Theory of the electron spin resonance in heavy fermion systems with non-Fermi-liquid behavior

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The theory of the electron spin resonance (ESR) in heavy fermion systems exhibiting a non-Fermi-liquid behavior is developed. It is shown that for the same values of the g factor of localized and itinerant electrons in the absence of the magnetic anisotropy the ESR signal has a δ-function shape if one does not take into account electron-lattice or electron-nuclear couplings. Magnetically anisotropic electron-electron interactions of localized electrons, together with the hybridization between wave functions of itinerant and localized electrons, yield a shift of the position of the ESR signal and change the linewidth. These changes in the characteristics of the ESR in heavy fermion systems are connected with interactions of low-energy quasiparticles. We have shown that there can be a Fermi-liquid contribution to the linewidth and a shift of the position of the ESR (the effective g factor) and a non-Fermi-liquid one, governed by the quantum critical point. Obtained results are compared with recent experimental ESR data for the heavy fermion compound $YbRh_2Si_2$.

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I. INTRODUCTION

Some rare-earth compounds exhibiting properties of heavy fermions[1] and the so-called non-Fermi liquids (NFLs) (Ref. 2) have been the topic of many studies because of their large and very interesting variety of low-temperature properties. The low-energy physics of these systems is determined by a hybridization of rare-earth localized electrons of $4f$ states, where electrons strongly interact with each other, with conduction electrons. Such a hybridization in metals with magnetic impurities produces the Kondo effect,[3] i.e., the screening of the spin of a localized electron by spins of conduction electrons due to the antiferromagnetic coupling between the spin of a localized electron and spins of itinerant ones. In heavy fermion compounds, localized $4f$ electrons build up a regular Kondo lattice whose properties are determined by strong electron-electron correlations. It is usually believed that, in heavy fermion compounds, this gives rise to spin fluctuations of localized spin moments, which are completely screened below some characteristic (crossover) temperature, i.e., the ground state is a singlet with a finite magnetic susceptibility. Due to that screening, effective masses of carriers are enhanced compared to normal metals. It manifests itself in large values of the low-temperature magnetic susceptibility, the linear in temperature Sommerfeld coefficient of the electronic specific heat, and a low-temperature coefficient of the resistivity. Such a behavior can be described in the framework of a standard Fermi-liquid (FL) theory[4] with the enhanced effective electron mass. On the other hand, for compounds exhibiting a non-Fermi-liquid behavior the magnetic susceptibility and the Sommerfeld coefficient are usually divergent at low temperatures, while the resistivity often reveals a power-law low-temperature behavior with exponents of less than 2 (the latter is characteristic for Fermi liquids and it is observed in heavy fermion compounds[1]). It turns out that mostly there is no magnetic ordering in heavy fermion or non-Fermi-liquid compounds (they are metals with zero order parameter). However, very often, by tuning some parameters, such as external pressure, or by a chemical substitution, such systems undergo phase transitions to ordered magnetic states.[1,2] In that case, a competing magnetic interaction, the so-called RKKY interaction between the localized $4f$ electrons via the sea of itinerant ones, favors a magnetically ordered ground state.

The electron spin resonance (ESR) spectroscopy is widely used as a valuable experimental tool to probe selectively local electronic properties of magnetic ions in condensed matter and to study the intrinsic spin dynamics of correlated electron systems. In ESR experiments, a dc magnetic field is applied to the investigated system and one measures the absorption of an ac magnetic field, polarized perpendicular to the dc field direction. Due to such a geometry, the ESR appears as a very sensitive method to study the anisotropy of magnetic interactions. The ESR potentially can be also very useful in addressing directly the spin dynamics and the magnetic interactions of itinerant electrons in metallic systems. However, the majority of such studies were restricted mainly to light metals since the spin-orbit coupling that scales with the atomic number Z as $\sim Z^4$ drastically shortens the electron spin lifetime.[5] This yields a strong broadening of the ESR response rendering it in many cases experimentally undetectable. From this point of view, the occurrence of a narrow ESR signal in the heavy fermion metal $YbRh_2Si_2$ (see Refs. 6 and 7) comprising heavy elements seems to be incompatible with conduction electrons. On the other hand, despite the pronounced anisotropy it would indicate an ESR of localized Yb^{3+} $4f$ moments; a nonlocal character of resonating spins is suggestive by the persistence of this signal even at sub-Kelvin temperatures[8] where, at least in the single-ion Kondo scenario, the local $4f$ moments are expected to be screened. (See, though, Ref. 9, where the low-temperature theory of the ESR in the Kondo situation was developed.)

The current experimental situation calls apparently for an adequate ESR theory for a heavy fermion compound comprising a regular (Kondo-like) lattice of localized strongly correlated $4f$ electrons, hybridized with conduction electrons. The goal of the present work has been to develop such a theory and, in particular, to provide possible explanations

of the main features of ESR in $YbRh_2Si_2$ reported in Refs. 6 and 7.

