

The tunnelling current in heavy-fermion systems

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1993 J. Phys.: Condens. Matter 5 6189

(<http://iopscience.iop.org/0953-8984/5/34/007>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 11/05/2010 at 01:39

Please note that [terms and conditions apply](#).

The tunnelling current in heavy-fermion systems

Yu Kagan and N V Prokof'ev†

'Kurchatov Institute' Russian Science Centre, Moscow 123182, Russia

Received 18 January 1993

Abstract. The role of *f*-electron charge fluctuations in heavy-fermion systems is discussed, and the tunnelling current as a probe of charge spectral density near the Fermi level is calculated within perturbation theory using the transfer Hamiltonian approach. It is shown that in the case of integer valence systems only *c* electrons from a wide conduction band contribute to the tunnelling current. One finds only a weak reflection of the strong mass enhancement in the $I(U)$ curves, but the tunnelling conductance (and its derivative) can still be used for the study of spin excitations in the liquid formed by *f* spins. An examination is then made of the mixed-valence-type heavy-fermion compounds. In this case *f* electrons dominate in the current, and in some regimes the exact results for the arbitrary Coulomb interaction between the *c* and *f* electrons are derived. It is shown that because of the 'shaking up' of the polaron cloud around the *f* electron during the tunnelling process the current acquires a non-analytic dependence on electric potential and temperature. Both narrow *f*-band and *c*-*f* hybridization peaks are studied in detail.

1. Introduction

The question of whether charge or spin degrees of freedom dominate in the heavy-fermion (HF) ground state seems to be of primary importance in understanding the nature of HF systems. In this connection tunnelling properties of these systems, which are governed by tunnelling transitions of charged particles, might be very interesting.

Universal behaviour of the HF systems, which can be characterized by a single energy parameter T_K , makes one think about the common nature of these systems (see, for example, [1, 2]). However, even a brief analysis reveals two classes of HF systems with quite different microscopic properties. The first class is characterized by nearly integer valence of the *f* ion, the deep position of the *f* level and strong on-site Coulomb repulsion. Ce-based compounds are the typical examples. It is generally believed that these systems are adequately described by the Kondo-lattice Hamiltonian considered as the limiting version of the periodic Anderson model. One can expect that electrons from the deep *f* shell will give negligible contribution to the tunnelling current at small voltages $|U| \ll \epsilon_F - \epsilon^f$. In this case the current is defined by the tunnelling of electrons from the wide conduction band which, itself, is strongly renormalized by inelastic scattering on the spin sub-system. In [3, 4] the idea was proposed to ascribe the low-frequency HF peak in the density of states to neutral excitations of the spin liquid. Low-temperature excitations in this liquid obey the Fermi statistics and carry no charge. In its turn, the interaction between the conduction electrons and spin liquid results in a strong electron mass enhancement, $m_c^* \gg m_B$ (where

† Present address: Physics Department, University of British Columbia, 6224 Agricultural RD, Vancouver BC, Canada V6T 1Z1.

m_B is the bare band mass) which, however, in the general case is smaller than the effective mass, m_H , characterizing the low-temperature thermodynamics of HF systems.

Below, we show that large enhancement of the conduction band density of states at energies $\epsilon < T_K$ is only slightly reflected in the structure of the tunnelling current. This important result should be compared with mean-field theory (see, for example, [5, 6]), which predicts a noticeable contribution of f electrons to the current with strong dependence $I(U)$ at small U . As discussed in [3] we believe that the appearance of the f -electron charge near the Fermi energy in this case is connected with the artificial charge transfer to the spin degrees of freedom. Nevertheless, the derivatives of the current over voltage are directly related to the spectral density of spin excitations. In fact, one can use this possibility for studying the low-temperature properties of the spin liquid.

An itinerant (mixed-valence) type of f -electron excitations is characteristic of the case with the f level close to the Fermi energy. The formation of the HF state could then be connected with the f -electron charge degrees of freedom. An extremely narrow peak (10 K) in the density of states could result from a strong electron (and phonon) polaron effect due to the Coulomb interaction between the f electrons in a moderately narrow band and the conduction electrons in a wide band. The same effect of polaron narrowing is found for the conventional hybridization Hamiltonian [7, 8]. In both cases the f electrons may give the dominant contribution to the tunnelling current. One can clearly reveal polaron renormalizations in the non-trivial current-voltage curves which appear to be the result of 'shaking up' the polaron cloud around the f electron during the tunnelling. The important thing is that $I(U)$ (or dI/dU) reflects the existence of the HF peak in the density of states. Thus, the tunnelling current behaves quite differently in the Kondo-lattice and mixed-valence regimes, and can be used for the comparative analysis between HF systems with the goal to reveal the role of charge fluctuations in formation of the HF state.

2. Tunnelling current in the integer valence case (Kondo lattice)

Let us consider the tunnelling between the HF and usual metal. We assume an idealized picture, implying unperturbed electronic properties of both metals up to the boundary of the barrier, which could be either a vacuum separation or a dielectric layer. In this case the current can be calculated within the lowest-order perturbation theory using the transfer Hamiltonian approach:

$$H_T = \sum_{k\sigma} T_{kk'} (c_{k'\sigma}^\dagger a_{k\sigma} + a_{k'\sigma}^\dagger c_{k\sigma}). \quad (1)$$

Here $T_{kk'}$ is the tunnelling matrix element, $c_{k\sigma}$ and $a_{k\sigma}$ are the electron annihilation operators in HF and usual metals respectively. Within the framework of perturbation theory in the tunnelling amplitude the general expression for the tunnelling current has the form [9]

$$I = 4\pi e \sum_{pp'} |T_{pp'}|^2 \int d\omega d\omega' \delta(\omega + U - \omega') (n_\omega - n_{\omega'}) A_c(\mathbf{p}, \omega) A_a(\mathbf{p}', \omega') \quad (2)$$

where

$$A_i(\mathbf{p}, \omega) = -\frac{1}{\pi} \text{Im} G_i^R(\mathbf{p}, \omega) \quad i = a, c. \quad (3)$$

Here $G_c^R(\mathbf{p}, \omega)$ is the retarded Green function, the indexes c, a are related to the HF and usual metals, and n_ω is the Fermi distribution function. Coulomb blockade effects in tunnelling between the HF and normal metal are ignored in this paper assuming not too small a size for the tunnel junction.

