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FORMATION OF HEAVY-FERMION STATES IN NON-FERMI-LIQUID IMPURITY SYSTEMS

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A mechanism for the occurrence of heavy-fermion states in non-Fermi-liquid (NFL) metals with f-shell impurities is proposed. The impurity with an unstable valency is suggested to have the energy spectrum consisting of a deep f-level and quasicontinuum states (narrow band) in resonance with the Fermi energy. Depending on the impurity concentration, the single-site NFL states are generated by the two-channel Kondo scattering for the low concentration (the «Kondo regime») or by the screening interaction for a relatively high concentration (the «X-ray edge regime»). It is shown that the NFL states are unstable against the scattering of the NFL excitations by electron states of the narrow band. This scattering generates additional narrow Fermi-liquid (FL) resonances at/near the Fermi level in the «Kondo regime» and in the «X-ray edge regime». The mixed-valence states are shown to be induced by new FL resonances. The mixed valency mechanism is local and is related to the instability of single-site NFL states. The FL resonances lead to the existence of additional energy scales and of pseudogaps near the Fermi level in the mixed-valence states. They also considerably narrow the region with a nearly integer valency.

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1. INTRODUCTION

At present, intermetallic compounds with the f-shell atoms Ce or U are an important class of alloys in which the NFL behavior is observed (see [1, 2] for a review). The anomalous temperature dependences of their linear specific heat, magnetic susceptibility, and resistivity strongly support the NFL scenario. The Ce and U ions carry magnetic dipole or electric quadrupole moments that interact with the spins and charges of the conduction electrons, thereby giving rise to the Kondo effect and the NFL behavior at low temperatures. The f-electron compounds of interest have been alloyed with nonmagnetic elements (with a few possible exceptions) [2, 3]. The thermodynamic measurements evidence in favor of the quadrupole two-channel Kondo model introduced in [4]. We note that according to photoemission spectra, the U-based compounds look much more like the mixed-valence ones (see references in [5, 6]). Recently [7], it was shown that the temperature behavior of the specific heat and magnetic susceptibility is governed by nonuniversal power-law dependences for a relatively high concentration of the f-shell atoms.

Taking the foregoing into account, it would be highly desirable to have the unified treatment involving the explanation of two essential facts:

(1) the coexistence of the single-ion two-channel Kondo effect and the mixed-valence state;

(2) the possibility of non-universal power-law energy dependences on the parameters.

It should be noted that the role of instabilities of the NFL states in forming the heavy-fermion (HF) states has not been completely clarified. At the same time, it is well known that the single-ion NFL state is unstable against any perturbation that eliminates the orbital or spin degeneracy of the impurity. Two instability mechanisms are presently known in the two-channel quadrupole and orbital Kondo model. In [4], the instability is induced by the Jahn–Teller distortions of the impurity site. The second mechanism [8] attributes the instability to the channel anisotropy. As shown in [9] and [10], there occurs a new physical realization of the two-channel quadrupole Kondo model and of the NFL

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state instability against the scattering generated by the tunnel process in the doped size-quantized structures. The physical reason of the instability is the existence of the additional narrow FL resonances induced by tunneling.

For a metal containing orbitally degenerated deep impurity states, it was shown in [11] that the NFL state can be unstable against the scattering of the multiparticle excitations having different z projections of the quadrupole moment.

In this paper, we propose a new mechanism for the occurrence of HF states in NFL metals with the f-shell impurities. We assume that a specific feature of atoms with an unstable valency is the energy spectrum that contains two unfilled shells: the orbitally degenerate deep f-level states and the atomic quasicontinuum states (narrow band) near the Fermi level. As shown below, the scattering of the NFL excitations by atomic quasicontinuum states, which is potential in its character, generates additional FL resonances near the Fermi level. Along with the NFL excitations, new FL resonances form an additional branch of heavy-fermion states with the characteristic energy that is much smaller than the width of the NFL resonance (even in the case of the Kondo effect). New FL resonances generate the mixed-valence state. The heavy-fermion states have a local origin within the treatment proposed below.

In conclusion, we briefly discuss the temperature transitions within the proposed framework and the role of single-site NFL fluctuations in the «concentrated» heavy-fermion systems.

2. THE IMPURITY MODEL AND THE SCATTERING PROBLEM FOR AN INTERACTING SYSTEM

2.1. It is commonly known that an ion with unfilled d- or f-shells partially retains its atomic properties in a crystal. This is possible due to the presence of a centrifugal barrier separating the region A in which the atomic forces act from the region B where the lattice potential acts. The height of the barrier is comparable to other characteristic energies of the system, i.e., the Fermi energy and the interatomic interaction energy. The typical energy spectrum of lanthanide and actinide ions with an unstable valency seems to contain quasilocal deep f-levels together with the quasicontinuum states under the centrifugal barrier. The atomic quasicontinuum may be formed by the d-shell states being in resonance with the conduction band states at the

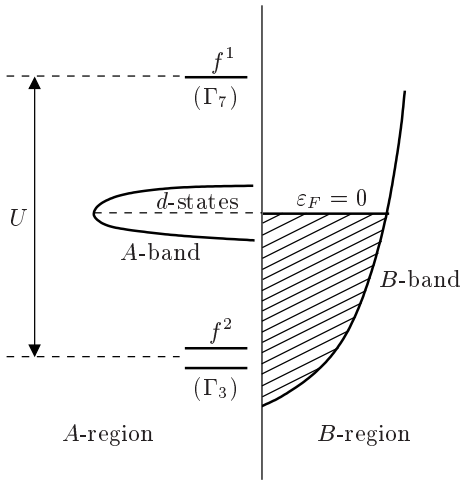

Fig. 1. The initial electron spectrum. A and B are the impurity region and the conduction band, respectively, U is the Hubbard repulsion. The A-band consists of the impurity states in resonance with the Fermi level

Fermi level. A similar impurity model with a highly degenerate f-level was also considered in [12]. The initial electron spectrum before mixing is depicted in Fig. 1.

The Hamiltonian of the system is given by

$$H = H_A + H_B + H_{AB}, \tag{2.1}$$

where H_B and H_A are the Hamiltonians of the conduction band and of the impurity region. The Hamiltonian H_{AB} describes the hybridization H_h and the scattering H_{sc} between electron states of the conduction band and the impurity region. The Hamiltonian of the impurity region is given by

$$H_A = H_0^f + H_0^d + H_U^f,$$

where H_0^f is the Hamiltonian of the deep level, H_U^f is the Hubbard repulsion, and H_0^d is the Hamiltonian of the narrow A-band. In what follows, we do not consider the intraband interactions assuming that they are weak compared to the interaction between the deep level and the band electrons. Therefore, H_0^d is the Hamiltonian of the noninteracting d-electrons. It is also assumed that the d- and f-shells are not mixed in the impurity region. We start from the low-lying electron configuration of the isolated ion and then take the mixing with the conduction electrons into account in the spirit of the Anderson model with two unfilled shells.

We consider the situation where the deep level is a Γ_3 quadrupole (non-Kramers) doublet of the crystal field interacting with the Γ_8 quartet of the conduc-

tion electrons. However, we emphasize that the mechanism proposed here can be applied for all compounds in which the symmetry allows the local quartet of conduction states to couple to the two-fold degenerate level and an additional potential scattering of the multiparticle excitations exists.

For U-based compounds, the Γ_3 doublet in the $5f^2$ configuration is formed as a result of splitting the multiplet with the total moment $J = 4$ with the cubic crystal field. The Γ_3 doublet has an electric quadrupole moment and no magnetic dipole moment. The quantum numbers of the Γ_3-level electron are the numbers of lines μ for the irreducible representation of the point group $\mu_{\Gamma_3} = \pm 1$. The two quantum number values $\mu = \pm 1$ correspond to the projections of the quadrupole moment on the z-axis, i.e., $Q_{zz} = \pm 8$.

The multiparticle configuration of the unfilled shell is denoted by $|n;\mu\rangle$, where n indicates the number of electrons and μ is the set of quantum numbers characterizing the configuration.