II. FRAMEWORK OF THE MODEL

Let us start with the consideration of the Anderson lattice model (which is believed to be one of the basic models for heavy fermion metals) in the external ac and dc magnetic fields, in the geometry, characteristic for ESR, with the Hamiltonian

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} a^{\dagger}_{\mathbf{k},\sigma} a_{\mathbf{k},\sigma} + \sum_{j,\sigma} \epsilon_f a^{\dagger}_{f,j,\sigma} a_{f,j,\sigma} + \mathcal{H}_{int} + V \sum_{\mathbf{k},j,\sigma} [\exp(i\mathbf{k}\mathbf{r}_j) a^{\dagger}_{\mathbf{k},\sigma} a_{f,j,\sigma} + \text{H.c.}] - \mu_B H \left[\frac{g}{2} \sum_{\mathbf{k}} (a^{\dagger}_{\mathbf{k},\uparrow} a_{\mathbf{k},\uparrow} - a^{\dagger}_{\mathbf{k},\downarrow} a_{\mathbf{k},\downarrow}) + \frac{g_f}{2} \sum_{j} (a^{\dagger}_{f,j,\uparrow} a_{f,j,\uparrow} - a^{\dagger}_{f,j,\downarrow} a_{f,j,\downarrow}) \right] - \mu_B h(t) \times \left[g \sum_{\mathbf{k},\sigma,\sigma'} a^{\dagger}_{\mathbf{k},\sigma} \sigma^{x,y}_{\sigma,\sigma'} a_{\mathbf{k},\sigma'} + g_f \sum_{j,\sigma,\sigma'} a^{\dagger}_{f,j,\sigma} \sigma^{x,y}_{\sigma,\sigma'} a_{f,j,\sigma'} \right], \tag{1}$$

where $a^{\dagger}_{\mathbf{k},\sigma}$ ($a_{\mathbf{k},\sigma}$) are creation (destruction) operators of conduction electrons $\sigma = \uparrow, \downarrow$, $a^{\dagger}_{f,j,\sigma}$ ($a_{f,j,\sigma}$) are creation (destruction) operators of a $4f$ electron localized at the jth lattice site with the position $\mathbf{r}_j$, g_f is the effective g factor of localized electrons, g is the effective g factor of conduction electrons, μ_B is the Bohr magneton, H is the dc magnetic field, $h(t)$ is the ac magnetic field, V is the matrix element of the hybridization between conduction and localized electron wave functions, and $\mathcal{H}_{int}$ is the term that describes the electron-electron interaction between $4f$ localized electrons. We shall focus on the situation of $g_f \sim g$ in what follows using for this purpose the units in which $g_f = g = 2\pi\hbar = \mu_B = 1$ and bearing in mind a possibility of a generalization to the case $g_f \neq g$ (see below).

Consider the circular time dependence of the ac magnetic field, i.e., the $h(t)$-dependent part of Eq. (1) has the form $(h/2)[\exp(i\omega t) S^{+}_{tot} + \text{H.c.}]$, where $h \ll H$ is the magnitude of the ac field, $\omega/2\pi \sim H$ is its frequency, and $S^{\pm}_{tot} = S^{x}_{tot} \pm i S^{y}_{tot}$ are linear combinations of the projections of the total spin of the system. In such a case we can use a unitary transformation (turn all spins about the z axis) to remove the explicit time dependence from the term of the Hamiltonian proportional to h. It is clear that if $\mathcal{H}_{int}$ does not contain magnetically anisotropic terms (say, it has the usual Hubbard-like interaction only), the explicit time dependence is totally removed by such a unitary transformation from the Hamiltonian. It means that the ESR signal would have resonance at $\omega/2\pi = H$, with zero linewidth (δ-function peak) and no shift of the resonance, compared to the noninteracting electron, due to spin-spin interactions. Naturally, additional interactions, not included in Eq. (1), e.g., an electron-lattice coupling or electron-nuclear one, will produce the broadening of such a δ-function line and/or a shift of the position of the resonance. A similar situation would appear if the magnetic field H is directed exactly along the axis of the uniaxial magnetic anisotropy: one can remove the explicit time dependence from the Hamiltonian with the help of the unitary transformation. Observe that if the polarization of the ac field is not circular, one can drop other (nonresonance) proportional to h terms present in the Hamiltonian, after the unitary transformation, because $h \ll H, \omega/2\pi$.

In the case of, e.g., linear polarization of the ac field, i.e., $h\cos(\omega t) S^{x}_{tot}$, a resonance-antiresonance situation is possible with $\omega/2\pi = \pm H$, usual for the ESR case. However, we shall consider only the resonance with $\omega/2\pi = H$ in detail in what follows. In our work we study the general case, when $\mathcal{H}_{int}$ *has* magnetically anisotropic terms, considering a weak magnetically anisotropic electron-electron interaction as a perturbation.