Suppose, that the density of states in the metal a is a weak function of energy near the Fermi level with small electron-phonon renormalizations. Then the function $A_a(\mathbf{p}', \omega')$ can be written in the form

$$A_a(\mathbf{p}', \omega') \approx \delta(\omega' - \epsilon_{\mathbf{p}'})$$

at least in the small frequency range characteristic of the HF metal. Substituting this expression into (2) we find

$$I = 4\pi e \sum_{\mathbf{p}\mathbf{p}'} |T_{\mathbf{p}\mathbf{p}'}|^2 \int d\omega \delta(\omega + U - \epsilon_{\mathbf{p}'}) (n_\omega - n_{\omega+U}) A_c(\mathbf{p}, \omega). \quad (4)$$

It is essential that the answer depends only on the one-particle Green function. This is an obvious simplification as compared with the usual conductivity, which must be calculated from the two-particle Green function.

In this section we consider HF systems with the f level deep enough under the Fermi energy. If we assume as well the on-site Hubbard repulsion between f electrons to be much larger than $\epsilon_F - \epsilon^f$, we then come to the typical limiting case of the periodic Anderson model usually described by the Kondo-lattice Hamiltonian:

$$H = H_B + H_{\text{int}} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma} + J \sum_i \sigma_i S_i \quad (5)$$

where $\sigma_i = c_{i\sigma}^+ \sigma c_{i\sigma}$ is the conduction electron spin operator at the site i , σ is the Pauli matrix, and S_i is the f -electron spin operator. The interaction term in the Hamiltonian (5) corresponds to the spin exchange between the wide-band electrons and the localized f shell. This Hamiltonian results in an indirect interaction between the spins, the local Kondo-renormalization of the spin exchange etc. These interactions connected with the virtual high-frequency excitations in the wide band lead to the adiabatic spectrum of spin excitations in the narrow energy interval of order of T_K . In close analogy with the well known problem of deriving the adiabatic phonon spectrum in metals [10] one can neglect afterwards all non-adiabatic corrections to the spectrum of spin excitations. Bearing this fact in mind we can write down the effective low-frequency Hamiltonian in a form corresponding to the two-component Fermi liquid:

$$H = H_B + H_{\text{SL}} + H_{\text{int}} \quad (6)$$

where H_{SL} is the spin liquid Hamiltonian, and H_{int} contains only the low-energy part of the interaction (in the general case with another exchange coupling \bar{J}). Below, we assume a weak exchange interaction, $\rho_c \bar{J} \ll 1$, where ρ_c is the c -electron density of states on the Fermi surface. In this case we can neglect vertex renormalization in H_{int} .

For the Kondo-lattice Hamiltonian the tunnelling current is entirely defined by conduction electrons renormalized through their interaction with the spin liquid. To find the Green function $G_c^R(\mathbf{p}, \omega)$ we have to evaluate its self-energy part, which to the lowest order in $\rho_c \bar{J}$ is described by the diagram

$$\Sigma_n(\mathbf{p}) = \bar{J}^2 T \sum_m \int \frac{d\mathbf{p}'}{(2\pi)^3} \frac{\Pi(\mathbf{p} - \mathbf{p}', \omega_m)}{i\epsilon_{n-m} - \xi_{\mathbf{p}'} - \Sigma_{n-m}(\mathbf{p}')} \quad (7)$$

Here $\epsilon_n = \pi T(2n + 1)$ and $\omega_m = 2\pi Tm$ are the Matsubara frequencies, and $\xi_p = \epsilon_p - \mu$ is the energy of the electron excitations. In the general case the spin liquid polarization operator has the form

$$\Pi(\mathbf{q}, \omega_m) = \int_0^\infty dE P(\mathbf{q}, E) \frac{2E}{\omega_m^2 + E^2}. \quad (8)$$

The spectral density $P(E)$ is the internal characteristic of the spin liquid. If excitations in this liquid are fermions, then

$$P(\mathbf{q}, E) = \sum_{kk'} (n_k - n_{k'}) \delta(E_k - E_{k'} - E) \delta_{\mathbf{k}+\mathbf{q}, \mathbf{k}'}. \quad (9)$$