For relatively large values of the Hubbard repulsion in the absence of hybridization, the ground state configuration of the ion U^{4+} is the singly occupied Γ_3 doublet with the electron configurations $|1;+1\rangle$ and $|1;-1\rangle$ and the energy E_f. The electron creation operators and electron numbers correspond to the singly occupied states:

$$
\begin{aligned}
&f^+_{\mu=+1} = |1;+1\rangle\langle 0;0|; \quad f^+_{\mu=-1} = |1;-1\rangle\langle 0;0|;\\
&n_{f\mu} = f^+_\mu f_\mu; \quad \sum_\mu n_{f\mu} = 1;\\
&H^f_0 = \sum_{n,\mu} E_{n,\mu}|n;\mu\rangle\langle n,\mu| \equiv \sum_\mu E_{f\mu} f^+_\mu f_\mu,\\
&H^f_U = \sum_{\mu\mu'} U_{\mu\mu'} n_{f\mu} n_{f\mu'}(1-\delta_{\mu\mu'}).
\end{aligned}
\tag{2.2}
$$

The Γ_3 states are hybridized with the partial conduction band waves having the total angular momentum $j = 5/2$. Taking the splitting of the $j = 5/2$ multiplet by the cubic crystal field into account amounts to the transition from the angular momentum representation to the irreducible representations of the point group of the crystal. The latter representation has the quartet Γ_8 that can be hybridized with the Γ_3 doublet. The Γ_8 quartet possesses two groups of the states: $\Gamma_8^{(+)}$, $\Gamma_8^{(-)}$ with $\Gamma_8^{(+)} = |\Gamma_8;2\rangle$, $|\Gamma_8;1\rangle$ and $\Gamma_8^{(-)} = |\Gamma_8;-2\rangle$, $|\Gamma_8;-1\rangle$. The groups $\Gamma_8^{(+)}$ and $\Gamma_8^{(-)}$ correspond to different signs of j_z. Different signs of j_z correspond to different sings of the spin projection σ_z. In addition, the states $|\Gamma_8;\pm 2\rangle$ and $|\Gamma_8;\pm 1\rangle$ have the respective z components of the quadrupole moment $Q_{zz} = \pm 8$.

In other words, the quartet Γ_8 of partial waves decomposes into the tensor product $\Gamma_3 \otimes \Gamma_7$. It is therefore described by a combination of the «orbital» (Γ_3) and the «spin» (magnetic) (Γ_7) indices.

The partial states of the conduction electrons mixed with the Γ_3 doublet can therefore be classified by the quantum numbers $|\varepsilon;\gamma,\alpha\rangle$, where $\varepsilon = v_F k - \varepsilon_F$, with k being the wave vector modulus and ε_F being the Fermi energy. In what follows, we choose the position of the Fermi level as zero. The quantum number $\gamma = 2, 1 \equiv \mu$ corresponds to the two values of the quadrupole moment within the groups $\Gamma_8^{(+)}$ and $\Gamma_8^{(-)}$; the magnetic quantum numbers $\alpha = \pm$ distinguish the respective groups $\Gamma_8^{(+)}$ and $\Gamma_8^{(-)}$. The operators $a^+_{B\mu\alpha}(\varepsilon)$ describe the states $|\varepsilon;\mu,\alpha\rangle$ in the B-band.

In terms of these states, the hybridization Hamiltonian

$$
H_h = \sum_{\mathbf{k}\sigma n} \sum_{\mu_{n+1}\mu_n} \left(V^f_{\mu_{n+1}\mu_n\sigma}(\mathbf{k}) a^+_{B\sigma}(\mathbf{k}) |n+1;\mu_{n+1}\rangle\langle n;\mu_n| + \text{H.c.} \right),
$$

where $a^+_{B\sigma}(\mathbf{k})$ creates the conduction band electron with the spin σ and the wave vector $\mathbf{k}$, can be written as

$$
H_h = \sum_{\mu\alpha} \int_{-\infty}^{+\infty} d\varepsilon \rho_{0B}(\varepsilon) \left(V^f_{\mu\alpha}(\varepsilon) a^+_{B\mu\alpha}(\varepsilon) f_\mu + \text{H.c.} \right). \tag{2.3}
$$

Here, $\rho_{0B}(\varepsilon)$ is the density of states (DOS) in the B-continuum, the terms with $V^f_{\mu\mu'\alpha}(\varepsilon)$, $\mu \neq \mu'$, are neglected because of the cubic symmetry, and the matrix elements $V^f_{\mu\mu\alpha}(\varepsilon)$ are denoted by $V^f_{\mu\alpha}(\varepsilon)$.

In finding the interaction Hamiltonian in what follows, it is significant that because of the band state symmetry, the hybridization matrix elements $V^f_{\mu\alpha}(\varepsilon)$ are nonzero for both components of the Γ_3 doublet with $\mu = \pm 1$. This means that the matrix elements

$V^f_{\mu_{n+1}\mu_n\sigma}(\mathbf{k})$ are spatially nonlocal. We additionally assume the hybridization matrix elements to be independent of the sign of the z component j_z of the total momentum j, i.e., $V^f_{\mu\alpha} \equiv V^f_\mu$.

The Hamiltonian H_{AB} in Eq. (2.1) also involves the scattering between electron states of the A- and B-bands. In terms of the partial states, the scattering Hamiltonian is given by

$$H_{sc} = \sum_{\mu\alpha} \int_{-\infty}^{+\infty} d\varepsilon \rho_{0A}(\varepsilon) \times \\ \times \int_{-\infty}^{+\infty} d\varepsilon' \rho_{0B}(\varepsilon') T^{AB}_{\mu\mu}(\varepsilon,\varepsilon') a^+_{A\alpha\mu}(\varepsilon) a_{B\alpha\mu}(\varepsilon'), \quad (2.4)$$

where the operators $a_{A\mu\alpha}(\varepsilon)$ describe the states in the atomic continuum (A). The scattering with $\mu \neq \mu'$ is absent because of the cubic symmetry. We assume that the scattering matrix elements as well as the hybridization ones are independent of the quantum number α.

In defining the NFL states, it is important to account for the splitting of the f doublet ground state due to a local deviation from the cubic symmetry at the impurity site. In the Hamiltonian, the splitting is described by the term

$$H_\Delta = \Delta \hat{\tau}^z_f. \quad (2.5)$$

Because the Hubbard repulsion U is the largest parameter in the problem, it is convenient first to take the effective interaction induced by U into account and then to use the multi-particle states as a basis for solving the scattering problem. As shown below, the system described by the Hamiltonian H in (2.1) has two physical mechanisms generating singularities at/near the Fermi level. The Hubbard repulsion U generates the effective interaction between conduction electrons and the deep level. This interaction induces an NFL resonance at the Fermi level in the B-band. The scattering of the multiparticle excitations in the conduction band by the electron states of the A-band generated by H_{sc} results in the formation of additional Fermi-liquid (FL) resonances near the Fermi level.

2.2. In the system with the Hamiltonian H, the excitations are completely described by the Green's function

$$\hat{G}_{f\mu}(z) = \langle f_\mu | (z - \hat{H})^{-1} | f_\mu \rangle.$$

Because the energy U is dominant, it is essential to properly treat correlations on the site. To calculate $\hat{G}_{f\mu}(z)$, we use the method of the equations of motion [19] that correctly accounts for these on-site correlations. This gives

$$\hat{G}_{f\mu}(z) = \hat{G}^0_{f\mu}(z) \frac{1 - \Sigma_{A\mu}(z)\Sigma_{B\mu}(z)}{\hat{D}^{AB}_\mu(z)}, \quad (2.6)$$

where

$$\hat{G}^0_{f\mu}(z) = \left[z - \varepsilon_f - \hat{\Sigma}^h_{B\mu}(z) \right]^{-1}$$

is the Green's function of the interacting system without scattering; we then have

$$\hat{D}^{AB}_\mu(z) = 1 - \Sigma^{sc}_{A\mu}(z) \hat{W}_{B\mu}(z),$$

$$\hat{W}_{B\mu}(z) = \Sigma^{sc}_{B\mu}(z) + \Sigma^{sc}_{B\mu}(z)\Sigma^{sc}_{\mu B}(z)\hat{G}^0_{f\mu}(z).$$

Equation (2.6) implies that the full Green's function $\hat{G}_{f\mu}(z)$ has features of two types. The function $\hat{G}^0_{fr\mu}(z)$ describes the contributions of the multiparticle resonances at the Fermi level due to the interaction between the conduction electrons and the deep level. The second factor in Eq. (2.6) is generated by the scattering of the multiparticle excitations via the atomic quasicontinuum states. The scattering results in additional singularities, namely, simple poles near the Fermi level. The pole positions are determined by the equation $\hat{D}^{AB}_\mu(z) = 0$. The self-energy functions $\Sigma^h_{B\mu}(z)$ and $\Sigma^{sc}_{\nu\mu}(z)$ with $\nu = A, B$ are expressed as spectral expansions of multiparticle Green's functions of the A- and B-bands,

$$\Sigma^{sc}_{\nu\mu}(z) = |T^\nu_\mu(0)|^2 \sum_p \frac{1}{z - \varepsilon_\nu(p)} = \\ = |T^\nu_\mu(0)|^2 \int d\varepsilon \frac{\rho_\nu(\varepsilon) f(\varepsilon)}{z - \varepsilon}, \\ \Sigma^h_{B\mu}(z) = |V^f_\mu(0)|^2 \int d\varepsilon \frac{\rho_B(\varepsilon) f(\varepsilon)}{z - \varepsilon}, \quad (2.7)$$

where $\varepsilon_\nu(p)$ is the excitation spectrum at the Fermi level, $\rho_\nu(\varepsilon)$ is the DOS corresponding to this spectrum, and $f(\varepsilon)$ is the Fermi function. In Eqs. (2.7), it is assumed that $V^f_\mu(\varepsilon) \approx V^f_\mu(0)$ and the scattering matrix elements are separable:

$$T^{AB}_{\mu\mu}(\varepsilon,\varepsilon') \approx T_{AB}(0,0) = T^A_\mu(0) T^B_\mu(0),$$

where $T^A_\mu(0)$ is dimensionless.

