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CALCULATION OF THE FERMI LEVEL IN A CERTAIN TYPE OF DISORDERED METALLIC STRUCTURE

РАСЧЁТ ЭНЕРГИИ ФЕРМИ ДЛЯ ОДНОГО СЛУЧАЯ НЕУПОРЯДОЧЕННОЙ МЕТАЛЛИЧЕСКОЙ СТРУКТУРЫ

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It was found experimentally that many metallic glasses exhibit an interesting effect — the appearance of a minimum in the temperature dependence of electrical resistivity — usually considered to be connected with the Kondo effect [1—3]. It has been shown, however, that the presence of the minimum can be explained by using in the case of metallic glasses the theory of the so-called modified relaxation constant, under the assumption that the Fermi level approaches close enough to the levels of defects [4]. In the disordered metallic structures this effect has not been investigated yet either theoretically or experimentally. The aim of this paper is to show (by a calculation) that the drop of the Fermi level can be due to the disorder of the metallic structure.

Let us consider the model of free electron moving in a random potential. Their Hamiltonian has the following form

$$\hat{H} = -\frac{h^2}{2m}\nabla^2 + U_p(\mathbf{r}) ,$$

where $U_p(\mathbf{r})$ is a stationary random function defined by the multigaussian distribution function, so that $\langle U_p(\mathbf{r})\rangle = 0$. Let η^2 denote the dispersion of the random potenial. Using the formalism of the Feynman path integrals — applied in the treatment of similar problems also byEdwards [5, 6] — the density of states can be calculated as a series in the powers of ħ [7]. Considering the quasiclassical approximation only, the energy of electrons in a disordered metallic structure can be written as

$$E = \varepsilon + \xi\eta ,$$

where $\varepsilon = \hbar^2 k^2/2m$ and ξ is a random quantity with a gaussian distribution function.

The Fermi level will be determined using the relation for the concentration of electrons

$$n = \frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_0^{\infty}\frac{\varepsilon^{1/2}}{\exp\left(\frac{\varepsilon+\xi\eta-E_F}{kT}\right)+1}\,e^{-(1/2)\xi^2}\,d\varepsilon\,d\xi . \tag{1}$$

After integrating by parts and applying the transformation $x = \frac{\varepsilon+\xi\eta-E_F}{kT}$ one obtains

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\int_0^{\infty}\varepsilon^{3/2}\,e^{-(1/2)[(\varepsilon-E_F-kTx)/\eta]^2}\,\frac{e^x}{(1+e^x)^2}\,d\varepsilon\,dx . \tag{2}$$

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Further, using the translation operator $\hat{D} = d/dE_F$ we obtain

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{e^{-kT\hat{D}x}\,e^x}{(1+e^x)^2}\,dx\int_0^{\infty}\varepsilon^{3/2}\,e^{-(1/2)(\varepsilon-E_F/\eta)^2}\,d\varepsilon\,. \tag{3}$$

Introducing the following substitutions $\varepsilon = \eta y$, $z = -E_F/\eta$ we have

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\eta^{3/2}\int_{-\infty}^{\infty}\frac{e^{kT/\eta\hat{D}'x}\,e^x}{(1+e^x)^2}\,dx\int_0^{\infty}y^{3/2}\,e^{-(1/2)y^2+yz-(1/2)z^2}\,dy\,, \tag{4}$$

where $\hat{D}' = d/dz$.

The integration of (4) over x after introducing the parabolic cylinder function $D_{-5/2}(z)$ yields

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{2/3}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\eta^{3/2}\Gamma\left(\frac{5}{2}\right)\left[\frac{\pi kT}{\eta}\hat{D}'\,\mathrm{cosec}\,\frac{\pi kT}{\eta}\hat{D}'\right]e^{-z^2/4}D_{-5/2}(z)\,. \tag{5}$$

When expanding the expression in brackets into a series and taking into account the first and the second terms only, one obtains

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\eta^{3/2}\Gamma\left(\frac{5}{2}\right)\left[1+\frac{1}{6}\left(\frac{\pi kT}{\eta}\right)^2\frac{d^2}{dz^2}\right]e^{-z^2/4}D_{-5/2}(z)\,. \tag{6}$$

The differentiation of the parabolic cylinder function can be performed using the recursion formula

$$\frac{d^m}{dz^m}e^{-z^2/4}D_r(z) = (-1)^m\,e^{-z^2/4}D_{r+m}(z)\,,$$

with $m = 1, 2, 3, \ldots$ Then the expression (6) reads

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}\frac{1}{\sqrt{2\pi}}\eta^{3/2}\Gamma\left(\frac{5}{2}\right)\left[e^{-z^2/4}D_{-5/2}(z)+\frac{1}{6}\left(\frac{\pi kT}{\eta}\right)^2 e^{-z^2/4}D_{1/2}(z)\right]. \tag{7}$$

Taking the two first terms in the asympotic expression of the parabolic cylinder function one obtains [8]

$$n = \frac{2}{3}\frac{\sqrt{2}}{\pi^2}\frac{m^{3/2}}{\hbar^3}E_F^{3/2}\left[1+\frac{\pi^2}{8}\left(\frac{kT}{E_F}\right)^2\right]\left[1+\frac{3}{8}\left(\frac{\eta}{E_F}\right)^2\right]. \tag{8}$$

It is known that in crystalline metals the Fermi level is given by an approximative formula $E_F^{cr} = E_{F_0}\left[1-\frac{\pi^2}{12}\left(\frac{kT}{E_{F_0}}\right)^2\right]$ with $E_{F_0} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$ being the Fermi level at $T = 0\,K$. Then the relation (8) can be written as

$$E_F\left[1+\frac{3}{8}\left(\frac{\eta}{E_F}\right)^2\right]^{2/3} = E_F^{cr}\,. \tag{9}$$

After solving Eq. (9) the following result for the Fermi level is obtained

$$E_F = \frac{1}{2}E_F^{cr} \pm \frac{1}{2}(E_F^{cr\,2}-\eta^2)^{1/2}. \tag{10}$$

Since at $\eta = 0$ there must be $E_F = E_F^{cr}$, only the singn + is allovable, thus

$$E_F = \frac{1}{2}E_F^{cr}\left[1+\sqrt{1-\left(\frac{\eta}{E_F^{cr}}\right)^2}\right]. \tag{11}$$

The obtained result can be interpreted as a drop of the Fermi level in glassy metals due to the disorder of structure. The rate of the decrease is given by the dispersion of the random potential as a parameter of disorder. The relation (11) shows that a considerable decrease of E_F^{cr} requires fair oscillations of the random potential. This is illustrated in Fig. 1, where the Fermi level (in units E_F^{cr}) is plotted as a function of η.

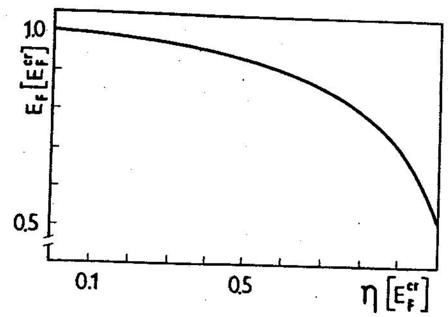

Fig. 1. The Fermi level of a disordered metallic structure vs η as the parameter of disorder.

It should be noted that the obtained result is a rough approximation only, which describes qualitatively the dependence $E_F = E_F(\eta)$. In the following it is desirable to perform a calculation which would consider not only the quasiclassical expression of the density of states but also the first (second) quantum mechanical correction (s).

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