In the framework of the linear-response theory, the absorption of the ac magnetic field is equal to

$$I(\omega) = \frac{h^2 \omega}{2} \chi''_{aa}(\mathbf{q} = 0, \omega), \tag{2}$$

where $a \perp z$ is the direction of the polarization of the ac field and $\chi''(\mathbf{q}, \omega)$ is the imaginary part of the dynamical magnetic susceptibility. Here we consider the case of $\mathbf{q} = 0$ because the ESR is a local characteristics (usually in the ESR experiments, the wavelength of the ac field is larger than the size of a sample).[10–12] We point out that if the magnetic anisotropy is along the x direction, then $\omega^2 \chi''_{xx}(0,\omega) = 4\pi^2 H^2 \chi''_{yy}(0,\omega)$ [or, if there is an angle ϕ between the axis x and a, one has $\omega^2 \chi''_{aa}(0,\omega) = (4\pi^2 H^2 \cos^2\phi + \omega^2 \sin^2\phi)\chi''_{yy}(0,\omega)$]. The dynamical magnetic susceptibility can be calculated using spin-spin correlation functions of the problem.

III. MAIN RESULTS

To proceed further, let us first diagonalize the noninteracting part of Hamiltonian (1) (for the case $H = h = 0$). The standard unitary transformation yields two bands of collective quasiparticles (which appear due to the hybridization between itinerant and localized electrons) with the dispersion laws

$$2\epsilon^{(1,2)}_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \epsilon_f \pm \sqrt{(\epsilon_{\mathbf{k}} - \epsilon_f)^2 + 4V^2}. \tag{3}$$

Suppose that the $4f$ levels are lying in the lowest band close to the Fermi surface, and, as usual, one has a weak hybridization $V^2 < (\epsilon_{\mathbf{k}} - \epsilon_f)^2$. Besides, we suppose that the number of electrons is close to the half filling. In this case, when all $4f$ shells are almost occupied, each by one electron, the Anderson lattice model is in the situation of the Kondo lattice. In our approach the FL and the NFL behaviors of the model follow from the nesting of some sections of the Fermi surface,[13] which is related to the quantum phase transition (quantum critical point). At low energies, the main contribution to all characteristics of our heavy fermion metal comes from the quasiparticle states in the vicinity of the Fermi surface, i.e., of the lowest band of Eq. (3). The effective model, which we use in the following,[14] describes two pieces of that Fermi surface (e.g., one electron and one hole pocket) of the

studied heavy electron system (with the preformed heavy effective mass of quasiparticles, caused by the hybridization of the localized $4f$ electrons with the conduction ones; see above). Those two pieces are separated by the wave vector $\mathbf{Q}$. The latter is connected with the induced by the RKKY coupling (mostly antiferromagnetic) fluctuations of the order parameter, with the linearized about Fermi-surfaces dispersion laws. As a result, the noninteracting part of the effective low-energy Hamiltonian, responsible for the ESR signal in heavy fermion systems, is supposed to be

$$\mathcal{H}_0 = \sum_{\mathbf{k},\sigma,j=1,2} \varepsilon_j(\mathbf{k}) c^\dagger_{j,\mathbf{k},\sigma} c_{j,\mathbf{k},\sigma}, \tag{4}$$

where $c^\dagger_{j,\mathbf{k},\sigma}$ ($c_{j,\mathbf{k},\sigma}$) are creation (destruction) operators of the low-energy quasiparticle (or quasihole) in the jth pocket; $\varepsilon_1(\mathbf{k}) \approx v_F(k-k_{F1})$; $\varepsilon_2(\mathbf{k}) \approx v_F(k_{F2}-k)$; k is the magnitude of the quasimomentum $\mathbf{k}$, measured from the center of the respective pocket; and $v_F \approx v_F^{(0)} V^2/(\epsilon^F_{\mathbf{k}}-\epsilon_f)^2 \sim v_F^{(0)}(m/m^*) < v_F^{(0)}$, where $v_F^{(0)}$ and $\epsilon^F_{\mathbf{k}}$ are the bare Fermi velocity and the bare energy at the Fermi level of conduction electrons, m is their bare mass, and m^* is the effective mass of quasiparticles. For heavy fermion systems one has $m^* > m$. It is supposed that both of pieces have the same Fermi velocity, while their Fermi quasimomenta, $k_{F,1,2}$, are different. One can speculate that such pieces of the Fermi surface are present in $YbRh_2Si_2$ (see, e.g., the recent *ab initio* calculations).[15,16]

In Refs. 14, 17, and 18, the model was successfully applied for the description of the low-temperature dependencies of the magnetic susceptibility, the specific heat,[14] the resistivity,[17] and the dynamical magnetic susceptibility,[18] respectively, of heavy fermion systems with the NFL behavior, in particular, to $YbRh_2Si_2$. It was supposed that the interactions among electrons inside the same pocket and between pockets essentially determine those dependencies.