Without the interaction, we have $\rho_\nu(\varepsilon) = \rho_{0\nu}$ and $\hat{G}^0_{f\mu}(z) = [z - \bar{\varepsilon}_{f\mu} - i\gamma_{f\mu}]^{-1}$, where $\bar{\varepsilon}_{f\mu}$ is the energy of the deep level renormalized by the hybridization and $\gamma_{f\mu}$ is the width of this level. In this case, both $\hat{G}^0_{f\mu}(z)$ and $\Sigma^0_{\nu\mu}(z)$ have no singularities near the Fermi level.

In the interacting system as $U \to \infty$, we are interested in the case where the dominant effect of the interaction is the generation of a multiparticle resonance

(the f_r-level) near the Fermi level. The Green's function $\hat{G}^0_{f_r\mu}(z)$ of this resonance must then be inserted in Eq. (2.6). The multiparticle peaks in $\hat{G}^0_{f_r\mu}(z)$ at the Fermi level determine the properties of the DOS $\rho_B(\varepsilon)$ and of the self-energy functions $\Sigma^{sc,h}_{B\mu}(z)$.

To obtain the density of states at the Fermi level in the interacting system, the following consideration can be used. It is known [19] that the exact Green's function of the conduction electrons in the impurity Anderson model is given by (in our notation)

$$G_{\mu\alpha}(k,k';z) = \delta_{\mu\mu'}\delta_{\alpha\alpha'}\delta(k-k')G_{0\mu\alpha}(k,k';z) + \\ + G_{0\mu\alpha}(k;z)V^{f*}_{\mu\alpha}(k)G^{(0)}_{f\mu\mu}(z)V^{f}_{\mu\alpha}(k')G_{0\mu\alpha}(k;z), \quad (2.8)$$

where $G_{0\mu\alpha}(k;z)$ is the Green's function of noninteracting electrons (in accordance with the definition given above, the variables k and ε are identical). Because of the symmetry properties, the function $G^{(0)}_{f\mu\mu}(z)$ can have only diagonal components. The Green's function of an impurity state $G^{(0)}_{f\mu\mu}(z)$ involves all the interactions induced by the Hubbard repulsion U. Near the Fermi level, the multiparticle resonance Green's function $\hat{G}^0_{f_r\mu}(z)$ must be inserted in Eq. (2.8). Thus, the DOS of multiparticle excitations at the Fermi level takes the form

$$\rho_B(\varepsilon) - \rho_{0B}(\varepsilon) = -\frac{1}{\pi}A_\rho \operatorname{Im}\operatorname{Sp}\hat{G}^0_{f_r\mu}(\varepsilon), \quad \varepsilon > 0,$$

where $A_\rho \propto \gamma_B\rho_{0B}$, $\gamma_B \equiv \sum_\mu \gamma_{B\mu}$ and $\gamma_{B\mu} \equiv \equiv |V^f_\mu|^2\rho_{0B}$.

With the foregoing taken into account, the complete solution of the scattering problem requires determining the main interaction and calculating the Green's function $\hat{G}^0_{f_r\mu}(z)$.

3. THE INTERACTION HAMILTONIAN AND THE NON-FERMI-LIQUID STATE

3.1. To derive the effective interaction between the deep f-doublet and the conduction electrons, we suppose that for relatively large values of the Hubbard repulsion, the ground state configuration of the ion U^{4+} is the singly occupied Γ_3 doublet with the electron configurations $|1;+1\rangle$, $|1;-1\rangle$ and the energy E_f. Taking virtual transitions into the excited states with the energies $E_2 = 2E_f + U$ into account and using either the projection operator techniques or the Schriffer–Wolff transformation for the Hamiltonian $H^f_U + H^f_0 + H_h$, we obtain the standard expression

$$H_{int} = \sum_{\mu\mu'\alpha\alpha'} \iint d\varepsilon d\varepsilon' \rho_{0B}(\varepsilon)\rho_{0B}(\varepsilon') \times \\ \times V_{\mu\mu'}(\varepsilon,\varepsilon')a^+_{B\alpha\mu}(\varepsilon)a_{B\alpha'\mu'}(\varepsilon')f^+_\mu f_{\mu'}. \quad (3.1)$$

As $U_{\mu\mu'} \to \infty$, the matrix elements in Eq. (3.1) become

$$V_{\mu\mu'}(\varepsilon,\varepsilon') \sim \frac{V^{f*}_\mu(\varepsilon)V^f_{\mu'}(\varepsilon')}{\varepsilon_f}, \quad \varepsilon_F - E_f \equiv \varepsilon_f.$$

The doubly degenerate f-level containing one electron can be conveniently described in terms of the pseudospin variable $\hat{\tau}_f$. The projections of the pseudospin operator $\hat{\tau}_f$ on the coordinate axes coincide with the components of the quadrupole moment tensor. The projection $\hat{\tau}^z_f \sim Q_{zz}$ on the z axis has two values corresponding to the occupation of the different orbitals of the doublet. The operator $\hat{\tau}^x_f \propto J^2_x - J^2_y$ inverts the pseudospin, and we can therefore write

$$\hat{\tau}^i_f = \sum_{\mu\mu'=\pm1} f^+_\mu \sigma^i_{\mu\mu'} f_{\mu'},$$

where σ^i are the Pauli matrices.

The index $\alpha = \pm$ is magnetic, and therefore, it cannot change under the scattering by the electric quadrupole moment of the impurity nonmagnetic Γ_3 doublet described by (2.4). In other words, for Hamiltonian (2.4) to possess the time reversal property, the quantum number α must be conserved during the scattering. The scattering processes change only the states belonging to the same group ($\Gamma^{(+)}_8$ or $\Gamma^{(-)}_8$) and these states form a representation for the pseudospin $\hat{\tau}_f = 1/2$.

The time reversal symmetry therefore guarantees the transfer from Hamiltonian (2.4) to the two-channel quadrupole exchange Hamiltonian with the channel index α,

$$H_{int} = \sum_{\mu\mu'\alpha}\sum_{i=x,y,z} \iint d\varepsilon d\varepsilon' \rho_{0B}(\varepsilon)\rho_{0B}(\varepsilon') \times \\ \times V_i(\varepsilon,\varepsilon')a^+_{B\alpha\mu}(\varepsilon)\sigma^i_{\mu\mu'}a_{B\alpha\mu'}(\varepsilon')\hat{\tau}^i_f, \\ V_i(\varepsilon,\varepsilon')\sigma^i_{\mu\mu'} \equiv V_{\mu\mu'}(\varepsilon,\varepsilon'). \quad (3.2)$$

Because the hybridization matrix elements are complex in general, Eqs. (3.1) and (3.2) contain the term involving $\hat{\tau}^y_f$ along with the term involving $\hat{\tau}^x_f$. We are interested in the case where the dominant effect of the interaction is the generation of a multiparticle resonance at the Fermi level. The Green's function corresponding to this resonance can be calculated using

the bosonization method by reducing the Hamiltonian H_0 to the resonance-level model proposed in [14]. To reduce the Hamiltonian $H_0 = H_{00} + H_{int} + H_\Delta$ with the two-channel exchange in Eq. (3.2) to the resonance-level model, it is convenient to rewrite H_0 as

$$H_0 = iv_F \sum_{\mu\mu'\alpha} \int_{-\infty}^{+\infty} \psi^+_{\mu\alpha}(x)\partial_x \psi_{\mu\alpha}(x) + \\ + \frac{1}{2}\sum_{\mu\alpha}\sum_{i=x,y,z} V_i \psi^+_{\mu\alpha}(0)\hat{\sigma}^i_{\mu\mu'}\psi_{\mu'\alpha}(0)\hat{\tau}^i_f + \Delta\hat{\tau}^z_f, \quad (3.3)$$

where

$$\psi_{\mu\alpha}(x) = \int_{-\infty}^{+\infty} dk\, e^{ikx} a_{B\mu\alpha}(k)$$

and

$$\psi_{\mu\alpha}(0) = \psi_{\mu\alpha}(x=0).$$

The bosonic representation of the fermion fields $\psi_{\mu\alpha}(x)$ takes the form

$$\psi_{\mu\alpha}(x) = \hat{\eta}_{\mu\alpha}\frac{e^{-i\Phi_{\mu\alpha}(x)}}{(2\pi a)^{1/2}}, \quad \hat{\eta}^2_{\mu\alpha} = 1, \\ \Phi_{\mu\alpha}(x) = (\pi)^{1/2}\left[\int_{-\infty}^{x} dx' P_{\mu\alpha}(x') + \varphi_{\mu\alpha}(x)\right], \quad (3.4)$$

where $\varphi_{\mu\alpha}(x)$ is the boson field, $P_{\mu\alpha}(x')$ is the canonically conjugate momentum, $[\varphi_{\mu\alpha}(x), P_{\mu'\alpha'}(x')] = i\delta(x-x')\delta_{\mu\mu'}\delta_{\alpha\alpha'}$, and a is the lattice constant. The operators $\hat{\eta}_{\mu\alpha}$ ensure the anticommutation relations between different species of fermions. The boson fields $\varphi_{\mu\alpha}(x)$ and $P_{\mu\alpha}(x)$ can be rewritten in terms of the collective variables that are introduced by means of the canonical transformation of $\varphi_{\mu\alpha}(x)$ and $P_{\mu\alpha}(x)$:

$$\varphi_{c,f} = \frac{1}{2}[(\varphi_{11}+\varphi_{12}) \pm (\varphi_{21}+\varphi_{22})], \\ \varphi_{s,(sf)} = \frac{1}{2}[(\varphi_{11}-\varphi_{12}) \pm (\varphi_{21}-\varphi_{22})]. \quad (3.5)$$