We are interested in the renormalization of the electron spectrum at energies and temperatures within the interval $\sim T_S$. In this case the integration over small ξ gives the main contribution to the self-energy part, therefore one can integrate separately over the energy $\xi_{p'}$ and the momentum direction \mathbf{p}'/p' on the Fermi surface. Neglecting the contributions of order of $(\rho_c \bar{J})^2$ and T_S/W (where $W \sim \epsilon_F$ is the electron bandwidth) one has the universal expression for the self-energy part

$$\Sigma_n = -i\pi \rho_c \bar{J}^2 T \sum_{m=-n}^n \Pi_m \quad (10)$$

$$\Pi_m = \langle \Pi(\mathbf{p} - \mathbf{p}', \omega_m) \rangle \quad (11)$$

where $\langle \dots \rangle$ stands for the average over the angle between the vectors \mathbf{p} and \mathbf{p}' on the Fermi surface. The sum over m from $2E/(\omega^2 + E^2)$ in (8) is a standard one (see [11]). Thus we get

$$\Sigma_n = -\rho_c \bar{J}^2 \int dE P(E) \left(i\pi \coth \frac{E}{2T} + \Psi \left(\frac{1}{2} + \frac{\epsilon_n - iE}{2\pi T} \right) - \Psi \left(\frac{1}{2} + \frac{\epsilon_n + iE}{2\pi T} \right) \right) \text{sgn}(n) \quad (12)$$

where Ψ is the logarithmic derivative of the Γ -function. To find the retarded Green function which is analytic in the upper half-plane we make use of the analytic properties of the Ψ function and simply replace ϵ_n in this expression with $-i\omega$.

We now return to (4) and complete the averaging over the momenta \mathbf{p} and \mathbf{p}' on the Fermi surface, making use of the fact that the self-energy part is independent of \mathbf{p} . Then

$$I = 4\pi e \int d\omega (n_\omega - n_{\omega+U}) \int d\xi T^2(\xi, \omega + U) \rho_c(\xi) \rho_a(\omega + U) A_c(\xi, \omega). \quad (13)$$

Here $T^2(\xi, \xi')$ is the averaged value of the tunnelling matrix element modulus, squared. Assuming a weak non-singular dependence of $T^2 \rho_c \rho_a$ on ξ and ξ' for small arguments, we can restrict ourselves by linear expansion:

$$T^2(\xi, \xi') \rho_c(\xi) \rho_a(\xi') = t^2 (1 + \alpha \xi + \beta \xi'). \quad (14)$$

Usually the coefficients α and β reflect the exponential dependence of the tunnelling amplitude on the electron energy [12]. Substituting this expansion back into (13), and using the fact that the A_c function has a sharp peak at $\xi \approx \omega$, we find

$$I = 4\pi e t^2 \int d\omega (n_\omega - n_{\omega+U}) \rho_\omega \quad (15)$$

$$\rho_\omega = 1 + \alpha(\omega - \text{Re} \Sigma_\omega^R) + \beta(\omega + U) + \gamma \text{Im} \Sigma_\omega^R. \quad (16)$$

The last term arises from the difference between the $\text{Im } G^R$ and the real δ function. Note that there is no special smallness in γ with respect to the coefficients α and β .

In the absence of electron renormalization the expression for the current takes the form

$$I = 4\pi e t^2 U [1 - \frac{1}{2}(\alpha - \beta)U]. \tag{17}$$

Taking into account that α , β and γ are of the order of $1/W$ (or S/W , where S is the tunnelling exponent) we find that correction to the zero-order expression is small if the scale of the electron spectrum renormalization is small compared with the bandwidth. However, one can easily extract this correction

$$\Delta I = 4\pi e t^2 \int d\omega (n_\omega - n_{\omega+U})(-\alpha \text{Re } \Sigma_\omega^R + \gamma \text{Im } \Sigma_\omega^R) \tag{18}$$

experimentally because its dispersion is concentrated in the region of very small electric potential $U \sim T_K$. Thus, all information about the interaction can be obtained by measuring the conductance, $\sigma(U) = dI/dU$ and its derivative, d^2I/d^2U . The essential fact is that studying odd, σ_o , and even, σ_e , conductances we can separate the contributions from real and imaginary self-energy parts. In particular, at $T \rightarrow 0$ the conductance takes a very simple form

$$\sigma(T \rightarrow 0) = 4\pi e t^2 (-\alpha \text{Re } \Sigma_U^R + \gamma \text{Im } \Sigma_U^R). \tag{19}$$

From (12) we have

$$\text{Re } \Sigma_U^R = -\rho_c \bar{J}^2 \int dE P(E) \ln \left| \frac{E+U}{E-U} \right|. \tag{20}$$

In the limit $U \ll T_K$

$$\text{Re } \Sigma_U^R = -\lambda U \quad \lambda = 2\rho_c \bar{J}^2 \int dE P(E)/E. \tag{21}$$

In the opposite limiting case $U \gg T_K$

$$\text{Re } \Sigma_U^R = -2\rho_c \bar{J}^2 \int dE EP(E) \frac{1}{U}. \tag{22}$$

The expression (21) defines the electron mass renormalization

$$m_c^* = m_B(1 + \lambda). \tag{23}$$

According to the analysis made in [4] the effective coupling constant is large $\lambda \sim \rho_c \bar{J}^2 / T_K \gg 1$. It follows from (19) and (20) that the study of odd conductance makes it possible to determine only the energy scale for spin excitations, T_K . Note that strong mass renormalization leading to the sharp increase of the electron density of states near the Fermi level is reflected in the tunnelling current only as a small perturbation. The reason is that, with the self-energy part depending only on frequency, there is a strict cancellation between the density of states renormalization and the Z factor of the Green function. This result is well known, for example, in the case of the electron-phonon interaction.

Measuring the even conductance, σ_e , we directly obtain the behaviour of the spin liquid spectral function $P(E)$. Indeed, the general expression for the imaginary part of the self-energy (12) at the real axis and arbitrary temperature has the form

$$\text{Im } \Sigma_U^R = -\pi \rho_c \bar{J}^2 \int dE P(E) (2N_E + n_{E+U} + n_{E-U}) \quad (24)$$

where N_E is the Bose distribution function. In the limit $T \rightarrow 0$

$$\text{Im } \Sigma_U^R = -\pi \rho_c \bar{J}^2 \int_0^U dE P(E) \quad (25)$$

and

$$\frac{d\sigma_e}{dU} = -4\pi e t^2 \gamma \pi \rho_c \bar{J}^2 P(U). \quad (26)$$

This result is very important because it allows us to investigate experimentally the character of the spin liquid excitations at low temperatures and their evolution with the increase of energy in the interval of order T_K .