In the present work we will address, however, very important specifics of ESR that distinguishes it from the above mentioned experimental methods. We will be interested only in those type of interactions, which reveal the magnetic anisotropy, because the operators of magnetically *isotropic* interactions between electrons commute with the total spin of the system and, hence, *do not contribute* to the shift of the ESR resonance and the linewidth. That is why here we limit ourselves with the only two kinds of interactions between quasiparticles, caused by electron-electron interactions $\mathcal{H}_{int}$ between localized $4f$ electrons:

$$\mathcal{H}_{12} = \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} U_\parallel(\mathbf{Q}) c^\dagger_{1,\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{2,\mathbf{k}'-\mathbf{q},\sigma} c_{1,\mathbf{k},\sigma} c_{2,\mathbf{k}',\sigma} + \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\sigma} U_\perp(\mathbf{Q}) c^\dagger_{1,\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{2,\mathbf{k}'-\mathbf{q},\bar{\sigma}} c_{1,\mathbf{k},\bar{\sigma}} c_{2,\mathbf{k}',\sigma}, \tag{5}$$

where $U_\parallel$ and $U_\perp$ define the constants of electron-electron interactions with the momentum transfer (nesting vector) $\mathbf{Q} \gg \mathbf{q}$ with and without spin flip, respectively. The difference between $U_\parallel$ and $U_\perp$ can be caused by the spin-orbit interaction. It turns out that the spin flip is impossible for a small momentum transfer between pockets.

The renormalization-group analysis ($|\mathbf{Q}|$ is assumed large compared to the quasimomenta of pockets) yields[14,17,18]

$$\tilde{U}_\parallel \pm \tilde{U}_\perp = \frac{(U_{\parallel 0} \pm U_{\perp 0})}{1 + t\rho_F(U_{\parallel 0} \pm U_{\perp 0})}, \tag{6}$$

where overtildes denote the renormalized values of couplings (with respect to the initial values, denoted by the index 0), $\rho_F = (2\pi^2 v_F)^{-1}$ is the total density of states at the Fermi surface, and $t = \ln D/(|\omega| + 2T + \delta)$. Here $D = v_F\Lambda_0$ is the renormalization cutoff, T is the temperature, ω is the frequency of the external field, and the parameter $\delta = v_F(k_{F1}-k_{F2})/2 \pm H$ (here we supposed that the external dc magnetic field of the value H was switched on) determines the nesting mismatch. Due to the mismatch of the Fermi surfaces, the integration in Eq. (6) may proceed, generally speaking, until the vertex diverges or the critical point is reached. The latter is reached at $\delta = \delta_0$ (i.e., at the zero Néel temperature, $T_N = 0$). If $T_N > 0$, there is a transition to a magnetically ordered phase with magnetic moments aligned along the z axis and T_N is the temperature of the phase transition to the magnetically ordered state. On the other hand, if $T_N < 0$, the system remains paramagnetic and the long-range magnetic order cannot develop. The quantum critical point corresponds to the mismatch $\delta_0 \approx D\exp(-1/U\rho_F)$ determined here in the approximation of the Hubbard model (within that model one has $U_\parallel = U_\perp = U$, and they are equal to the values of the electron-electron interactions with the small momentum transfer).[14] Notice, that $U \gg |U_\parallel - U_\perp|$, and in Eq. (6) the denominator does not become zero in our case. The nesting condition implies that $\varepsilon_{2\mathbf{k}-\mathbf{Q}} = -\varepsilon_{1\mathbf{k}} + 2\delta$; hence, at $\delta = 0$ one has the perfect nesting. One can see that the external magnetic field H changes δ and, hence, it can change the behavior of the model, reminiscent to the observations in $YbRh_2Si_2$. We emphasize that the ESR response, studied in our work, is caused, in fact, by the Stoner continuum of collective quasiparticles formed by the hybridization of conduction electrons with the localized $4f$ ones, but *not* by spin waves in a metal. We note also that most of interactions, considered here, are antiferromagnetic ones, which correlates with the AFM order observed in $YbRh_2Si_2$. On the other hand, standard Fermi-liquid interactions, present in heavy fermion systems can also lead to a ferromagnetic contribution to the spectrum, which also may play a role in the ESR characteristics.

The intensity of the ESR signal (or the imaginary part of the magnetic susceptibility) in our approach is determined by the Green's functions of quasiparticles at $\mathbf{q} = 0$. Our calculations of the imaginary part of the dynamical magnetic susceptibility of the effective model are simplified, compared to the general situation,[18] because only the homogeneous case, $\mathbf{q} = 0$, and only transverse components of the magnetic susceptibility, relevant for the ESR, are considered here. The pole of the imaginary part of the homogeneous dynamical magnetic susceptibility determines the resonance frequency and the linewidth, as usual.