Similar expressions can be written for the conjugate fields $P_{\mu\alpha}(x)$, $\mu,\alpha = 1,2$. The Fourier components of the boson fields $k^{1/2}\varphi_l(k)$ correspond to the charge (c), flavour (f), pseudospin (s), and mixed (flavour-quadrupole, sf) density operators $\rho_l(k)$. The flavour is generated by the channel index α.

In terms of the collective bosonic variables, the spinless fermion collective fields are given by

$$\psi_l(x) = \frac{e^{-i\Phi_l(x)}}{(2\pi a)^{1/2}}, \quad l = c, f, s, (sf). \quad (3.6)$$

The Hamiltonian H_0 can be represented as a sum of four terms corresponding to the four spinless fermion collective channels. The charge and flavour channels are not coupled to the impurity pseudospin. The other channels give the following terms in the Hamiltonian $H_0 = H_{00} + H_{int} + H_\Delta$:

$$H_{00} = iv_F \sum_{l=s,(sf)} \int_{-\infty}^{+\infty} dx \psi^+_l(x)\partial_x\psi_l(x),$$

$$H_{int} + H_\Delta = \frac{V_x}{(2a\pi)^{1/2}}[\psi^+_{sf}(0) + \psi_{sf}(0)]\hat{\tau}^x_f + \\ + \tilde{V}_z\psi^+_s(0)\psi_s(0)\hat{\tau}^z_f + \Delta\hat{\tau}^z_f, \quad \tilde{V}_z \equiv 2(V_z - \pi v_F). \quad (3.7)$$

The Hamiltonian in Eq. (3.7) corresponds to the resonance-level model that yields a multiparticle resonance (the f_r level) at the Fermi level. The f_r level can be described in terms of the fermion operators d^+ and d coupled to the pseudospin operator $\hat{\tau}_f$ via the Majorana representation: $d^+ = \hat{\tau}^+_f\hat{\eta}$, $\hat{\tau}^z_f = d^+d - (1/2)$, where $\hat{\eta}$ is the Majorana (real) fermion operator such that $\hat{\eta}^2 = 1$. The Green's function $\hat{G}^{(0)}_{f_r}(z)$ of the resonance level contains the anomalous components $\propto \langle dd\rangle$ and $\propto \langle d^+d^+\rangle$ in addition to the normal components $\propto \langle dd^+\rangle$ because the number of fermions is not conserved in the models described by Eq. (3.7).

3.2. It is known [15,16] that the two-channel model described by Eqs. (3.3) and (3.7) has two regions with essentially different physical properties depending on the relation between T_K and Δ, where T_K is the exponential Kondo temperature.

We consider the region of the parameters where the Kondo physics plays the key role. This case is referred to as the «Kondo regime» in what follows. It occurs under the condition

$$T_K \gg \Delta. \quad (3.8)$$

In this case, the model described by (3.7) renormalizes to the strong coupling limit [15,16]. In this limit, the quantites $\Gamma_K = \pi\rho_{0B}V_x^2$ and Δ renormalize to T_K and Δ^2/T_K, respectively. The fixed point lies on the line $\tilde{V}_z = 0$ [8] (the Emery–Kivelson line) and the screening interaction is not essential for small energies. The quantity T_K is defined on the Emery–Kivelson line and depends on V_x only. For this reason, the parameters T_K and Δ are independent. The NFL state is generated by the impurity degrees of freedom that are not hybridized with the conduction electrons [14,17]. Near the Fermi level at $T = 0$, the Green's function becomes

$$\hat{G}^{(0)}_{f_r}(z) = \pm\left[\frac{\hat{\sigma}_0 - \hat{\sigma}_x}{z - \Sigma_K(z)} + \frac{\hat{\sigma}_0 + \hat{\sigma}_x}{z}\right], \quad (3.9)$$

where $\Sigma_K(z)$ is the self-energy part determined by the hybridization term in Eq. (3.7), and $\pm$ corresponds to $\mathrm{Re}(z)\gtrless 0$. As usual, the exponential pole at $|z| \propto T_K$ in the first term of $\hat{G}^{(0)}_{f_r}(z)$ has the exponentially small residue $Z_K \propto \exp(-\varepsilon_{\Gamma_3}/\gamma_B)$, $T_K \propto \varepsilon_F Z_K$.

On the other hand, under the conditions

$$T_K \ll \Delta, \quad \tilde{V}_z \gg V_{x,y}, \tag{3.10}$$

the model does not renormalize to the strong coupling limit (or equivalently, to the fixed point at $\tilde{V}_z = 0$) for low temperatures because of a very weak renormalization of Δ [15]. In this case, the NFL state is generated by the screening interaction in Eq. (3.7) and by the non-hybridized impurity degrees of freedom. This mechanism is referred to as the «X-ray edge regime» in what follows. In this case, the hybridization occurring in the sf-channel can be treated as a perturbation of the ground state obtained at $V_x = 0$. At $V_x = 0$, the problem is solved exactly. To obtain the Green's function $\hat{G}^{(0)}_{f_r}(z)$ at $V_x = 0$, we use the technique that was previously applied to the well-known problem of the X-ray absorption in metals.

We first diagonalize the Hamiltonian $H^s_{00} + H_s + H_\Delta$ in (3.7) at $V_{x,y} = 0$. For this, we introduce the boson operators $b_{sk} = k^{-1/2}\rho_s(k)$ and $b^+_{sk} = k^{-1/2}\rho_s(-k)$, where

$$\begin{aligned} \rho_s(k) &= \frac{1}{N^{1/2}} \sum_{q=0}^{k_D-k} \psi^+_s(q)\psi_s(q+k), \\ \rho_s(-k) &= \frac{1}{N^{1/2}} \sum_{q=k}^{k_D} \psi^+_s(q)\psi_s(q-k), \quad k \geq 0, \end{aligned} \tag{3.11}$$

are density operators, $\psi_s(k)$ are Fourier components of the fields $\psi_s(x)$, and the cut-off occurs at $k_D \sim a^{-1}$. Using the operators b_{sk} and b^+_{sk}, we write the Hamiltonian as

$$H^s_{00} + H_s + \Delta\hat{\tau}^z_f = v_F \sum_{k>0} k b^+_{sk} b_{sk} + \tilde{V}_z \left(d^+ d - \frac{1}{2}\right) \times \\ \times \sum_{k>0} \left(\frac{k}{N}\right)^{1/2} (b^+_{sk} + b_{sk}) + \Delta\hat{\tau}^z_f. \tag{3.12}$$

This is diagonalized by the canonical transformation

$$U_B = \exp\left(\tilde{V}_z \rho_{0B} \left(d^+ d - \frac{1}{2}\right) \sum_{k>0} (kN)^{-1/2} (b_{sk} - b^+_{sk})\right).$$

Under this operation, the Hamiltonian $H^s_{00} + H_s + \Delta\hat{\tau}^z_f$ is transformed to

$$\tilde{H}_s = v_F \sum_{k>0} k \tilde{b}^+_{sk} \tilde{b}_{sk} + \tilde{\Delta}\left(\tilde{d}^+ \tilde{d} - \frac{1}{2}\right), \tag{3.13}$$

where

$$\tilde{d}^+ = U_B d^+ U_B^{-1} \equiv U_{0B} d^+,$$

$$\tilde{b}^+_{sk} = U_B b^+_{sk} U_B^{-1} = b^+_{sk} + \frac{\rho_{0B}\tilde{V}_z}{(kN)^{1/2}} d^+ d,$$

$$U_{0B} = \exp\left(\tilde{V}_z \rho_{0B} \sum_{k>0} \frac{b_{sk} - b^+_{sk}}{(kN)^{1/2}}\right),$$

$\tilde{\Delta} = \Delta - \varepsilon_U$, and $\varepsilon_U = \tilde{V}_z^2 \rho_{0B}$ is the «polaron shift».

