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K. VLADÁR
A. ZAWADOWSKI

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Hungarian Academy of Sciences

CENTRAL RESEARCH INSTITUTE FOR PHYSICS

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K. Vladár and A. Zawadowski

Central Research Institute for Physics
H-1525 Budapest 114, P.O.B. 49, Hungary

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ABSTRACT

The crossover temperature T_K is calculated at which the motion of the tunneling atom and the conduction electron charge screening cloud is gradually coupled together. The first theoretical estimation is given to show that the formation of the resonance provides a realistic explanation for the electrical resistivity minimum and for the inelastic electron scattering rate relevant in localization theory if $T_K \approx 1 - 5$ K.

АННОТАЦИЯ

Вычислена температура кроссовера T_K, в окрестности которой туннелирующий атом и экранирующее облако электронов проводимости постепенно связываются. Дается теоретическая оценка, согласно которой возникновение резонансного рассеяния может объяснить минимум электрического сопротивления, если $T_K \approx 1 - 5$ K, а также число соударений при неупругом рассеянии электронов, имеющее важное значение в теории локализации.

KIVONAT

Kiszámitjuk azt a crossover hőmérsékletet, amely környékén az alagutazó atom és a vezetési elektronok töltésleárnyékoló felhője fokozatosan egymáshoz csatolódik. Első izben végzünk olyan elméleti becslést, amely igazolja, hogy a rezonanciaszórás kialakulása $T_K \approx 1 - 5$ K körül reális magyarázat lehet az elektromos ellenállás minimumára, és a rugalmatlan elektronszórásból adódó ütközési számra, mely utóbbi a lokalizáció-elméletben játszik fontos szerepet.

The concept of two level systems[1] (TLS) has proved to be a milestone in understanding the low temperature behavior of insulating and metallic glasses as well[2]. Considering the relaxation rate of TLS observed by ultrasound measurements on metallic glasses the importance of interaction between conduction electrons and TLS has first been pointed out by Golding et al[3] suggesting a Korringa-like relaxation mechanism. Earlier, Cochrane et al[4] called the attention to the possibility that the electron-TLS interaction may contribute to the formation of electrical resistivity minimum observed in many alloys[5]. The resistivity has been studied by Kondo[6] and by the authors[7] up to fourth order in the coupling and logarithmic contribution has been obtained in somewhat similar manner as in the case of dilute magnetic alloys. In order to get logarithmic contribution it was necessary to take into account the angular dependence of the coupling on the direction of the in- and outgoing electrons. Recently, the possible role of TLS in localization theory has been emphasized in the context of the inelastic electron scattering rate which by making hopping between localized states limits the applicability of the scaling arguments[8].

One of the present authors[9] has suggested a simplified model to demonstrate that in the leading logarithmic approximation the electron-TLS interaction scales to a strong coupling problem, namely, to the isotropic antiferromagnetic Kondo problem. This result has been interpreted as the indication that at low temperature a strongly correlated state is formed in which the tunneling of the TLS and the charge polarization cloud exhibiting the Friedel oscillation are moving rigidly tight together. The aim of the present letter is to give the first theoretical evidence that at low temperatures the resonant electron scattering on TLS may contribute to the electrical resistivity and to the inelastic scattering rate just in the range of values observed in experiments. These estimations are based on second order scaling arguments and it is shown that the crossover temperature dividing the weak and strong coupling regions is very sensitive on the values of the couplings but it may be in the range of $1K^{o}$.

The following Hamiltonian is considered

$$H = \sum_{ks} \varepsilon_k a^{+}_{ks} a_{ks} + \frac{1}{2} (\Delta \sigma^{z}_{TLS} + \Delta_o \sigma^{x}_{TLS}) + \sum_{\substack{kk's\\ \alpha\beta, i}} a^{+}_{k's} (f^{x}_{\alpha} (k') V^{i}_{\alpha\beta} f_{\beta} (k)) a_{ks} \sigma^{i}_{TLS} \tag{1}$$