A. Non-Fermi-liquid regime

The ESR linewidth Γ in our model is determined by the imaginary part of the self-energy of low-energy quasiparti-

cles, $\Sigma''(\mathbf{k},\omega)$. For our model, at low temperatures it can be given by the FL and the NFL contributions $\Gamma=\Gamma_{\mathrm{FL}}+\Gamma_{\mathrm{NFL}}$. In the second order in the magnetically anisotropic interactions, one obtains[19]

$$\Sigma''(\mathbf{k},\omega)=\int\frac{d\omega'}{2\pi}\left[\coth\left(\frac{\omega'}{2T}\right)-\tanh\left(\frac{\omega'-\omega}{2T}\right)\right]\times\int\frac{d^3q}{(2\pi)^3}\chi_s''(\mathbf{q},\omega')G''(\mathbf{k}-\mathbf{q},\omega'-\omega)(\tilde{U}_{\parallel}-\tilde{U}_{\perp}). \tag{7}$$

Here G'' and χ_s'' are the imaginary part of the Green's function and the staggered susceptibility, respectively. For the perfect nesting of the Fermi surfaces, at $\delta=0$, the main (NFL) contribution comes from $\mathbf{q}\approx\mathbf{Q}$. For that case the integration over $\mathbf{q}$ is performed over the Green's function and yields the density of states. In this approximation the main part of the staggered susceptibility can be written as

$$\chi_s''(\mathbf{Q},\omega)\approx\mathrm{Im}\ \psi\left(\frac{1}{2}+\frac{\Gamma_{\mathrm{NFL}}}{2\pi T}+i\frac{\omega}{4\pi T}\right), \tag{8}$$

where $\psi(x)$ is the digamma function. At low energies and for the imperfect nesting ($\delta\neq 0$) the staggered susceptibility has a gap. The dominant contribution to the staggered susceptibility corresponds to points $\tilde{\mathbf{Q}}$ on a sphere of radius $2\delta_0$ centered about $\mathbf{Q}$. In this approximation, one can write[13,17]

$$\chi_s''(\tilde{\mathbf{Q}},\omega)\approx\frac{\rho_F}{2}\mathrm{Im}[\psi_+ + \psi_-], \tag{9}$$

where

$$\psi_{\pm}(\omega)=\psi\left(\frac{1}{2}+\frac{\Gamma_{\mathrm{NFL}}}{2\pi T}+i\frac{\omega}{2\pi T}\pm i\frac{\delta-\delta_0}{2\pi T}\right). \tag{10}$$

The case $\delta=\delta_0$ of the perfect nesting corresponds to the gapless quantum critical point.

Then the NFL contribution to the ESR linewidth can be found from the equation

$$\Gamma_{\mathrm{NFL}}=\frac{\rho_F^2}{8}\int d\omega'\left[\coth\left(\frac{\omega'}{2T}\right)-\tanh\left(\frac{\omega'-\omega}{2T}\right)\right](\tilde{U}_{\parallel}-\tilde{U}_{\perp})\mathrm{Im}[\psi_+(\omega')+\psi_-(\omega')], \tag{11}$$

where for dressed vertices the analytical continuation was used, $t\rightarrow t+i\pi/2$. In the ground state, the NFL contribution vanishes for $|\omega|<2(\delta-\delta_0)$. For larger frequencies it is proportional to $|\omega|-2(\delta-\delta_0)$. For perfectly nested Fermi surfaces, the solution of Eq. (11) yields

$$\Gamma_{\mathrm{NFL}}=\alpha\rho_F^2(\tilde{U}_{\parallel}-\tilde{U}_{\perp})^2\max(|\omega|,\beta T), \tag{12}$$

where α and β are factors on the order of 1.

The change in the value of the effective g factor can be written as

$$g=\left(1+\frac{\delta\omega(T,\omega)}{H}\right). \tag{13}$$

[For the situation with the angle θ between the direction of the distinguished axis of the heavy fermion system and the direction of the applied ac magnetic field H, $\delta\omega$ has to be multiplied by a function of θ; the latter in the simplest case can be written, e.g., as $f(\theta)=1-3\cos^2\theta$.] So as to remind for the ESR situation, one is interested in the response with zero quasimomentum (see Sec. II). Then, Kramers-Kronig relations

$$\Sigma'(\omega,T)=\Sigma'(\infty,T)+\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}d\omega'\frac{\Sigma''(\omega',T)}{\omega'-\omega} \tag{14}$$

imply the connection between the lifetime (linewidth of the ESR) and the change in the energy of quasiparticles [notice that $\Sigma'(\infty,0)$ is related to the shift of the chemical potential due to interactions in the ground state]. The energy change in quasiparticles is obviously related to the temperature and the frequency dependencies of the shift of the resonance position under the conditions of the ESR in the NFL region,

$$\delta\omega(T,\omega)=\mathrm{const}-\frac{2\alpha\rho_F^2\omega}{\pi}(\tilde{U}_{\parallel}-\tilde{U}_{\perp})^2\ln\frac{D}{\max(|\omega|,\beta T)}. \tag{15}$$

We can see that according to the model the shift of the g factor due to the NFL contribution for $T\ll\omega$ is proportional to the logarithm of the temperature,

$$\delta g(T)\sim 4\alpha\rho_F^2(\tilde{U}_{\parallel}-\tilde{U}_{\perp})^2\ln(\beta T). \tag{16}$$

For $\omega\gg T$, it is proportional to the logarithm of the applied field H (so as to remind, in the ESR experiments one has the condition $\omega/2\pi=H$).