If HF at $E \ll T_K$ are the neutral Fermi excitations above the spin liquid ground state then the spectral function according to (9) behaves as

$$P(E) \sim E. \quad (27)$$

On the other hand, at high enough energies $E \sim T_K$ (or $T \sim T_K$) there is a tendency toward the appearance of independent localized spin excitations, and the $P(E)$ dependence must change. Apparently, the Fermi statistics is only a limiting property of the spin liquid at $E \rightarrow 0$, and one can expect a very early deviation from the linear dependence (27). As a possible scenario, another low-temperature scale characterizing this crossover sets in, $T_{\text{coh}} \ll T_K$. One can define T_{coh} as the temperature where the quadratic dependence of the resistivity $\rho \sim T^2$ breaks down. In many cases the quadratic law is replaced by the linear dependence $\rho \sim T$ which takes place in a relatively wide temperature interval $T_{\text{coh}} < T < T_K$. Taking into account the fact that in the same temperature region the specific heat is still a linear function of T , and the magnetic susceptibility is almost independent of T , the idea of describing the spin excitations as a set of two-level systems with the constant distribution function over energy splittings seems to be very attractive. Indeed, in this case $P(E) \sim \tanh(E/2T)$, and we get both the linear temperature dependence of the specific heat and resistivity and a very weak (as $\ln(T)$) temperature dependence of the magnetic susceptibility. Note that in the general case the same kind of behaviour results from the rather arbitrary condition

$$P(E) \sim f(E/2T) \quad (28)$$

(at $T \rightarrow 0$ this relation takes the form $P(E) = P_0 = \text{constant}$). Such a behaviour of the spectral function is reflected in the law $\sigma_e(U) \sim |U|$ for the tunnelling conductance in the region of intermediate U , and in the marginal behaviour of the self-energy part (see (20))

$$\text{Re } \Sigma_\omega^R = -\rho_c \bar{J}^2 P_0 \omega \ln(\omega) \quad T_{\text{coh}} < \omega < T_K. \quad (29)$$

This kind of behaviour could be realized if the system of quasi-independent spins with lower temperature transforms into the spin liquid with relaxation times of the effective

'molecular field' much longer than $1/T_K$. The latter could result from the long-range character of the indirect interactions between the spins ($\sim 1/R^3$).

The problem of spin excitations in the absence of long-range ordering at $T \rightarrow 0$ as well as the problem of a possible Fermi liquid ground-state in spin systems is one of the most interesting. It seems that we face the same difficulty in high-temperature superconductors (HTSC) where the interaction between the charge carriers and spin sub-system plays an essential role. We note that some properties following from (28) for the spin spectral function are observed in HTSC compounds (the linear law for the resistivity $\rho \sim T$, the linear dependence of the tunnelling conductance $\sigma \sim |U|$, the marginal self-energy part [13]). The theory is obviously incomplete at this point, thus we find the possibility of determining the spectral function $P(E)$ experimentally to be the real basis for the development of different theoretical approaches.

At finite temperature the tunnelling conductance depends on the ratio between U , T and T_K . If $T < U < T_K$ then all previous results remain valid. In the case $U < T < T_K$ only the even part of the conductance undergoes some change, which is effectively described by the replacement $U \rightarrow \pi T$. In the limit $T \gg T_K$ the even conductance σ_e acquires a constant value independent of T and U , while σ_o goes to zero. Indeed, at high temperature $P(E) \sim 1/T$ due to the finite energy interval of the spin excitations. On the other hand, the leading term in the general expression (24) is connected with the Bose distribution function $N_E \sim T/E$, thus cancelling the temperature dependence of $\text{Im } \Sigma^R$.

3. Tunnelling current in a narrow polaron band

In this section we consider the tunnelling properties of HF systems with the f level close to the Fermi level. Depending on the parameters the case of narrow f band or c - f hybridization may be considered. As mentioned above, the appearance of an extremely small energy scale in this case is connected with the electron (and phonon) polaron effect due to the Coulomb interaction with the wide conduction band. In its turn, the scattering of conduction electrons on the excitations from the narrow band results in a strong mass renormalization of the c electron in close analogy with the previous discussion. We thus end up with a two-component Fermi liquid with heavy masses of both components (which ratio, however, may be arbitrary).

We start a consideration of the case of two electron bands on the Fermi level. The Hamiltonian can be written as

$$H = H_B + H_{SL} + H_{int} \equiv \sum_{k\sigma} (\epsilon_k c_{k\sigma}^+ c_{k\sigma} + E_k^f f_{k\sigma}^+ f_{k\sigma}) + \sum_{kk'q\sigma\sigma'} V_q f_{k\sigma}^+ c_{k'\sigma'}^+ c_{k'-q\sigma'} f_{k+q\sigma}. \quad (30)$$

If the bare width of the f band, Δ , is small as compared with the c bandwidth, W , then the interaction described by the last term in (30) leads to a drastic narrowing of the f band down to the value, $\bar{\Delta} \ll \Delta$. The contribution of the narrow band to the tunnelling conductance has a sharp peak at $U \sim \bar{\Delta}$. In this respect the picture is quite different from that defined by the renormalized conduction band. In the previous section we found that in spite of a strong mass enhancement near the Fermi surface, $m_c^* \gg m_B$, which is present in the case under consideration as well, the tunnelling current from the conduction band is only slightly influenced by this renormalization. With the comparable values of the tunnelling matrix elements the current from the narrow band will dominate at small U , and we have to calculate only this particular contribution.