Equation (3.13) allows us to find the Green's function of the resonance level,

$$\hat{G}^{(0)}_{f_r}(t) = \hat{G}^{(00)}_{f_r}(t) \langle U^+_{0B}(t) U_{0B}(0)\rangle_D, \tag{3.14}$$

where $U_{0B}(t)$ is derived from $U_{0B}(0)$ by the substitution $b_{sk} \to b_{sk} e^{i\varepsilon_k t}$. In Eq. (3.14), $\langle \ldots \rangle_D$ denotes averaging over the states of the diagonalized Hamiltonian $H^s_{00} + H_s$ and $\hat{G}^{(00)}_{f_r}(t)$ is the Green's function with the s-channel interaction disregarded. The averaging is performed in the standard way using the relations

$$e^{\hat{A}} e^{\hat{B}} = e^{\hat{A}+\hat{B}+(1/2)[\hat{A},\hat{B}]},$$

$$\langle e^{[F(b^+,b)]}\rangle = e^{(1/2)\langle F^2(b^+,b)\rangle},$$

where F is an arbitrary linear combination of boson operators. As a result, we find that at large times $\varepsilon_F t \gg 1$, the function in Eq. (3.14) is given by

$$\hat{G}^{(0)}_{f_r}(t) \sim \hat{G}^{(00)}_{f_r}(t) t^{-\alpha_s}, \tag{3.15}$$

where $\alpha_s = (\delta_s/\pi)^2$ and δ_s is the phase shift for the scattering described by H_s in the pseudospin channel.

At $V_{x,y} = 0$, we use Eq. (3.15) with $\hat{G}^{(00)}_{f_r}(t) \propto e^{-i\tilde{\Delta}t}$ to obtain the known expression for the Green's function

$$G^{(0)}_{f_r}(z) = \frac{A_{(\pm)}\Gamma(1-\alpha_s)}{z - \tilde{\Delta}} \left(\frac{z - \tilde{\Delta}}{W}\right)^{\alpha_s}, \tag{3.16}$$

where $A_{(+)} = -1$ and $A_{(-)} = (-1)^{-\alpha_s}$ for $\mathrm{Re}(z - \tilde{\Delta}) \gtrless 0$, respectively, $\Gamma(x)$ is the gamma function, and W is the cut-off parameter of the order of the conduction band width.

We next recall (e.g., from [23]) that including the hybridization V_x as a perturbation in the «X-ray edge» Hamiltonian, we recover the previous «X-ray edge» results with the energy shifted as $i\omega \to i\omega + i\Gamma_K \operatorname{sign}\omega$, $\Gamma_K = \pi\rho_{0F} V_x^2$, in the resonance level Green's function $\hat{G}_{f_r}$. Within the framework of two-channel model (3.5), the width due to the hybridization appears only for a half of the impurity degrees of freedom $\tau^x_{\Gamma_3}$ hybridized with the conduction sf-channel.

The same result can be obtained by writting Hamiltonian (3.5) in terms of the hybridized states and then

considering the screening interaction for these states. One can readily show that additional interactions induced by the transition to the new basis are proportional to $\tilde{V}_z(V_x/W)$ and are therefore much smaller than the screening interaction. In the new basis, Hamiltonian (3.7) is reduced under condition (3.10) to a Hamiltonian of the «X-ray edge» type. In the present case, the hybridization in Eq. (3.7) gives the level width related to a half of the degrees of freedom of the impurities hybridized with the conduction electrons.

Using Eqs. (3.14) and (3.15) with

$$\hat{G}^{(00)}_{f_r} \sim (\hat{\sigma}_0 - \hat{\sigma}_x)e^{-i(\tilde{\Delta}-i\Gamma_K)t} + (\hat{\sigma}_0 + \hat{\sigma}_x)e^{-i\tilde{\Delta}t},$$

we thus obtain $\hat{G}^{(0)}_{f_r}(z)$ in the energy representation,

$$\hat{G}^{(0)}_{f_r}(z) = A_{(\pm)}\Gamma(1-\alpha_s) \times \left[\frac{\hat{\sigma}_0 - \hat{\sigma}_x}{z - \tilde{\Delta} + i\Gamma_K}\left(\frac{z - \tilde{\Delta} + i\Gamma_K}{W}\right)^{\alpha_s} + \frac{\hat{\sigma}_0 + \hat{\sigma}_x}{z - \tilde{\Delta}}\left(\frac{z - \tilde{\Delta}}{W}\right)^{\alpha_s}\right], \quad (3.17)$$

where

$$\Gamma_K \sim W\frac{\gamma_{B1}\gamma_{B2}}{\varepsilon_f^2}.$$

Because we calculate the retarded Green's function in Eq. (3.17), we must have $\operatorname{Im} z < 0$. If the radial parts of the wave functions entering the matrix elements V^f_μ are independent of μ, we readily obtain

$$\gamma_{B1} \sim \gamma_{B2} = \gamma_B, \quad \Gamma_K \sim W\frac{\gamma_B^2}{\varepsilon_f^2}. \quad (3.18)$$

The power-law dependence occurs in Eq. (3.17) under conditions (3.10).

It follows from (3.17) that the multiparticle NFL resonance at the Fermi level is generated by the mixed flavor-quadrupole (sf) mode. The interactions in the pseudospin channels having the screening character lead to the effective broadening of the resonance level. The second term in Eq. (3.17) is due to the impurity degrees of freedom that are not hybridized with the conduction electrons.

In conclusion of this section, we write the expression for the DOS $\rho_B(\varepsilon)$ near the Fermi level. The multiparticle resonances at the Fermi level are described by the Green's functions in Eqs. (3.9), (3.17), and (3.16). These Green's functions must be inserted in Eq. (2.8), after which $\rho_B(\varepsilon)$ is derived. In particular, inserting Eq. (3.17) in Eq. (2.8), we find the DOS in the «X-ray edge» regime

$$\rho_B(\varepsilon) - \rho_{0B}(\varepsilon) = -\frac{1}{\pi}A_\rho \operatorname{Im}\operatorname{Sp}\hat{G}^{(0)}_{f_r}(\varepsilon) = A_\rho \sum_{i=1,2}\frac{\sin\left[(1-\alpha_s)\operatorname{arctg}\dfrac{\Gamma_i}{\varepsilon - \tilde{\Delta}}\right]}{W^{\alpha_s}[(\varepsilon - \tilde{\Delta})^2 + \Gamma_i^2]^{(1-\alpha_s)/2}}, \quad \varepsilon > 0, \quad (3.19)$$

where $A_\rho \sim \gamma_B\rho_{0B}$. The widths $\Gamma_1 = \delta \to 0^+$ and $\Gamma_2 = \Gamma_K$ correspond to the two contributions into the Green's function $\hat{G}^{(0)}_{f_r}$ in Eq. (3.17).

In the Kondo regime, the DOS is determined by function (3.9).

4. THE FERMI-LIQUID RESONANCES NEAR THE FERMI LEVEL

4.1. The scattering of the multiparticle excitations due to the term H_{sc} results in simple poles near the Fermi level in the complete Green's function $\hat{G}_{f\mu}(z)$ in Eq. (2.6). The poles correspond to new Fermi-liquid resonances. The positions $z_r^{(\pm)} = \varepsilon_r^{(\pm)} - i\gamma_r^{(\pm)}$ of the poles are determined by the equation

$$D^{AB}_\mu(z_r^{(\pm)}) = 1 - \Sigma^{sc}_{A\mu}(z_r^{(\pm)})W_{B\mu}(z_r^{(\pm)}) = 0. \quad (4.1)$$

Because this equation is the same for all terms of the matrix $\hat{D}^{AB}_\mu$, the matrix indices are omitted in Eq. (4.1).

The expression for the Green's function (2.6) near the FL resonance with the energy $z_{r\mu}$ becomes

$$\hat{G}_{f\mu}(\varepsilon) = F_r^{-1}\frac{z_{r\mu}\hat{G}^{(0)}_{f_r}(z_{r\mu})}{\varepsilon - \tilde{\Delta} - z_{r\mu}}, \quad (4.2)$$

where we expanded the denominator in Eq. (2.6) near the resonance energy as $D(\varepsilon) = D'(z_{r\mu})(\varepsilon - \tilde{\Delta} - z_{r\mu})$, where $D'(z_{r\mu}) \approx F_r/z_{r\mu}$ (with the indices of the denominator omitted at the moment) and F_r is a function of the parameters of the order of unity. The energy dependences of $\Sigma^{hsc}_{\nu\mu}(z)$ in (2.6) are determined by the DOS $\rho_\nu(\varepsilon)$. In the model under consideration, the function $\Sigma^{sc}_{A\mu}(z)$ has no features at the Fermi level, which allows us to write

$$\operatorname{Re}\Sigma^{sc}_{A\mu}(0) \approx \rho_{0A}(0), \quad \operatorname{Im}\Sigma^{sc}_{A\mu}(0) = 0. \quad (4.3)$$

The self-energy functions $\Sigma^{sc}_{B\mu}(z)$ have the features corresponding to the NFL peaks in the DOS $\rho_B(\varepsilon)$.