B. Fermi-liquid regime

The FL contribution to the linewidth arises from the imaginary part of the staggered susceptibility for values of $\mathbf{q}$ different from $\mathbf{Q}$. The nesting does not play any role for that situation. Using the standard calculations, we get

$$\Gamma_{\mathrm{FL}}=\frac{\pi\rho_F^3}{8}[\omega^2+(\pi T)^2](U_{\parallel}-U_{\perp})^2. \tag{17}$$

Kramers-Kronig relations imply that in the FL regime the shift of the resonance frequency in the ground state and consequently the g shift has to be proportional to

$$\delta\omega\sim\mathrm{const}-\rho_F^2\omega(U_{\parallel}-U_{\perp})^2a(T^2)+b(T^2)\omega^3+\cdots, \tag{18}$$

where a and b are functions of T^2. Hence, the FL contribution to the shift of the ESR position roughly does not depend on temperature, compared to the NFL part. It is also important to point out that ferromagnetic magnetically anisotropic Fermi-liquidlike interactions, not only of type (5), present in the system, according to our theory will *reduce* the linewidth of the ESR in heavy fermion metals in a way similar to Eq.

(17) with $|U_{\parallel}-U_{\perp}|$ added by the magnetically anisotropic part of the ferromagnetic Fermi-liquid interactions (without nesting).

It turns out that the FL contribution is smaller than the NFL one, because it is proportional to $(U_{\parallel}-U_{\perp})$, but not to the renormalized value of the anisotropic coupling, as the NFL term. Also it is $\rho_F T$ (or $\rho_F \omega$) times smaller than the NFL contribution. However, the NFL correction exists only for the above mentioned conditions of nesting, while the FL part is present for all interactions. At the quantum critical point Γ_{NFL} dominates. On the other hand, for $\delta > \delta_0$, the NFL contribution is suppressed.

C. Special role of anisotropy for ESR

We emphasize that in the considered model similar mechanisms are responsible for the logarithmic temperature behavior of the specific heat, the magnetic susceptibility, and the resistivity, on one hand, and the shift of the ESR resonance frequency and the linewidth, on the other hand. However, the energy scales for the ESR and for thermodynamic and kinetic characteristics are different. For the ESR, all renormalizations are connected with the magnetic anisotropy of electron-electron interactions $(U_{\parallel}-U_{\perp})$. That is why the energy scale of the ESR shift and linewidth are much smaller than the energy scales for the specific heat and resistivity, which are determined by $U \propto U_{\parallel} \sim U_{\perp} \gg |U_{\parallel}-U_{\perp}|$, while their temperature dependencies are similar. On the other hand, as we have shown above, the magnetically isotropic part of the Hamiltonian of electron-electron interactions $\mathcal{H}_{int}$ exactly commutes with the projections of the total spin of the system and, therefore, cannot affect the position of the ESR and its linewidth, similar to the situation with the ESR in metals with Kondo impurities.[9] Therefore, possible influence of the magnetically isotropic part of electron-electron interactions in the framework of our and similar schemes of calculations would be the artifact of the approach. It also turns out that in this work, we calculated only the influence of electron-electron interactions on the linewidth of the ESR in heavy fermion metals. Obviously, their contribution has to be added by the electron-lattice and electron-nuclear relaxation parts.

D. Other consequences of the theory

The upper branch of quasiparticles (3) is separated from the lower one by the (perhaps indirect) gap

$$\Delta = \epsilon_{\mathbf{k}}^{min} - \epsilon_{\mathbf{k}}^{max} + \sqrt{(\epsilon_f - \epsilon_{\mathbf{k}}^{max})^2 + 4V^2} + \sqrt{(\epsilon_f - \epsilon_{\mathbf{k}}^{min})^2 + 4V^2}, \tag{19}$$

where $\epsilon_{\mathbf{k}}^{min}$ ($\epsilon_{\mathbf{k}}^{max}$) is the minimum (maximum) of the energy of bare conduction electrons. Notice that the external dc magnetic field splits the energy levels, and the lower-energy magnetic field-induced part effectively reduces the value of the gap as $\Delta(H) \approx \Delta(0) - H$. Those gapped electron excitations, together with the separated from the lowest orbital doublet of localized $4f$ electrons contributions of the higher orbital states, can produce an exponential in T contribution in the linewidth of the ESR, $\sim [e^{A/T}-1]^{-1}$, where A is proportional to Δ or C (which is the value of the crystalline electric field, separating the lowest orbital doublet from higher orbital states), in heavy fermion metals at high-enough temperatures (on the order of Δ or C).

The generalization of the proposed theory for the case of different g factors of localized $4f$ and conduction electrons is straightforward. The main difference with the case considered above appears to be in the onset of two different signals (but related to each other via hybridization) of ESR for localized and itinerant electrons. They manifest themselves theoretically in two poles of the Green's functions of quasiparticles, which determine the homogeneous dynamical magnetic susceptibility of the heavy fermion system and, hence, the absorption of the ESR rf field. The behavior of the shifts of the resonance fields and linewidths of the respective resonance modes could be related via the "bottlenecklike" effect.