where $i=x,y,z$, a_{ks} is the annihilation operator for conduction electron with spin s and energy ε_k , σ^{i}_{TLS} $(i=x,y,z)$ is the pseudospin Pauli matrices for TLS and $V^{i}_{k'k} = \sum_{\alpha\beta} f_{\alpha}(k') V^{i}_{\alpha\beta} f_{\beta}(k)$ is the coupling between electrons and pseudospin σ^{i}_{TLS} $f_{\alpha}(k)$'s form a complete set of functions (e.g. spherical harmonics), which depend on the direction of k only. It can be shown, that in the starting Hamiltonian one can take $V^{y}=0$ /6,7/ and V^{x} describes the electron assisted tunneling thus $V^{x}/V^{z} << 1$ as V^{x} is proportional to the tunneling rate $e^{-\lambda} << 1$. Furthermore, it can be seen[10/] by taking a representation where V^z is diagonal that only those two indices α,β are of importance for which the difference $V^z_{\alpha\alpha}-V^z_{\beta\beta}$ is the largest. In a simple model where one atom moves in a symmetric double well potential f_1 and f_2 have been found as linear combinations of s- and p- and d-like functions. The second order scaling equations are derived by changing the electron band width cut-off from value D to D' and they can be obtained in the framework of multiplicative renormalization group[11/]. In the following only two indices $\alpha=1,2$ are kept and $\rho_o V^i_{\alpha\beta} = v^i \sigma^i_{\alpha\beta}$ holds in the representation used where ρ_o is the conduction electron density of states at the Fermi level for one spin direction and v^i is the dimensionless coupling. The scaling equations for the symmetric case $\Delta=o$ are

$$x \frac{\partial}{\partial x} v^i(x) = -4\, v^j(x)\, v^k(x) + 8\, v^i(x) \left(v^j(x)^2 + v^k(x)^2 \right) \quad \text{with } i\neq j\neq k \tag{2}$$

$$x \frac{\partial}{\partial x} \ln \Delta_o(x) = 8 \left(v^z(x)^2 + v^y(x)^2 \right) \tag{3}$$

where $x=D'/D$. In the general case $\Delta\neq O$ scaling equation can be derived for the energy splitting $E(D') = \left(\Delta(x)^2 + \Delta_o(x)^2 \right)^{1/2}$, but the ratio Δ/Δ_o is changing as well[10/]. The second order scaling equations are correct as far as the scaled couplings are much smaller than unity, $v^i(x) \leq o{,}2$. For eq. (2) there is an isotropic fixed point $v^{x*} = v^{y*} = v^{z*} = 1/4$, but according to Anderson's argument the exact scaling equation must have stable fixed point only in the infinity (or at zero), thus $v^{x^*}=v^{y^*}=v^{z^*}=\infty$. By integrating the scaling eq. (2) $v^i \ll 1$ one get for the typical value of the cutoff between the weak and strong coupling regions which is known as the crossover (Kondo) temperature[12]

$$T_K = D\left(\frac{v^x}{4v^z}\right)^{\frac{1}{4v^z}} (v^x v^z)^{1/2} \tag{4}$$

at which $v^x=v^y=v^z\Big|_{D'=T_K} \sim 1/8$. The changes of the couplings are depicted in Fig. 1. The renormalization of Δ_o is shown also in the symmetric case where $\Delta=0$ in the representation used. Δ_o is screened by several order of magnitude.

Depending on the value of the parameters of an individual TLS two cases must be distinguished: (i) $T_K \gg E(T_K)$ thus a correlated state is formed, (ii) $T_K \lesssim E(T_K)$, therefore the correlated state can not be formed completely, because the scaling stops at $D' \sim E(T=D')$, thus the situation existing at $T'=D'$ is preserved even to very low temperatures.

In case (i) one can turn to the analogy of the Kondo problem for magnetic impurities. At $T=T_K$ $v^x=v^y \sim 1/8$ thus they are large and the electron scattering amplitude is large as well. For $T \ll T_K$ one must consider the scattering amplitude rather than the coupling. Its diagonal part proportional to unit operator I_{TLS} increases and tends to the unitarity limit, while the terms proportional to σ^i_{TLS} have a maximum at $T=T_K$ and they tend to zero as the temperature is lowered. These limits mentioned can be achieved only if $E=0$.