Let us start with the simplest case: T or U much larger than $\bar{\Delta}$. Then the problem is that of a localized f level and can be solved exactly. In this case $\rho_f(\xi) = \delta(\xi - \epsilon^f)$, and we can ignore the dependence of the tunnelling matrix element on the initial and final electron energies. Thus

$$I = -4eT^2(\epsilon_F, \epsilon_F)\rho_a(\epsilon_F) \int d\omega (n_\omega - n_{\omega+U}) \text{Im} G^R(\epsilon_F, \omega). \quad (31)$$

On the other hand, we can express the tunnelling current directly in terms of the transition probabilities between the localized f level and the usual metal state with energy ω :

$$I = 4e \int d\omega [n_f(1 - n_{\omega+U})W(\epsilon^f - \omega) - n_{\omega+U}(1 - n_f)W(\omega - \epsilon^f)]. \quad (32)$$

Using the equilibrium property $W(-E) = W(E) \exp(-E/T)$ we write this expression in the form

$$I = 2e \int d\omega (n_\omega - n_{\omega+U}) [n_f W(\epsilon^f - \omega) + (1 - n_f)W(\omega - \epsilon^f)]. \quad (33)$$

The probability of an incoherent tunnelling transition with energy transfer E was found for the case of an asymmetric double-well system in [14]:

$$W(E) = 2T^2(\epsilon_F, \epsilon_F)\rho_a \left(\frac{2\pi T}{W}\right)^{2\alpha} \frac{\Omega}{E^2 + \Omega^2} \frac{|\Gamma[1 + \alpha + iE/2\pi T]|^2}{\Gamma[1 + 2\alpha]} e^{E/2T}. \quad (34)$$

Here α is the dimensionless coupling constant which, in the Born approximation, has the form (note that the coupling is non-zero only in the HF metal)

$$\alpha = \rho_c^2 \langle |V_{k-k'}|^2 \rangle. \quad (35)$$

For an arbitrary scattering potential α is expressed in terms of phase shifts at the Fermi energy [15]

$$\alpha = \sum_l (2l + 1)(\delta_l/\pi)^2. \quad (36)$$

The relaxation width of the f level due to its interaction with the conduction band is defined by Ω :

$$\Omega = 2\pi\alpha T. \quad (37)$$

Now, comparing (31) with (33) and (34) we get

$$\text{Im} G^R = - \left(\frac{2\pi T}{W}\right)^{2\alpha} \frac{\Omega}{(\omega - \epsilon^f)^2 + \Omega^2} \frac{|\Gamma[1 + \alpha + i(\omega - \epsilon^f)/2\pi T]|^2}{\Gamma[1 + 2\alpha]} \frac{\cosh(\omega/2T)}{\cosh(\epsilon^f/2T)}. \quad (38)$$

At $T \rightarrow 0$ and $\epsilon^f > 0$:

$$\text{Im} G^R = - \begin{cases} \frac{\pi}{\omega - \epsilon^f} \left(\frac{\omega - \epsilon^f}{W}\right)^{2\alpha} \frac{1}{\Gamma[2\alpha]} & \omega > \epsilon^f \\ 0 & \omega < \epsilon^f. \end{cases} \quad (39)$$

This result coincides with the well known expression for the Green function of a deep hole, obtained by Nozieres and deDominicis [15]. Knowing the imaginary part, we can restore the Green function:

$$G^R = - \left(\frac{2\pi T}{W} \right)^{2\alpha} \frac{\Omega}{(\omega - \epsilon^f)^2 + \Omega^2} \frac{|\Gamma[1 + \alpha + i(\omega - \epsilon^f)/2\pi T]|^2}{\Gamma[1 + 2\alpha]} \times \frac{\sinh[(\omega - \epsilon^f)/2\pi T + i\pi\alpha] \cosh(\epsilon^f/2\pi T + i\pi\alpha)}{\cosh(\epsilon^f/2T)} \quad (40)$$

We now calculate the tunnelling current. This can be done analytically if one make use of the time integral representation for the transition probability (34):

$$W(E) = -\frac{1}{\pi} \text{Re} \int_0^\infty dt e^{iEt} \left(\frac{-i\pi T}{W \sinh(\pi T t)} \right)^{2\alpha} \quad (41)$$

As a result we find the following expression for the current

$$I = g \frac{1}{2\pi\Gamma(1 + 2\alpha)} \left(\frac{2\pi T}{W} \right)^{2\alpha} |\Gamma[1/2 + \alpha + i(U + \epsilon^f)/2\pi T]|^2 \frac{\sinh(U/2T)}{\cosh(\epsilon^f/2T)} \quad (42)$$

where

$$g = 4\pi e T^2(\epsilon_F, \epsilon_F) \rho_a(\epsilon_F) \quad (43)$$

It is obvious that $I(U, \epsilon^f) = -I(-U, -\epsilon^f)$.