IV. COMPARISON WITH EXPERIMENTS

Let us now discuss our theoretical results, comparing them with the recently observed ESR characteristics in the heavy fermion metal $YbRh_2Si_2$.[6,7] This clean stoichiometric intermetallic compound has attracted a great attention owing to its reach electronic phase diagram.[20–24] In the heavy fermion state, depending on temperature and magnetic field, one finds an antiferromagnetically ordered phase adjacent to a quantum critical point, as well as regions of FL and NFL behaviors. Specifically, there, FL and NFL regimes have been identified in the temperature and the magnetic field dependencies of the electronic specific heat, the resistivity,[20] as well as the ^{29}Si-nuclear-magnetic-resonance (NMR) relaxation rates and the Knight shift.[21]

The ESR experiments in $YbRh_2Si_2$ manifest the following features. The strong anisotropy of the ESR response corresponds to the magnetic anisotropy of this compound, which agrees with our theory. The experiment[6] observed a negative shift in the effective g factor, related by the authors to the antiferromagnetic electron-electron coupling. Distinct regimes with different temperature dependencies of the effective g factor and the linewidth ΔH in the temperature range $\sim 2-25$ K were observed in the field range $\mu_0 H \sim 0.2-8$ T.[6,7] For all studied fields, the effective g factor varies with temperature approximately as $\ln(T)$, whereas the magnitude of this variation decreases with increasing H. Remarkably, in the field range $\sim 5-6$ T, the $g(T)$ dependence levels off below $\sim 4-5$ K. For the same fields, one observes a crossover in the temperature dependence of $\Delta H(T)$ from a T^2-like at $T \lesssim 7-8$ K to the linear in T dependence plus an additional exponential term $[\exp(A/T)-1]^{-1}$ that becomes relevant in the high-temperature regime (see below).[6,7]

The above temperature crossovers of the ESR g factor and the linewidth ΔH can be straightforwardly explained in our theory as a manifestation of the crossover between the NFL and the FL regimes in $YbRh_2Si_2$. The NFL regime is characterized by the $\ln(T)$ shift of the g factor [Eq. (16)] and the linear in T dependence of ΔH [Eq. (12)], whereas the $g \approx$ const [Eq. (18)] and the $\Delta H \sim T^2$ [Eq. (17)] behaviors are predicted for the FL regime. It is interesting to note that the behavior of the Sommerfeld coefficient of the specific heat is

also proportional to ln T in the NFL regime, and it manifests the crossover at similar temperatures to the FL regime,[20] like the observed shift of the ESR position, but with a different energy scale.[6,7] On the other hand, the crossover from the linear in T behavior in the NFL regime to T^2 in the FL one was observed in the behavior of the ^{29}Si NMR relaxation rate[21] and resistivity (though at lower temperatures for the latter),[20] also with a different energy scale, compared to that observed in the ESR linewidth.[6,7] According to the previous theoretical results,[14,17] the Sommerfeld coefficient of the specific heat and the resistivity in a heavy fermion metal are also determined by the real and the imaginary parts of the self-energy of quasiparticles, like the shift of the position and the linewidth of the ESR. However, as we have shown in Sec. III C, the energy scales for the ESR characteristics are determined by the magnetically anisotropic part of interactions between quasiparticles only and, thus, are much smaller than those of the Sommerfeld coefficient and resistivity, which are determined by all interactions including isotropic ones. This theoretical finding is crucial for the explanation of the occurrence in the heavy fermion state of $YbRh_2Si_2$ of a well-defined narrow ESR mode that manifests the energy scale much smaller compared to the total scale of electron-electron interactions.

One should also note that in $YbRh_2Si_2$, together with the crossover from the FL to the NFL states, an additional crossover was observed,[24] probably related with the change in the volume of the Fermi surface from a smaller to a larger value. It implies the presence of additional (with respect to ones taken into account in our theory) large pieces of the Fermi surface. However, there is no nesting for those large pieces of the Fermi surface and, hence, the contribution from them to the ESR characteristics is of the FL type only and renormalizes the coefficients in Eq. (17), affecting the linewidth and the shift of the ESR position in the FL regime. This fact implies that the ESR phenomenon in $YbRh_2Si_2$ can be more complicated than our simplified description. As we discussed in Sec. III B, ferromagnetic correlations between quasiparticles, which can follow from the standard Fermi-liquid interactions can also play an important role in the ESR in that heavy fermion metal.

