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EXACTLY SOLVABLE MODEL OF TOPOLOGICAL TRANSITIONS IN METALS

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Summary. *In this paper, we consider ETP using a precisely solvable model of an electron in a crystal. The main characteristics of the transition are given by analytical functions that contain only the parameters of the potential. The results of calculations are compared with experimental data on the Lifshitz phase transition (genus transition) in normal metals. The practical significance of the work is to increase the accuracy of quantitative predictions of the physical properties of alloys of various transition metals.*

Keywords. *Electron-topological transitions (ETP), Fermi surface, Lamé potential, phase transition, Weierstrass function.*

1. Introduction

The basic properties of metals, such as electrical conductivity or thermal conductivity, are determined by the shape of the Fermi surface and the free path of electrons on this surface. The curvature of this surface changes the density of the allowed electronic states near it, as a result the thermodynamic and kinetic properties of metals change.

Changes in the topology of Fermi surfaces are not accompanied by changes in the crystal lattice or its symmetry, so they do not belong to the phase transitions of the 2nd kind. Such phase transitions were provided by I.M. Lifshitz and called as electron-topological transitions (ETP) 2.5 genus [1]. In his work, I.M. Lifshitz pointed to the change in the following properties of the metal during its phase transition: paramagnetic susceptibility, electronic heat capacity, coefficient of compressibility, thermal coefficient of pressure, anomalies of electrical resistance in a strong magnetic field.

ETPs associated with changes in the topology of the Fermi surface were first observed for the superconducting characteristics of metals in the region of high pressures and low temperatures [2]. Later ETPs were observed in metals in the normal state. New research in the field of ETP is associated with the development of new materials with high-temperature superconducting properties, changes in the magnetic order in metals during elastic deformations, etc. With the development of technology there is a need for a new elemental base of electronic equipment built on the basis of superconductors. Therefore, there is a need to increase the accuracy of quantitative predictions of the physical properties of alloys of various transition metals.

The article describes a method for constructing qualitative and quantitative properties Lifshitz transition from single-band model exactly solvable separable

potential Λ . The considered model allows to describe all parameters of transition by means of exact analytical functions using simple parameters.

2. ETP 2.5 kind

I.M. Lifshitz showed [1] that under the action of external pressure in a single-crystal metal, an electronic phase transition can occur. This transition changes the topology of the Fermi surface (TPF). For example, it is possible to move from a closed Fermi surface to an open Fermi surface or vice versa (see Fig. 1). The value of the Fermi energy at which the isoenergetic surface touches the face of the Brillouin zone is called the critical value of the Fermi energy.

If $\varepsilon_c > \varepsilon_F$, then the Fermi surface is closed (A).

If $\varepsilon_c < \varepsilon_F$, then the Fermi surface is open (B, C).

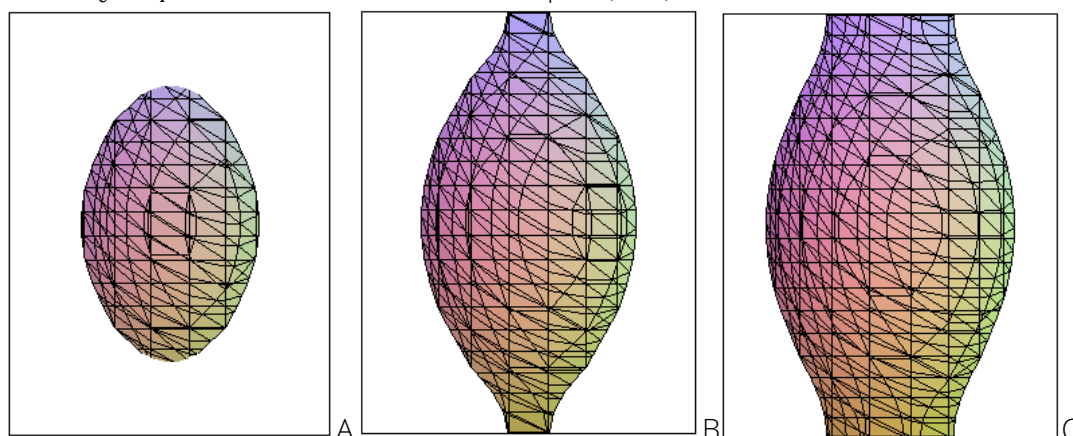


Fig. 1 Transition from a closed (A) Fermi surface to an open one (B, C) with a change in the Fermi energy for a crystal with tetragonal symmetry in a precisely solvable model of an electron in a metal. [3]

Neither the lattice itself, nor its symmetry at such transition does not change, and in electronic properties at zero temperature there is a phase transition when the third derivative of thermodynamic potential goes to infinity. More precisely, the feature has 2.5 derivatives of thermodynamic potential. The finite temperature "blurs" the feature and the third derivative of the thermodynamic potential becomes finite at (see Fig. 2). The effect of finite temperature was first taken into account in a precisely solvable model of an electron in a crystal [3].