The polaron effect which is T - and U -dependent influences the tunnelling current. In the absence of the polaron effect, when $\alpha \rightarrow 0$ the general expression (43) transforms into the trivial case corresponding to the δ -functional peak in the f -electron density of states:

$$I = \frac{g}{2} \left[\tanh\left(\frac{U + \epsilon^f}{2T}\right) - \tanh\left(\frac{\epsilon^f}{2T}\right) \right] \quad (44)$$

With $\alpha \neq 0$ simple formulae can be obtained in the limit $T \rightarrow 0$:

$$I = g \frac{1}{2\Gamma(1 + 2\alpha)} \left(\frac{U + \epsilon^f}{W} \right)^{2\alpha} \theta(U + \epsilon^f) \quad \epsilon^f < 0 \quad (45)$$

and $U, \epsilon^f \ll T$:

$$I = g \frac{\Gamma^2(1/2 + \alpha)}{4\pi\Gamma(1 + 2\alpha)} \left(\frac{2\pi T}{W} \right)^{2\alpha} \frac{U}{T} \quad (46)$$

Thus at $T \rightarrow 0$ the current is a non-analytic function of the electric potential over a wide range of U . The δ -functional peak effectively spreads out and the essential part of the spectral density is concentrated in relatively slow decaying tails. It is interesting that, for strong enough coupling, when $\alpha = 1/2$ the localized f level is seen in the tunnelling current just like an ordinary wide band. Physically, the reason is the strong shaking up of the polaron cloud around the f electron during its transition to the normal metal state. In the typical case $\alpha < 1/2$. The non-analytic dependence on U and T allows one to reveal

the narrow band in the structure of charge fluctuations and to understand the role played by the interband Coulomb interaction in the formation of the HF state.

Consider now the narrow band of finite width with the Fermi level inside the band. In the general case the situation does not change after polaron narrowing, and ϵ_F still lays inside the $\bar{\Delta}$ interval. Within the framework of the tight-binding approximation the bare f-electron spectrum has the well known form

$$E_p = \epsilon^f - \Delta_0 \sum_g e^{ipg} \quad (47)$$

where g is the displacement vector to the neighbouring equivalent site (for simplicity we assume here the cubic crystal symmetry). In [7] the relationship between the electron motion in a narrow band and the band motion of a heavy particle (e.g. a proton) was discussed in detail. The only difference is that the non-adiabatic interval of the conduction band excitations interacting with the f electron is spread over the entire energy spectrum while this interval is very narrow in the case of a heavy particle. Assuming that for a dense system the value of the polaron bandwidth has the same order of magnitude as that in the one-particle case, we find [7, 14]

$$\bar{\Delta} \approx \Delta \left(\frac{\Delta}{W} \right)^{b/(1-b)} \quad (48)$$

Here Δ is the bandwidth corresponding to the dispersion law (47). The dimensionless coupling between the heavy and light electrons has the form (compare it with the expression for α , equation (35))

$$b = 2\rho_c^2 \langle |V_{k-k'}|^2 [1 - \cos(\mathbf{k} - \mathbf{k}')g] \rangle. \quad (49)$$

Let $T \ll \bar{\Delta}$. Then in the narrow band we have a Fermi liquid state, and neglecting the interaction between f electrons we may write the Green function in the form

$$G^R = \frac{Z}{\omega - \bar{E}_p + i\delta} \quad (50)$$

where \bar{E}_p is the f-electron dispersion law corresponding to the bandwidth $\bar{\Delta}$, and the Z factor corresponds to the overlap integral of the light electrons. We substitute $\text{Im } G^R$ into the general expression for the current (31). With $U < \bar{\Delta}$ we find

$$I \approx gZ \frac{U}{\bar{\Delta}}. \quad (51)$$

Comparing this result with (45), which should be the continuation of the band expression to the region $U \geq \bar{\Delta}$, we obtain an approximate formula for the Z factor:

$$Z \approx \left(\frac{\bar{\Delta}}{W} \right)^{2\alpha}. \quad (52)$$

We thus find that $\bar{\Delta}$ is the crossover point where the linear dependence of the current on voltage is replaced by an interaction-dependent power law $I \sim U^{2\alpha}$. This result allows one to define the f-electron energy scale directly from the $I(U)$ curves. The same crossover

takes place if we increase the temperature up to the $\bar{\Delta}$ value when temperature fluctuations destroy the coherent motion in the f band [7].

One might wonder why the enormous mass renormalization in the Kondo-lattice case is not seen in the tunnelling current, while the heavy mass in the polaron band strongly influences the $I(U)$ dependence. There are two reasons for this. First, in the case of a narrow band the bare f-electron mass is supposed to be large irrespective of the interaction effects. Second, for the momentum-independent self-energy part (which is the case of the conduction band renormalization) the effective mass enhancement is compensated by a small Z-factor. In the polaron picture the self-energy part is also a function of momentum. It follows from (35) and (49) that Z-factor and $\bar{\Delta}$ renormalizations are governed by different coupling constants. Note that band narrowing depends on the geometry of the particle motion in the crystal, while the transition probability between the two metals and the Z-factor are sensitive only to the on-site interaction with the conduction band.

4. Tunnelling current in the case of c-f hybridization

The hybridization Hamiltonian leading to the f-electron delocalization in a crystal has the well known form

$$H_h = \sum_{k\sigma} V_h(k) (f_{k\sigma}^+ c_{k\sigma} + c_{k\sigma}^+ f_{k\sigma}). \quad (53)$$

The interband interaction leads to renormalization of the hybridization vertex which, contrary to widespread opinion, is essentially influenced by the momentum dependence of $V_h(k)$. In the general case there are two interaction channels having infrared divergence. The first one is connected with the orthogonality catastrophe for the overlap integral between the many-electron wavefunctions of the wide band and is governed by the sum of all scattering phase shifts (see (36)). The second channel is connected with the c electron rescattering in the final state due to its interaction with the extra hole in the f shell. This process, which is well-known in the theory of x-ray absorption and in the Kondo effect, results in the infrared enhancement of the transition matrix element [15]:

$$(W/\omega)^{\delta_j/\pi}. \quad (54)$$

The phase shift δ_j characterizing the scattering between the hybridized c electron and f hole is defined mainly by the symmetry of the hybridization matrix element. Indeed, the spherically symmetric part of the hybridization potential is zero due to the orthogonality between the c and f states in the absence of the hybridization potential. This means that in (54) we have $j \neq 0$. For a wide-enough conduction band with dominant s-symmetry of electron wavefunctions the phase shift in (54) has the symmetry of a deep f hole, $\delta_j = \delta_3$. The admixture of p- and d-symmetry waves in the wide band leads to a linear superposition of different contributions to the hybridization vertex, which renormalization is defined by the phase shifts δ_2 and δ_1 respectively.