In the Kondo regime, the main singular term appears in $\Sigma^{sc}_{B\mu}(z)$ because of the δ-like contribution to

the spectral function induced by the second term in the Green's function (3.9) as $z \to \varepsilon + i0^+$. In other words, this singular term is due to the impurity degrees of freedom that are not hybridized with the conduction electrons. The self-energy $\Sigma^{sc}_{B\mu}(z)$ takes the form

$$\Sigma^{sc}_{B\mu}(z) \approx \text{const} + V^f_\mu T^{B*}_\mu \frac{\gamma_B \rho_{0B}}{z}. \qquad (4.4)$$

In the «X-ray edge» regime, using the density of states in Eq. (3.19), we obtain the contribution of the resonance levels to the self-energy function at zero temperature,

$$\Sigma^{sc}_{B\mu}(z) \approx A_{B\mu}\left(\gamma_B \gamma_{B\mu} \rho_{0B}\right)\left(\frac{T^{B*}_\mu}{V^{f*}_\mu}\right) \times \times \left(\frac{W}{z - \tilde{\Delta} + i\Gamma_K}\right)^{1-\alpha_s} (-1)^{\alpha_s - 1}, \qquad (4.5)$$

where $|A_{B\mu}| \sim 1$.

In the Kondo regime, inserting (3.9) and (4.4) in (4.1) and taking the most singular term $\propto 1/z^3$ in $W_{B\mu}(z)$ into account, we readily obtain two resonances above and below the Fermi level that occur due to the scattering of the non-hybridized impurity degrees of freedom. The energies of these resonances are determined by

$$\frac{|z^{(\pm)}_r|}{W} = A_r \left(\gamma_{A\mu} \rho_{0A}\right)^{1/3} \left(\gamma_B \rho_{0B}\right), \qquad (4.6)$$

where $A_r \sim 1$ and $\gamma_{A\mu} = |T^B_\mu|^2 \rho_{0A}$. The resonance width above the Fermi level is much smaller than the resonance width below the Fermi level. The former width is determined by the terms in Eq. (4.1) that are much smaller than the leading singular term $\propto 1/z^3$. Therefore, the pseudogap exists near the Fermi level for $|\varepsilon^{(-)}| \gg \gamma^{(-)}_r$ and for $|\varepsilon^{(-)}| \ll \gamma^{(-)}_r$.

In addition, Eq. (4.1) has two solutions above and below the Fermi level with $|z + i\gamma_K| \ll \gamma_K$. For this reason, the shape and the width of the Kondo peak change weakly at the Fermi level. In particular, the width of the Kondo peak has a small additional term $\sim T_K \left(\gamma_{A\mu} \rho_{0A}\right)\left(\gamma_B \rho_{0B}\right) \ll T_K$ due to the scattering.

The qualitative picture of the DOS in the Kondo regime near the Fermi level is shown in Fig. 2. We see that the FL resonances generate both the additional energy scale $\gamma_r \ll T_K$ and the pseudogap near the Fermi level.

We thus obtained the essential result that the scattering of the non-hybridized impurity degrees of freedom by the electron states of the narrow band leads to the existence of new resonances near the Fermi level.

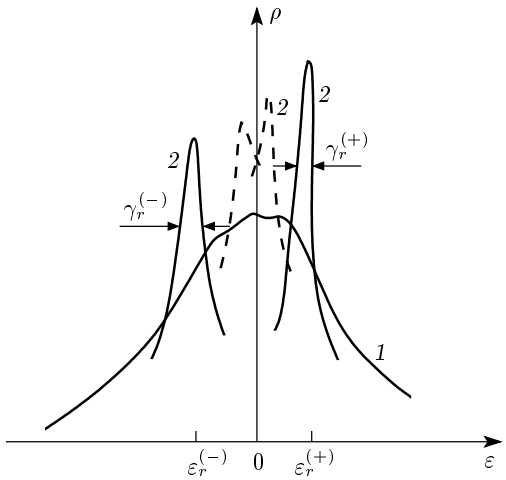

Fig. 2. The Kondo resonance (curve *1*) and new FL resonances (curves *2*) show the respective FL resonances with $|\varepsilon^{\pm}_r| \gg \gamma^{\pm}_r$ and $|\varepsilon^{\pm}_r| \ll \gamma^{\pm}_r$

According to the experimental data [2], there exists a concentration region where the Kondo energy T_K exponentially increases with decreasing the impurity concentration. At the same time, the hybridization matrix elements and, consequently, the widths γ_B and $\gamma_{A\mu}$ remain approximately constant in this region. We can therefore expect that the condition $|z_r| \ll T_K$ is satisfied at sufficiently low cocentration of the impurity atoms.

4.2. Using expressions (2.7) and (3.17), it is easy to verify that in the «X-ray edge» regime, Eq. (4.1) possesses solutions of two types with their energies satisfying the respective conditions

$$|z^{(\pm)}_r| \ll \Gamma_K, \quad \text{the narrow resonances,}$$

$$|z^{(\pm)}_r + i\Gamma_K| \ll \Gamma_K, \quad \text{the «wide» resonances.}$$

For simplicity, we here used the condition

$$\tilde{\Delta} \ll \Gamma_K, z^{(\pm)}_r.$$

The signs «±» correspond to the resonances above and below the Fermi level. For $|\varepsilon^{(\pm)}_r| \ll \gamma^{(\pm)}_r, |\gamma^{(\pm)}_r - \Gamma_K|$, the widths of the FL resonances are determined by

$$\frac{\gamma^{(\pm)}_r}{W} = A_1 \left(\gamma_{A\mu} \gamma_{B\mu} \rho^2_{0B}\right)^{1/(1-\alpha_s)} \times \times \left(\gamma_B \rho_{0B}\right)^{2/(1-\alpha_s)} \left(\frac{\varepsilon_f}{\gamma_{B\mu}}\right)^4, \quad \gamma^{(\pm)}_r \ll \Gamma_K, \qquad (4.7)$$

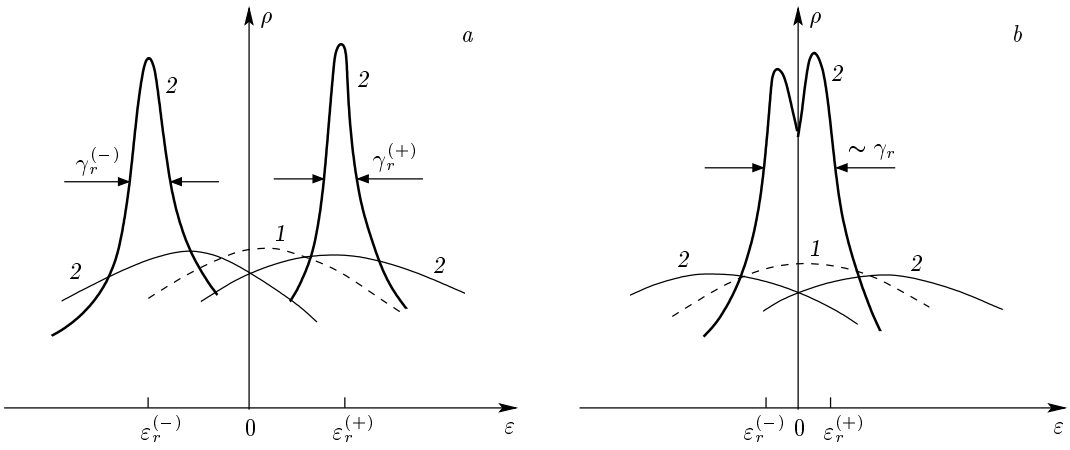

Fig. 3. The NFL (curves *1*) and FL resonances in the «X-ray edge» regime: (*a*) the narrow resonances for $|\varepsilon_r^{\pm}| \gg \gamma_r^{\pm}$; (*b*) these resonances for $|\varepsilon_r^{\pm}| \ll \gamma_r^{\pm}$

$$\frac{|\gamma_r^{(\pm)} - \Gamma_K|}{W} = A_2 \left(\gamma_{A\mu}\gamma_{B\mu}\rho_{0B}^2\right)^{1/3(1-\alpha_s)} \times \\ \times \left(\gamma_B\rho_{0B}\right)^{2/3(1-\alpha_s)}, \quad |\gamma_r^{(\pm)} - \Gamma_K| \ll \Gamma_K, \quad (4.8)$$

where $A_{1,2} \sim 1$. In this case, the FL resonances merge into a single weakly split resonance at the Fermi level (Fig. 3*b*). For $|\varepsilon_r^{(\pm)}| \gg \gamma_r^{(\pm)}, |\gamma_r^{(\pm)} - \Gamma_K|$, the energies $|\varepsilon_r^{(\pm)}|$ are determined by the expressions in the right-hand sides of Eqs. (4.7) and (4.8) and by $\gamma_r^{(\pm)} = |\varepsilon_r^{(\pm)}| \sin\varphi$ with $\varphi \ll 1$. In this case, pairs of the FL resonances appear above and below the Fermi level (Fig. 3*a*). Pairs of the FL resonances can exist because the Green's function $\hat{G}_{f\mu}(z)$ has two branches above and below the Fermi level. For $|\varepsilon_r^{(\pm)}| \gg \gamma_r^{(\pm)}$, there are well-determined pseudogaps near the Fermi level in the case of the narrow resonances.