In case (ii) the elastic (e.g. v^z for the case $\Delta_o=0$) and the inelastic (v^x and v^y) scattering amplitudes (or couplings) remain roughly the same even at very low temperatures.

Considering different physical quantities in case (ii) a fairly good approximation can be obtained by carrying out the calculations in the lowest orders of perturbation theory but with the enhanced couplings $v^i \lesssim 1/8$ $(i=x,y)$ depicted in Fig. 1.

In order to estimate T_K one can use the model where only one atom is moving. For this model Black et al[13] obtaines $v^z \sim Uv\rho_o(k_F d)$ where U is the pseudopotential of the atom, v is the atomic volume, d is the separation distance between the two equilibrium positions and k_F is the Fermi momentum. Considering the electron assisted tunneling through the barrier one obtains[14] $v^x \sim (k_F d)^2 \lambda v U \rho_o \Delta_o/V$ where $\lambda = w(2MV)^{1/2}$ with the width and height of the square potential barrier, w and V respectively, and M is the mass of the atom, furthermore, the factor $(k_F d)^2$ is due to the fact that the change in the barrier height must be measured from the average of the two potential minima. Using typical values $\rho_o v = 0.2\ eV^{-1}$, U=1eV, d=0.3-0.5, $M=50M_{proton}$, $k_F = 1\mathring{A}^{-1}$, $\lambda=6$,[15] then $v^z = 0.2(k_F d)$ and $v^x/v^z \sim 10^{-3}-10^{-4}$. In order to get $T_K \sim 1K^o$ one must have $v^z \sim 0.3$ for D=10eV. It must be emphasized that T_K may change by several orders of magnitude due to small changes of the parameters, especially in v^z.

Let us consider now different physical quantities. Minimum in the electrical resistivity: Assuming a uniform distribution

$P(E)=P_o$ for TLS energies $E=(\Delta^2+\Delta_o^2)^{1/2}$, the number of TLS for which case (i) holds is $T_K P_o$. For these TLS the total scattering amplitude is in the range of unitarity limit. For $T>T_K$ the temperature dependence of the resistivity can be estimated by assuming that there is only one electron in the finite state thus the scattering rate is proportional to the enhanced couplings, actually to $(v^x)^2+(v^y)^2+(v^z)^2\big|_{x=T/D}$. In this range of temperature the resistivity changes logarithmically at least in one decade of T. As $T\to 0$, the total increase ΔR in the resistivity can be estimated as the scattering amplitude in the unitarity limit $2\rho_o^{-1}/\pi$ multiplied by the number of TLS in case (i), thus

$$\Delta R\sim \frac{m}{ne^2}\left(\rho_o^{-1}\frac{2}{\pi}\right) 2P_oT_K = \frac{P_oT_K}{N}\,\frac{1}{e^2}\,\frac{8\pi}{k_F} \qquad (5)$$

where m and e are the electron mass and charge, N is the total number of electrons and the factor 2 is due to the two channels $\alpha=1,2$, furthermore, $\rho_o=\frac{mk_F}{2\pi^2}$. In order to explain $\Delta R\sim 10^{-7}\,\Omega\mathrm{cm}$ with $T_K=5K^o$ and $k_F\sim 1\mathring{A}^{o-1}$ and $N=10^{-23}/\mathrm{cm}^3$ one need $P_o=2.10^{18}K^{o-1}\mathrm{cm}^{-3}$,[16] which is an acceptable amount of TLS. It should be noted that ΔR increases with T_K.

<u>Inelastic electron lifetime:</u> Black et al[13] suggested that the inelastic electron scattering rate due to TLS must be proportional to those number of TLS which can be excited by thermal electrons (E<T). Using the golden rule e.g. for the case $\Delta_o=0$

$$\tau_{in}^{-1} = \frac{2\pi}{\hbar}\left\{ (v^x)^2 + (v^y)^2 \right\} \rho_o^{-1}\, P_o\, T \qquad (6)$$

In order to estimate τ_{in}^{-1} one can use $P_o\sim 4.10^{17}K^{o-1}\mathrm{cm}^{-3}$ [17] and

$\rho_o = 0.6\ 10^{34}\ cm^{-3}\ erg^{-1}$ and assuming $T \sim T_K$, thus $v^x \sim v^y \sim 0.12$ the one gets $\tau_{in}^{-1} = 1.2.10^{10} s^{-1} K^{o-1}.T$. The explicite factor T dominates the weak dependence of the couplings v^x and v^y on the temperature. The order of magnitude is the one suggested on the basis of resistivity measurements on thin wires [18]. If one uses bare couplings, the estimated τ_{in}^{-1} is less by a factor 50 and that is the source of discrapancy previously quoted [18].