Finally, we remark on the exponential contribution to the linewidth of the form $[\exp(A/T)-1]^{-1}$ observed in $YbRh_2Si_2$ at higher temperatures and assigned to a relaxation channel via an excited state of Yb^{3+} at the crystal-field (CF) energy C above the ground state.[6,7] The parameter A was significantly reduced down to $\sim 50-60$ K for large resonance fields (Ref. 7) compared to the value of ~ 115 K at small resonance fields (Ref. 6). Since from the neutron scattering the CF energy C was found to be much higher ($C \sim 200$ K),[25] we can suppose that the interaction with the upper band of quasiparticle excitations, calculated in our theory [see Eq. (19)], can play a major role in the high-T relaxation process, which also agrees with the reduction in the value of A with the growth of the resonance magnetic field.

V. COMPARISON WITH OTHER THEORIES

After this study had been finished, we became aware of the recent theoretical works,[26,27] devoted to the problem of the ESR in a Kondo lattice. In the work in Ref. 26, the responses of the Anderson impurity and the Anderson lattice models to the ac magnetic field were studied. On the other hand, Ref. 27 considers the ESR in the Kondo impurity and the Kondo lattice models. Anderson and Kondo models are related to each other: the Kondo situation appears at the value of the chemical potential (for lattice models) or the energy of the impurity site (for impurity models), at which the fillings of the localized orbitals are close to 1, i.e., only one electron (or one hole) is situated there. In this case the localized orbital is in the magnetic state. From this viewpoint, Refs. 26 and 27 and our work study similar situations. In Ref. 26, as in our work, the authors considered the ESR as the response to the collective excitations, i.e., quasiparticles, which appear due to the hybridization of the f-electron (localized) levels with the conduction electrons. The interaction between quasiparticles was taken into account in Ref. 26 in the framework of the Fermi-liquid-like approach, while in Ref. 27 it was calculated in the second order in the f-c exchange coupling.

For impurity models (not studied in our work) both theories[26,27] predict a broad ESR line, on the order of the Kondo temperature. In Ref. 26, the narrow line of the ESR resonance of the Anderson lattice model is the consequence of the hybridization between localized and conduction electrons (narrow band) and possible ferromagnetic fluctuations, which can appear in the Fermi-liquid approach. In Ref. 27, on the other hand, a similar narrow ESR line is also the consequence of the possible nonlocal ferromagnetic interactions between localized spins of the Kondo lattice model.

One of the main differences between our approach and that of Refs. 26 and 27 is related to the fact that in our study we consider the situation with the same g factors of localized and itinerant electrons. In that sense our theory and those in Refs. 26 and 27 are complimentary to each other. The shift of the ESR resonance field and the linewidth in our work are related to the magnetic anisotropy of electron-electron interactions together with the effect of the narrow band of quasiparticles due to the hybridization of conduction electrons with the localized ones. The smallness of the magnetic anisotropy determines in our theory the narrow line of the ESR response. On the other hand, the results of Refs. 26 and 27 correspond to the case of different g factors of conduction and localized electrons and magnetically isotropic Fermi-liquid interactions between electrons.

Also, the calculations in Refs. 26 and 27 were performed for the Fermi-liquid situation only, while our theory describes both the Fermi-liquid and the non-Fermi-liquid cases. Our study presents the results for the temperature and the magnetic field dependences of the shifts and linewidth broadenings of the ESR in the non-Fermi-liquid and the Fermi-liquid regimes. On the other hand, Refs. 26 and 27 present the results for the temperature dependence of the linewidth only in the Fermi-liquid regime.

VI. CONCLUSIONS

Summarizing, we have developed in the framework of the Anderson lattice model the low-temperature theory of the

ESR for heavy fermion metallic systems with magnetically anisotropic electron-electron interactions. We have shown that, for the same values of the g factor of localized and itinerant electrons in the absence of the magnetic anisotropy, the ESR signal has a δ-function shape if one does not take into account electron-lattice or electron-nuclear couplings. We note that the theory enables a straightforward generalization to the case of different g factors. We have shown that the magnetically anisotropic electron-electron interactions of localized electrons, together with the hybridization between wave functions of itinerant and localized electrons, can yield a shift of the position of the ESR signal and can change its linewidth. These changes of the characteristics of the ESR are connected with the interactions of low-energy quasiparticles (Stoner continuum) of the heavy fermion system. We have shown that there can be a Fermi-liquid contribution to the linewidth and the shift of the position of the ESR signal (effective g factor) and a non-Fermi-liquid one. These contributions are characterized by a much smaller energy scale compared to the total scale of electron-electron interactions that enables a narrow ESR mode to occur in a heavy fermion metal. Their relative values are governed by the quantum critical point of the phase transition to the magnetically ordered phase. We compare our results with recent ESR experiments on the $YbRh_2Si_2$ heavy fermion compound. In particular, our theory agrees with the quadratic in temperature change of the ESR linewidth and the almost T-independent g factor at low temperatures, where the FL behavior was observed. Our theory explains the crossover at higher temperatures to the logarithmic in T regime for the g shift and the linear in T dependence of the linewidth at higher temperatures, where the NFL regime takes place. Finally, for higher temperatures our theory agrees with the exponential in T behavior of the linewidth, whose exponent reduces with the value of the external magnetic field, as observed in the experiment.

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