Two types of the FL resonances correspond to the existence of the hybridized and non-hybridized impurity degrees of freedom. In particular, the narrow resonances, which determine a new small energy scale near the Fermi level, are generated by the interband scattering of the non-hybridized impurity degrees of freedom. In other words, the narrow resonances result from broadening and displacement of the zero-width term in the spectral function $\hat{G}_{f_r}^{(0)}$ (see the second term in Eq. (3.17)) due to the interband scattering.

Equations (4.7) and (4.8) imply that the FL resonances exist for the deep level ($\varepsilon_f \gg \gamma_B$) under the condition

$$\frac{\gamma_{A\mu}}{\gamma_{B\mu}} \ll \left(\gamma_{B\mu}\rho_{0B}\right)^{2-6\alpha_s} \left(\frac{W}{\varepsilon_f}\right)^{6(1-\alpha_s)}, \quad (4.9)$$

which is the same for the resonances of both types.

Condition (4.9) is satisfied for all values of α_s in the following cases. First, for $\gamma_{A\mu} \gg \gamma_B$ and sufficiently «shallow» f-levels such that

$$\gamma_B \ll \varepsilon_f \ll W \left(\frac{\gamma_B}{W}\right)^{(1-3\alpha_s)/3(1-\alpha_s)}, \quad (4.10)$$

and second, for $\gamma_{A\mu} \ll \gamma_B$ and $\varepsilon_f \sim W$.

On the other hand, the widths of the NFL resonance and, correspondingly, the characteristic binding energy of the collective states forming the NFL resonance can be estimated as

$$\varepsilon_K \sim \Gamma_K \left(\frac{\varepsilon_F}{\Gamma_K}\right)^{\alpha_s}. \quad (4.11)$$

This estimate is derived from the NFL DOS in Eq. (3.19). As α_s increases, the binding energy ε_K also increases.

The FL resonance can appear if the collective states defined in Eqs. (3.6) and (3.11) decay. Taking the foregoing into account, we must bear in mind that the decay of collective states becomes more difficult as α_s increases. Therefore, the structure of the FL resonances near the Fermi level essentially depends on the magnitude of the parameter α_s that describes the scattering in the quadrupole (pseudospin) channel. From the imaginary part of Eq. (4.1), we readily find that the narrow resonances exist for $\alpha_s \leq 3/5$. For $1/7 < \alpha_s \leq 1/3$, the narrow resonances appear above

and below the Fermi level. For $\alpha_s > 5/7$, FL resonances are absent.

In addition to condition (4.9), we thus find that the narrow FL resonances can exist when the pseudospin channel interaction $\tilde{V}_z$ is not very strong.

In the limiting case where $V_{x,y} = 0$, the FL resonance exists above the Fermi level for $\alpha_s \leq 1/3$. Its energy is determined by

$$\frac{|z_r^{(\pm)}|}{W} \sim (\gamma_{A\mu}\rho_{0A})^{1/(1-\alpha_s)} \times \\ \times (\gamma_B\rho_{0B})^{1/(1-\alpha_s)} \ll \gamma_B. \quad (4.12)$$

In the «X-ray edge» regime, the narrow FL resonances provide peaks in the DOS with the widths much smaller than those of the NFL resonance (see Fig. 3). Thus, their existence allows us to obtain a new mechanism for the appearance of the small energy scale.

We also mention that as shown in [11], the model without the continuum in the impurity region does not give narrow FL resonances, and therefore, does not lead to the small energy scale. The «wide» resonances above and below the Fermi level and a local state above the Fermi level have been obtained in this model. Additional mechanisms are required for broadening local states.

At the same time, the existence of the narrow FL resonances leads to the appearance of pseudogaps near the Fermi level in the «X-ray» regime. The pseudogap occurs under the Fermi level for a single narrow FL resonance at $1/3 < \alpha_s \leq 3/5$. At $\alpha_s \leq 1/3$ for the split FL resonances, the pseudogap also splits into two branches above and below the Fermi level. The pseudogaps are well determined for $|\varepsilon_r| \gg \gamma_r$. The minimum value of the DOS inside the pseudogaps is of the order of the magnitude of the «wide» resonances. The maximum widths of the pseudogaps are of the order $|\varepsilon_r^{(\pm)}|$ and are determined by the expression in the right-hand side of Eq. (4.7).

The conditions required for the appearance of pseudogaps are identical to those for the existence of the narrow FL resonances.

5. THE MIXED-VALENCE AND NEARLY INTEGER STATES

5.1. The criterion that enables us to choose between the two types of states involves the partial f-component $\rho_{f_r}(0)$ of the DOS at the Fermi level and the DOS $\rho_f(\varepsilon_{f\mu})$ at the deep level. For $\rho_{f_r}(0) \gg \rho_f(\varepsilon_{f\mu})$, the charged excitations play the key role at the Fermi level, while the opposite inequality means that their role is negligible. The former case corresponds to the mixed-valence state, and the latter case leads to the state with a nearly integer valency.

The Green's function $G^{(0)}_{f\mu}(z)$ for $|z|$ close to the energy $\varepsilon_{f\mu}$ of the deep level can be represented as

$$G^{(0)}_{f\mu}(z) \approx \frac{Z_{f\mu}}{z - \varepsilon_{f\mu}}, \quad (5.1)$$

where $Z_{f\mu} \sim 1$ is the residue at the pole $z = \varepsilon_{f\mu}$. The energy $\varepsilon_{f\mu}$ renormalized by hybridization is determined by the equation

$$\varepsilon_{f\mu} = \varepsilon_f + \Sigma^{(0)}_{B\mu}(\varepsilon_{f\mu}) \equiv \bar{\varepsilon}_f + i\gamma_{f\mu}.$$

The maximum value of the DOS at the deep level can therefore be estimated as

$$\rho_f(\varepsilon_{f\mu}) \sim \rho_{0B}\left(\frac{\varepsilon_F}{\gamma_B}\right). \quad (5.2)$$

We now verify our criterion for the Kondo resonance. It is well known [19, 20] that in this case, the density of charged states is small at the Fermi level. Using the «resonance–level» formalism, one can see this from the small residue Z_K that determines the pole contribution to the Green's function at $|z|$ close to the Fermi energy,

$$G_K(z) \approx \frac{Z_K}{z - E_K}, \\ \rho_K(0) \sim \frac{Z_K}{\gamma_K} \sim \rho_{0B} \ll \rho_f(\varepsilon_{f\mu}), \quad (5.3)$$

where $E_K \sim i\gamma_K$ and $\gamma_K \sim T_K$. In accordance with our criterion, the inequality corresponds to a small contribution of the charged excitations at the Fermi level.

However, for new FL resonances with the widths $\gamma_r^{\pm}$ in Eq. (4.6), the following unequality holds:

$$\rho^{FL}_{f_r}(0) \sim \frac{W}{\gamma_r}\rho_{0B} \gg \rho_f(\varepsilon_{f\mu}). \quad (5.4)$$

Therefore, additional FL resonances lead to the existence of a mixed-valence state in the Kondo regime.

In the «X-ray edge» regime, the NFL resonance is generated by the flavor-quadrupole and the quadrupole (pseudospin) modes that have a charge due to the quadrupole contribution. The component $\rho^{NFL}_{f_r}(0) = -(1/\pi)\,\mathrm{Im}\,\mathrm{Sp}\,\hat{G}^{(0)}_{f_r}(0)$ is then estimated as

$$\rho^{NFL}_{f_r}(0) \sim \rho_{0B}\left(\frac{W}{\Gamma_K}\right)^{1-\alpha_s} \sim \\ \sim \rho_{0B}\left(\frac{\bar{\varepsilon}_f}{\gamma_B}\right)^{2(1-\alpha_s)}. \quad (5.5)$$

For the narrow FL resonances, using expression (2.6) for the Green's function $G_{f_r\mu}(z)$, we readily arrive at the estimate

$$\rho_{f_r}^{FL}(0) = -\frac{1}{\pi}\sum_{\mu}\operatorname{Im}\operatorname{Sp}\hat{G}_{f\mu}(0) \sim \sim \rho_{0B}\left(\frac{W}{\gamma_r}\right)^{(1-\alpha_s)}. \quad (5.6)$$

Assuming $\bar{\varepsilon}_f \sim W$ and comparing (5.2) with (5.5) and (5.6), we find

$$\begin{aligned} &\rho_{f_r}^{NFL}(0) \gg \rho_f(\varepsilon_{f\mu}) \quad \text{at} \quad \alpha_s < \frac{1}{2}, \\ &\rho_{f_r}^{NFL}(0) \ll \rho_f(\varepsilon_{f\mu}) \quad \text{at} \quad \alpha_s > \frac{1}{2} \end{aligned} \quad (5.7)$$

and also the inequality

$$\rho_{f_r}^{FL}(0) \gg \rho_{f_r}^{NFL}(0), \quad \rho_f(\varepsilon_{f\mu}) \quad (5.8)$$

that holds for all values of the parameters at which FL resonances exist.