TLS relaxation rate $T_2^{-1} = 8\pi\, \hbar^{-1} \{(v^y)^2 + (v^x)^2\ \Delta^2/E^2 + (v^z)^2\ \Delta_o^2/E^2\}_{x=T/D} kT$ [19] can be observed in ultrasonic measurements which provide the most direct information on the couplings [20]. Using the notation $N(E)K_e = vN(E)V^{\perp}$ for the expression in the curly bracket above (where $N(E) = 2\rho_o$ and the other factor of two is due to the Pauli operators instead of spin 1/2 operators in eq. (1)), NK_e has previously been found in the order of 0.2 for several alloys [20]. It has recently been pointed out [21] that the experiment on superconducting materials are especially conclusive if the anomaly at the superconducting transition is considered. In $Pd_{0.7}Zr_{0.3}$ the observed coupling is $N(E)K_e = 0.9$, thus if $E \sim \Delta$ then $v^x \sim v^y = 0.16$ which correspond to enhanced couplings near T_K in Fig. 1. or if $E \sim \Delta_o$ and $v^x \sim v^y \ll v^z$ then $v^z = 0.32$ for which T_K must be large. These experiments give the first direct evidence that the enhanced couplings can really be found in the intermediate strong coupling range thus T_K 1-5K^o may occur.

The conclusion of our letter is that if v^z is large enough then a charge polarization cloud strongly coupled to the TLS atom can be built up at $T = T_K$. If $T_K \sim 1K^o$ then the couplings are enhanced anomalously and that may result in well observable contribution to the bulk resistivity minimum, to τ_{in}^{-1} relevant in localization theory and to T_2^{-1} determining the ultrasound absorbtion. As the first two of these experimental results might have different explanation, therefore, the performance of these experiments on samples prepared or treated (annealing, by radiation, by hydrogen) in the same way would be of crucial importance to test the presence of absence of the correlated state. It must finally be emphasized that these effects should not occur in all of the materials because a small change in the couplings can push T_K out of the range of interest. One may raise the idea that the largest v^z can be expected when in the electron-tunneling atom scattering the d-level resonance scattering dominates at the Fermi energy and the in numerical calculations $v\rho_o \sim 0.5$ can be reached e.g. for Zr based alloys[22].

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12. The factor $(v^x v^z)^{-1/2}$ is the correction to T_K derived in leading logarithmic approximation in Ref. 9, furthermore, a numerical error in eq. 10 of Ref. 9 has been corrected.

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14. See Ref. 9. and the results are similar as those in Ref. 6.

15. $\lambda=6$ corresponds to $\Delta_o=1K^o$ on the basis $\Delta_o=\hbar\omega_d \exp(-\lambda)$ with $\hbar\omega_d=400K^o$.

16. This value is five times larger that the value quoted in Ref. 17. for $Zr_{0.7}Pd_{0.3}$.

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19. In order to diagonalize the TLS part of the Hamiltonian given by eq. (1) one must perform a rotation around the y axis by angle α for σ^i_{TLS} in i=x,y,z, space and $tg\alpha=\Delta/\Delta_o$

20. See Ref. 3. and further references can be found in the papers quoted in Ref.s 2. and 21.

21. The $N(E)K_e=0.9$ value is obtained for $Zr_{0.7}Pd_{0.3}$ by W.Arnold, P. Doussineau, Ch. Frenois and A. Levelut (preprint) and G. Weiss and S. Hunklinger (private communication) on the basis of theory given in J.L. Black and P. Fulde, Phys. Rev. Lett. 43, 453 (1979).

