$$

$$m_{k-1} = r_k + 2r_{k+1} + \dots + (n+1-k)r_n.$$

In the thermodynamic limit the centers of the complexes $\lambda_{\alpha}^{(j)}$ are described by the

distribution $\rho_j(\lambda)$. We denote by $\tilde{\rho}_j(\lambda)$ the hole distribution (see Ref. 7 for a rigorous definition). After some laborious but straightforward algebraic manipulations we find the equations

$$\frac{\Gamma_j}{\pi} + \frac{1}{L} a_j \left(\lambda - \frac{\epsilon_f}{2\Gamma} \right) = \tilde{\rho}_j(\lambda) + \int_{-\infty}^{B_k} \mathcal{F}_{jk}(\lambda - \lambda') \rho_k(\lambda') d\lambda', \quad (6)$$

$$j = 1, \dots, n$$

where

$$\mathcal{F}_{jk}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega \epsilon^{-i\omega\lambda - \frac{k\omega}{2}(\max(j, k) - 1)} \frac{\text{sh}(\min(j, k) \frac{\omega}{2})}{\text{sh} \omega/2}, \quad (7)$$

$$a_j(\lambda) = \frac{2}{\pi} \frac{j}{(4\lambda^2 + j^2)}.$$

The parameters B_j are determined from the conditions

$$r_j/L = \int_{-\infty}^{B_j} \rho_j(\lambda) d\lambda. \quad (8)$$

4. The function $\rho_j(\lambda)$ are exponentially small in the limit $\lambda \rightarrow -\infty$ ($j \neq n$). In contrast, we have $\sigma(\lambda) \equiv \rho_n(\lambda) \rightarrow \text{const}$ in the limit $\lambda \rightarrow -\infty$, and the integrals in (6) and (8) diverge. The reason is that the lower bound on the conduction band has been ignored in Eqs. (4)–(6). It should be noted that $D^{(-)}/2\Gamma < \lambda^{(n)} < D^{(+)}/2\Gamma$, where $D^{(\pm)}$ are the band boundaries, and the state density of conduction electrons should be assumed to be zero outside the interval $(D^{(-)}, D^{(+)})$. Integrating Eq. (6) with $j = n$, we then find a condition on the limit $Q \equiv B_n$:

$$\int_Q^{\infty} \tilde{\sigma}(\lambda) d\lambda = n D^{(+)} / 2\pi.$$

The region $1 \ll |\lambda| \ll D^{(-)}/2\Gamma$ contributes to this integral. It follows from (6) that at $|\lambda| \gg 1$ we have

$$\tilde{\sigma}(\lambda) = \frac{\Gamma n}{\pi} \left(1 - \frac{n-1}{2\pi} \frac{1}{|\lambda|} + \dots \right).$$

We then find

$$Q = -\frac{n-1}{2\pi} \ln \frac{D^{(+)}}{2\Gamma} + O(1).$$

Shifting the arguments of the functions $\rho_j(\lambda)$ by Q , we find universal equations which depend exclusively on the renormalized level ϵ_f^* .

5. **Valence.** In the absence of a magnetic field ($H = 0$) the limits are $B_k = -\infty$ ($k = 1, \dots, n-1$), and system (6) can be solved explicitly by the Wiener-Hopf method. The solution leads to Eq. (3). It is a simple matter to derive the asymptotic behavior of the valence at $|\epsilon_f^*| \gg \Gamma$:

$$n_f = 1 + \sum_{k=1}^{\infty} a_k Z^k \quad (\epsilon_f^* < 0), \quad n_f = \sum_{k=1}^{\infty} b_k Z^k \quad (\epsilon_f^* > 0), \quad (9)$$

where

$$Z = \frac{\Gamma}{\pi \epsilon_f^{**}}, \quad a \quad \epsilon_f^{**} = \epsilon_f^* - \Gamma \frac{(n-1)}{\pi} \ln \frac{|\epsilon_f^{**}|}{2\Gamma n^{n/n-1}}.$$

The first coefficients, $a_1 = 1$ and $b_1 = n$, have been calculated previously by perturbation theory.^{2,3,8,9} The reason for the asymmetry of a_1 and b_1 is the difference between the degrees of degeneracy of the impurity ground state at $\epsilon_f^* < 0$ and at $\epsilon_f^* > 0$.