Usually the s-wave phase shift is the largest one for a short-range interaction. In most cases the sum of phase shifts squared in (36), which of course contains δ_0 , turns out to be larger than the linear term $\delta_{j \neq 0}$. We make use of this notion and neglect below the scattering processes leading to (54). Thus, in the general case, we come to the polaron narrowing of the hybridization peak which might be responsible for the charged HF component.

In some model considerations the hybridization vertex is considered as a momentum-independent constant. From the above discussion it is clear that in the general case this is a wrong starting point. Indeed, the constant value in k -space means the δ -functional form of the hybridization potential in a coordinate space. But this is in contradiction with the on-site orthogonality between the c and f states. Nevertheless, if we neglect this point, the renormalization (54) will be defined by the s -scattering phase shift, and the value δ_0/π may exceed the parameter 2α , especially in the perturbation approach. In this case one can imitate the broadening of the hybridization peak instead of narrowing.

In the mixed-valence regime far from the integer occupation of the f level the most important role is played by the interband c - f Coulomb interaction. Neglecting all intraband interactions we can write down the expression for the f -electron Green function as (see e.g. [8]):

$$[G_f^R(\omega, \mathbf{k})]^{-1} = [G_f^R(\omega)]^{-1} + |V_h(\mathbf{k})|^2 G_c^R(\omega, \mathbf{k}) \quad (55)$$

where G_f^R is the Green function of the localized f level, (41). Remember that in deriving (55) we neglected the rescattering of the hybridized c electron on the f hole because of a small value of the scattering phase shift $\delta_{j \neq 0}$ in (54). Equation (55) can be rewritten in the form

$$G_f^R(\omega, \mathbf{k}) = \frac{[\omega - \epsilon_{\mathbf{k}} - \Sigma^R(\omega, \mathbf{k})] G_f^R(\omega)}{\omega - \epsilon_{\mathbf{k}} - \Sigma^R(\omega, \mathbf{k}) - |V_h(\mathbf{k})|^2 G_f^R(\omega)} \quad (56)$$

where Σ^R is the self-energy part of c electrons.

The tunnelling current is defined by the integral over k from the Green function (see (4)). The hybridization peak is connected with the k -regions, where $\epsilon_{\mathbf{k}}$ is much larger than the characteristic frequency of the problem. On the other hand, at small electric potentials we can drop the energy dependence of the tunnelling matrix element. Under these conditions the sum over k from the Green function has the form

$$G_f^R(\omega) = \sum_{\mathbf{k}} G_f^R(\omega, \mathbf{k}) \approx G_f^R(\omega) \left(1 - G_f^R(\omega) \sum_{\mathbf{k}} \frac{|V_h(\mathbf{k})|^2}{\omega - \epsilon_{\mathbf{k}} - \Sigma^R(\omega, \mathbf{k}) - |V_h(\mathbf{k})|^2 G_f^R(\omega)} \right). \quad (57)$$

The basic contribution to this sum comes from large $\epsilon_{\mathbf{k}}$ values of order W . The second term in the brackets is of the order of $G_f^R(\omega) V^2/W$. Obviously, one can define the characteristic frequency of forming the coherent state in the system from the relation

$$G_f^R(\omega) \frac{V^2}{W} \approx 1. \quad (58)$$

Taking into account (39) we come to the following estimation for the hybridization peak width

$$\Gamma^* \approx \Gamma \left(\frac{\Gamma}{W} \right)^{2\alpha/(1-2\alpha)} \quad (59)$$

where Γ is the bare hybridization width.

With $U \gg \Gamma^*$ the second term in (57) can be omitted and the tunnelling current is essentially the same as in the case of a localized f level. In the region T , $U \leq \Gamma^*$ the current is described by (51) with the replacement of $\bar{\Delta}$ by Γ^* . Just as in the case of a narrow band Γ^* is the characteristic energy scale, where the crossover from the temperature-independent constant conductance to the interaction-dependent power law $I \sim U^{2\alpha}$ (or $I \sim U T^{2\alpha-1}$) is observed. Thus, both the narrow f -electron band and the hybridization peak are clearly seen in the tunnelling current in the mixed-valence case.

5. Concluding remarks

So far we have ignored the electron-phonon interaction. However, considering the HF state in the case of a narrow band or hybridization peak with the characteristic frequency much less than Debye temperature, Θ_D , we also have to include into the theory the phonon polaron effect. At low temperatures and small electric potentials the interaction with the phonon sub-system reveals itself only through the constant renormalization of the bare parameters Δ and Γ [7]:

$$\bar{\Delta} \rightarrow \Delta \exp\left(-\frac{\Phi}{1-b}\right) \quad \Gamma^* \rightarrow \Gamma \exp\left(-\frac{\Phi}{1-2\alpha}\right) \quad (60)$$

where Φ is the conventional phonon polaron exponent. Analogously, at U or $T > \bar{\Delta}$, Γ^* the expressions (42), (45) and (46) must be multiplied by the small polaron factor $\exp(-\Phi)$. The situation changes significantly only at high temperatures or large electric potentials comparable with the Debye temperature when the polaron cloud is excited during the tunnelling transition. Obviously, in this limit the tunnelling current is that corresponding to the localized f level and can be obtained from the relation (33). The transition probability incorporating the particle coupling to phonons was found in a number of papers (see, for example, [16]). In the context of the present discussion we shall not reproduce here the whole theory, but rather point out some essential results allowing us to estimate the role of the electron-phonon interaction in the formation of the HF state.