It is interesting to note that under the conditions $\gamma_{A\mu} \gg \gamma_B$ and

$$W\left(\frac{\gamma_B}{W}\right)^{(1-2\alpha_s)/2(1-\alpha_s)} \ll \varepsilon_f \ll \ll W\left(\frac{\gamma_B}{W}\right)^{(1-3\alpha_s)/3(1-\alpha_s)}, \quad (5.9)$$

the mixed-valence state and FL resonances exist simultaneously for all values of α_s.

Inequalities (5.7)–(5.8) imply that, first, the state with a nearly integer valency can be realized only when FL resonances are absent and the parameter α_s is sufficiently large. Second, two types of the mixed-valence states are generated in our system.

The NFL mixed-valence state occurs for $\alpha_s < 1/2$ if FL resonances are absent.

In the extreme case where $V_{x,y}^{\Lambda} = 0$, the mixed-valence state exists only owing to the additional FL resonance.

The FL mixed-valence states are generated by the instability of the NFL state against the interband scattering. These states are formed under the same conditions that are necessary for the existence of FL resonances at the Fermi level. The type of the FL mixed-valence state depends on the type of the FL resonance (narrow or «wide») that can be realized for a given set of parameters.

As shown above, narrow FL resonances exist for all values $\alpha_s < 1/2$. Thus, the main features of the FL mixed-valence state are the appearance of a small energy scale and the formation of pseudogaps.

The transitions between the NFL and FL mixed-valence states are characterized by changing the valency from one noninteger value to another. Taking the foregoing into account, we conclude that condition (4.9) alone is necessary for the transitions between two mixed-valence states.

When condition (4.9) is not satisfied, the direct transition between the NFL mixed-valence state and the state with a nearly integer valency occurs at $\alpha_s \approx 1/2$.

Apparently, the most realistic way to generate the transitions experimentally is to change the lattice parameter by doping [3]. This leads to changing the hybridization between conduction electrons and the Γ_3 level that enters the interaction matrix elements and the widths γ_B. We can thus obtain a series of transitions, which are considered in detail elsewhere.

6. CONCLUDING REMARKS

6.1. The above results allow us to understand the mechanisms of two important properties of HF NFL metals.

(1) The single-site two-channel Kondo effect and the mixed valence state coexist because of additional FL resonances at/near the Fermi level. The scattering of the non-hybridized impurity degrees of freedom by the narrow A-band electrons generates these resonances. Therefore, two energy scales T_K and γ_r exist at the Fermi level. The FL resonance with the width γ_r corresponds to the local mixed-valence state.

(2) There are two possible energy dependence types in a system with the two-channel quadrupole exchange interaction. In the Kondo regime ($T_K \gg \Delta$), one obtains the known universal energy dependences [14, 17, 22] because the Green's function in Eq. (3.9) has a single energy scale T_K.

In the «X-ray edge» regime ($T_K \ll \Delta$), nonuniversal power-law energy dependences must occur in accordance with the form of the Green's function in Eqs. (3.16) and (3.17).

It follows from the experimental data [2] that the increase of the impurity concentration x in the U-compounds results in (a) decreasing $T_K(x)$, (b) increasing the concentration of the impurity atoms by a noticeable value Δ, and (c) increasing the anisotropy of the exchange parameters. Therefore, increasing the impurity concentration must enable crossing over from the Kondo regime with the universal energy dependences to the «X-ray edge» regime with nonuniversal energy dependences.

As shown above, characteristic features of the NFL compounds with f-shell impurities are the different types of the mixed-valence states with the NFL and FL excitation spectra and the fact that the heavy-fermion state type depends on the interaction parameter α_s. In the other words, this parameter determines the role of the charge and spin excitations in the formation of heavy fermions.

Small energy scales and the pseudogaps are induced by the narrow FL resonances. Therefore, the instability of the NFL state provides a new physical mechanism for the small energy scale. Unlike in the previous works [6, 21], this mechanism is especially appropriate for impurities with an unstable valency.

Thus, the instability of the NFL state induced by the interband scattering of multiparticle excitations considerably changes the mechanisms of the formation of heavy-fermion states.

6.2. We now briefly consider the features of the temperature dependences within the framework of the mechanism proposed in the present paper. The energy dependences of the Green's functions (2.6), (3.9), (3.16), and (3.17) imply that new types of the temperature transitions (crossovers) occur in the system. When new FL resonances generated by scattering are not formed, a transition occurs from the universal temperature dependences of the physical quantities in the Kondo regime to nonuniversal power-law dependences in the «X-ray edge» regime. The characteristic temperature of this crossover is $T_{c1} \sim \Delta$. In particular, the logarithmic dependence of the linear specific heat $C/T \propto \ln(T_K/T)$ must be transformed into the power-law dependence $C/T \propto T^{-1+\alpha_s}$. The former dependence was calculated in [14, 17] using expression (3.9) within the framework of the two-channel Kondo model. The power-law dependences follow from Eqs. (3.16) and (3.18) for the Green's functions in the «X-ray edge» regime. As mentioned in this section, the condition $T_K \ll \Delta$ can be realized at a relatively high concentration of the f-shell impurities. The power-law dependences of C/T observed in $U_xY_{1-x}Pd_3$ at $x = 0.2$ in [7] can therefore be generated by the mechanism discussed here. We recall that historically, the alloys $U_xY_{1-x}Pd_3$ were the first systems where the NFL behavior induced by the two-channel quadrupole Kondo model was observed [3, 5].

In the two-channel quadrupole Kondo model, the magnetic susceptibility is known [2] to have the van Vleck contribution between the Γ_3 groundstate and the first excited crystalline electric field. The van Vleck susceptibility is described by the temperature dependence $\chi \sim \chi_0 - \alpha(T/T_K)^{1/2}$. According to the experimental data [7], this dependence is also transformed into a power-law one as the impurity concentration increases.

The quadrupole susceptibility χ_Q has the logarithmic divergence $\propto \ln(T_K/T)$ in the Kondo regime. It is experimentally determined from the nonlinear magnetic susceptibility χ_3 [24]. Correspondingly, χ_Q and χ_3 must exhibit the same crossover as the specific heat.

We emphasize that the crossover discussed here corresponds to the transition between the state with a nearly integer valency and the mixed-valence state.

The existence of the FL resonances generated by the scattering of NFL excitations results in crossovers between the FL and NFL temperature dependences within both the Kondo regime and the «X-ray edge» regime. The characteristic temperatures of these crossovers are $T_{c2} \sim \gamma_r$, where γ_r are the widths of the FL resonances determined in Eqs. (4.6), (4.7). We note that the low-temperature transition to the FL state usually occurs at $T \sim \Delta^2/T_K$ in the two-channel Kondo model [3, 25]. The maximum value of the linear specific heat is equal to $(C/T)^{max} \sim T_K/\Delta^2$. Within the framework of our mechanism, it must be $(C/T)^{max} \sim \gamma_r^{-1}$ for $\gamma_r \gg \Delta^2/T_K$. It is possible that the additional small scale γ_r enters the scaling dependences in the FL–NFL transition region. The appearence of a new small energy scale is observed in the low-temperature scaling law of resistivity in [24]. In the «X-ray edge» regions, the crossover at $T \sim T_{c2}$ corresponds to the transition between the FL and NFL mixed-valence states.

The temperature transitions between FL mixed-valence states of the different origins were considered in [26].

6.3. The above results are obtained for single-ion NFL effects. We now show that these effects can also be considerable in «concentrated» systems.

The ground state of these systems significantly depends on the competition between the intersite interaction, i.e., the indirect exchange of the RKKY type for pseudospins, and the on-site Kondo scattering leading to the screening of the quadrupole impurity moment by conduction electrons. The characteristic energy for the two-channel on-site Kondo scattering is determined by expression (4.11). The characteristic energy scale of the RKKY interaction is

$$\varepsilon_{RKKY} \sim c_i \left(\frac{V_{ex}^2}{\varepsilon_F}\right) \sim c_i \Gamma_K, \qquad (6.1)$$

where c_i is the concentration of the interacting atoms. In concentrated systems, i.e., at $c_i \sim 1$, the energies ε_K and ε_{RKKY} are such that

$$\varepsilon_K \gg \varepsilon_{RKKY} \quad \text{for} \quad \alpha_s \neq 0. \tag{6.2}$$

This implies that single-ion NFL effects can be very important even when the two-channel impurities form a sublattice.

The analysis presented here enables us to qualitatively understand two important aspects of the problem for the «concentrated» systems: the dependence of the HF properties on doping and a physical reasons that can satisfactorily explain a number of properties of the «concentrated» systems within the framework of the single-ion quadrupole Kondo model.

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