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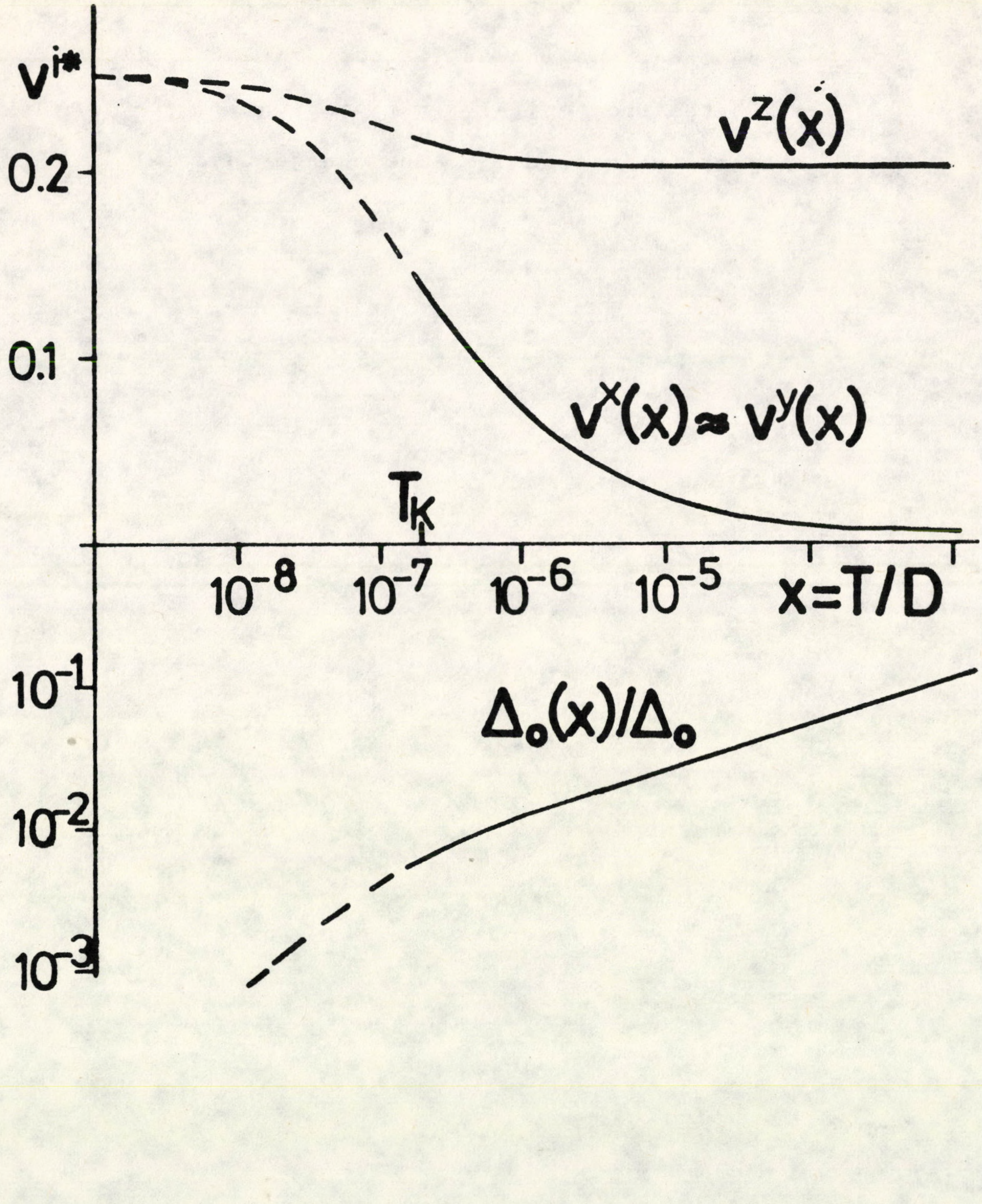
FIGURE CAPTION

Fig. 1. The scaling trajectories calculated using eq.s(2) and (3) are shown for $v^z=0.2$ and $v^x/v^z=10^{-3}$. Solid (dotted) curves show the parts where the second order scaling is (is not) valid. T_K is calculated from eq.(4). The logarithmic behavior is appearent around T_K. The change in $\Delta_o(x)$ is depicted as well.

Fig. 1.



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