6. Magnetic susceptibility in a zero field. To calculate the magnetic susceptibility it is sufficient to consider only those terms in the expansion of the functions ρ_j which are the leading terms with regard to $\exp(2\pi[B_k + \lambda])$. The calculations, which we omit, lead to Eq. (2). At $-\epsilon_f^* \gg \Gamma$ the impurity is magnetic ($n_f = 1$), and there is a Kondo effect:

$$\chi = \frac{n(n^2 - 1)}{12\pi T_k},$$

where

$$T_K = \frac{\Gamma}{\pi^2} \left(\Gamma (1/n) / (en)^{\frac{n-1}{n}} \right) \exp\left(\frac{\pi \epsilon_f^*}{n\Gamma}\right) \quad (10)$$

is the Kondo temperature.

The quantity $\Gamma_\chi = \sum_{p=2}^{\infty} C_p Z^p$ [$C_2 = n(n^2 - 1)/12\pi$] has been calculated by perturbation theory in the nonmagnetic case.^{9,10}

7. The limit $n \rightarrow \infty$. The nature of the transition from a state with a localized angular momentum to a mixed-valence situation changes with increasing n . As $n \rightarrow \infty$, with $\epsilon_f^*/n\Gamma = \text{const} < 0$, the terms in the perturbation-theory series (9) vanish; i.e., the state of an ion with $n_f = 1$ is stable in any order of perturbation theory. There are processes of a nonperturbative nature, however, which disrupt this state even in the limit $n \rightarrow \infty$. From (3) we have

$$n_f^\infty = 1 - \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{d\omega}{\omega + i0} \Gamma(1 + i\omega) \left(\frac{-i\omega + 0}{e} \right)^{-i\omega} e^{-i\omega \frac{\pi \epsilon_f^*}{n\Gamma}}. \quad (11)$$

If $\epsilon_f^* < 0$, the integral in (11) can be decomposed in $\exp(\pi \epsilon_f^*/12\Gamma)$, and the transition to the mixed-valence state should be sharper than the transition from the mixed-valence region to the nonmagnetic state ($n_f = 0$). At $\epsilon_f^* > 0$ we have

$$n_f^\infty = \frac{1}{\pi} \int_0^{\infty} \frac{dt}{t} \Gamma(1 + t) (t/e)^{-t} \sin \pi t e^{-t \epsilon_f^* \pi/n\Gamma}. \quad (12)$$

There is the erroneous opinion in the literature that the $1/n$ expansion simplifies the analysis of a mixed-valence state and that this expansion can be constructed by

summing the latter diagrams of perturbation theory. Actually, the $n \rightarrow \infty$ limit is determined by the sum of all planar diagrams, and it does not seem possible to treat this limit without an exact solution.

¹B. Coqblin and J. R. Schrieffer, *Phys. Rev.* **185**, 847 (1969).

²A. F. Barabanov, K. A. Kikoin, and L. A. Maksimov, *Teor. Mat. Fiz.* **20**, 364 (1974).

³F. D. M. Haldane, *Phys. Rev. Lett.* **40**, 416 (1978); *J. Phys. C* **11**, 5015 (1978).

⁴H. Barth, M. Luszik-Bhadra, and D. Riegel, *Phys. Rev. Lett.* **50**, 608 (1982).

⁵P. B. Wiegmann, *Phys. Lett.* **80A**, 163 (1980).

⁶P. A. Scholtzmann, *Z. Phys.* **49**, 109 (1982).

⁷C. N. Yang and C. P. Yang, *J. Math. Phys.* **10**, 1115 (1969).

⁸A. Bringer and H. Lustfield, *Z. Phys.* **B28**, 213 (1977).

⁹A. M. Tselik and A. F. Barabanov, *Zh. Eksp. Teor. Fiz.* **75**, 153 (1978) [*Sov. Phys. JETP* **48**, 337 (1978)].

Translated by Dave Parsons

Edited by S. J. Amoretty