The typical feature of the strong phonon polaron effect is the exponential dependence of the transition probability on temperature and electric potential at T and $U \geq \Theta_D$. Assuming $\Phi \gg 1$ in the high-temperature limit $T \geq \Theta_D$, U we find

$$I \sim U \sqrt{\pi/E_p T} \exp\left(-\frac{E_p}{4T}\right) \quad (61)$$

where E_p is the polaron energy shift of the f level ($E_p \approx \frac{1}{2}\Theta_D\Phi$). On the other hand, at large electric potentials $U \geq \Theta_D$, T we find for the transition probability

$$W(U) \sim \frac{\sqrt{\pi}}{2\mathcal{E}} \exp\left(-\frac{(U-E_p)^2}{4\mathcal{E}^2}\right) \quad (62)$$

the Gauss exponential dependence on U with the width $\mathcal{E}^2 \sim \Theta_D^2\Phi$. As expected, at high temperatures and large electric potentials the exponentially small polaron factor is removed and the conductance has two specific peaks at $\epsilon^f - E_p$ and $\epsilon^f + E_p$ with the separation between them being twice the polaron energy shift, or the so-called Stocks shift (see (62) and (33)). The existence of such a shift and its magnitude are related to the phonon polaron narrowing of the f band.

In this work we discussed a rather idealized picture for the tunnelling current. The scanning tunnelling microscope seems to be the most suitable experimental system. First, with this technique we have the possibility of studying the current from different atoms on the metal surface and may hope to separate the contributions from c and f bands. In the conventional tunnelling experiment both the c and f electrons tunnel through the dielectric barrier, and the problem of current shunting by conduction electrons may present an obstacle in analysing the contribution from the narrow f band. Second, we have no extra inelastic interaction in the vacuum space that can modify the $I(U)$ dependence essentially

and which is the case for the dielectric barriers. Third, we expect the smallest distortion of the bulk electron properties for the case of a metal–vacuum surface. We have calculated the tunnelling current within the perturbation theory in the transition matrix element ignoring the Coulomb interaction effects between the HF and normal metal, which are of importance only in very small tunnel junctions. The physics of the tunnelling process is contained in the matrix elements $T_{kk'}$, which need to be calculated in a way that models the experimental setup.

The study of the f-electron spectral function with the use of x-ray absorption spectroscopy introduces an additional problem connected with the infrared renormalization of the transition matrix element [15], which has the typical form (54), and within the transfer Hamiltonian approach is equivalent to the substitution

$$T_{kk'} \rightarrow T_{kk'} \left(\frac{W}{\omega} \right)^{s_j/\pi - 2s'} \quad T = 0. \quad (63)$$

Obviously, this effect will influence the interpretation of the experimental data.

Acknowledgments

This research was supported by the 'Netherlands Organization for Scientific Research' NWO.

References

- [1] Stewart G R 1984 *Rev. Mod. Phys.* **56** 755
- [2] Ott H R 1987 *Prog. Low Temp. Phys.* **XI** 217
- [3] Kagan Yu, Kikoin K A and Prokof'ev N V 1992 *Physica B* submitted
- [4] Kagan Yu, Kikoin K A and Prokof'ev N V 1992 *Pis. Zh. Eksp. Teor. Fiz.* **56** 221 (Engl. Transl. *JETP Lett.* **56** 219)
- [5] Tesanovič Z and Valls O T 1986 *Phys. Rev. B* **34** 1918
- [6] Coleman P and Andrei N 1989 *J. Phys.: Condens. Matter* **1** 4057
- [7] Kagan Yu and Prokof'ev N V 1987 *Zh. Eksp. Teor. Fiz.* **93** 366 (Engl. Transl. *Sov. Phys.-JETP* **66** 211)
- [8] Liu S H 1987 *Phys. Rev. Lett.* **58** 2707; 1988 *Phys. Rev. B* **37** 3542
- [9] Wolf E 1985 *Principles of Electron Tunnelling Spectroscopy* (Oxford: Oxford University Press)
- [10] Browman E G and Kagan Yu 1968 *Zh. Eksp. Teor. Fiz.* **52** 557 (Engl. Transl. *Sov. Phys.-JETP* **25** 362)
- [11] Gradshteyn I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York: Academic)
- [12] Herman H and Schmid A 1968 *Z. Phys.* **211** 313
- [13] Varma C M, Littlewood P B, Schmitt-Rink S, Abrahams E and Ruckenstein A E 1989 *Phys. Rev. Lett.* **63** 1996
- [14] Kagan Yu and Prokof'ev N V 1986 *Zh. Eksp. Teor. Fiz.* **90** 2176 (Engl. Transl. *Sov. Phys.-JETP* **63** 1276)
- [15] Nozières P and deDominicis C T 1969 *Phys. Rev.* **178** 1097
- [16] Kagan Yu and Prokof'ev N V 1989 *Zh. Eksp. Teor. Fiz.* **96** 2209 (Engl. Transl. *Sov. Phys.-JETP* **69** 1250)