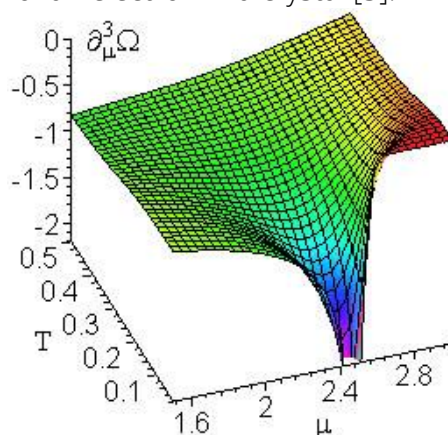


Fig. 2. The third derivative of the thermodynamic potential as a function of Fermi temperature and energy. The calculation was performed in a precisely solvable model of an electron in a metal [3].

Estimates suggested Lifshitz, pointed to the possibility of ETP pressure of several tens of thousands of atmospheres as critical energy, which changes the topology of the Fermi surface of the Fermi energy of the order for standard metals. For most superconductors, except thallium and rhenium, linear dependences of the superconducting transition temperature on pressure were obtained. The nonlinear dependence of the superconducting transition temperature for the waist in the region of low pressures had no explanation for the work [4].

Baryahtar V.G. and Makarov V.I. in their work [4] made assumptions about the existence near the Fermi level of critical energies corresponding to the fine structure of the electronic spectrum. If the Fermi level, changing under the influence of external factors, intersects these points, there is a change in the topology of the Fermi surface. In this case, ETP takes place at relatively low external pressures.

It turned out that the position of the Fermi level is relatively critical, can be influenced by several parameters - impurities of different valencies and pressure. This fact made it possible to create conditions for fairly accurate experiments to study electronic transitions. An impurity of greater valence increases the Fermi energy of the metal. An impurity of lower valence reduces the Fermi energy of the metal. The pressure, as well as impurities of greater valence, increase the Fermi level, as the compression of the metal increases the density of electrons in it. This allowed, combining the parameters of impurity and pressure, to adjust the Fermi level closer to the critical point of the impurity, and then, more smoothly changing the Fermi level by pressure, to observe the Lifshitz phase transition by the thermodynamic characteristics of the metal in normal or superconducting state. [5]

This theory describes the experiment well and makes it possible to obtain quantitative parameters of electronic transitions and to determine the fine structure of the electronic spectrum - the energy gap between the Fermi energy and the critical Fermi energy. An important result, both experimental and theoretical [5-9], was the observation of the extremum in the derivative dependence. This allowed further research to be used as a method for determining the critical values of the isoenergetic surfaces of electrons in metal.

3. Calculation of ETP parameters in the model of finite-band Lamé potentials.

V.G. Baryahtar, E.D. Bilokolos, A.M. Korostil for application to physical problems proposed to consider the Schrödinger equation with three-dimensional separable potential in the form of the sum of three one-dimensional finite-band potentials along orthogonal directions (orthorhombic crystal) [10]. The Schrödinger equation with such potentials has exact solutions, the wave functions and the spectrum are given by analytical functions. The parameters of the model have a simple physical meaning, they are related to the width of the slits at the edges of the Brillouin zone. Separable finite-band Lamé potentials are determined using Weierstrass functions.

$$U_n(x) = -n(n+1)\wp(ix + \omega; \omega, \omega'),$$

The elliptic Weierstrass function has two independent parameters - the half-periods of the potential ω, ω' . Having fixed the period of potential $2|\omega'|$, by means of parameter ω , it is possible to pick up width of cracks along the corresponding direction of the inverted lattice. In this model, the electron wave functions, energy, wave vector, and the number of conduction electron states are completely determined [10].

As already noted, the anomalies in the thermodynamic and kinetic characteristics of metals at low temperatures and high pressures are due to the peculiarities of the energy spectrum of conduction electrons. The density of electronic states as a function E has certain features (Van Hov singularities) near the critical point E_c , where the group velocity of electrons approaches zero.

$$v(E) = \frac{dN(E)}{dE} = \frac{2V}{(2\pi)^3} \int_{E(\mathbf{k})=E} \frac{dS}{|\nabla E(\mathbf{k})|}$$

In the model of the single-zone Lamé potential, the Schrödinger equation has the form:

$$-\Delta\Psi + W(x, y, z)\Psi = E\Psi,$$

$$W(x, y, z) = -2\wp(ix + \tilde{\omega} | \tilde{\omega}, \omega'^1 \tilde{\omega}') - 2\wp(iz + \omega | \omega, \omega') + e_3 + 2\tilde{e}_1$$

The half-periods of the Fermi potential and energy must be chosen so that in the first zone the Fermi surface has the form of a corrugated cylinder elongated along the axis k_z , (see Fig. 1B). Then the potential can be decomposed into a Taylor series of variables x , y and limited to the zero approximation. [11]

The spectrum of the Schrödinger equation

$$-\Delta\Psi + U(x, y, z)\Psi = \varepsilon\Psi,$$

$$U(x, y, z) = -e_3 - \wp(iz + \omega | \omega, \omega')$$

has the following form

$$\begin{cases} E(k_x, k_y, h_z) = k_x^2 + k_y^2 - e_3 + \wp(h_z), \\ k_z = \zeta(h_z) - \frac{\eta'}{\omega'} h_z. \end{cases}$$

The function $\varepsilon(k_x, k_y, k_z)$ in the first zone has two critical points: the minimum and the saddle point, in the second zone it has one critical point - the minimum. Only the first zone is considered below.

Let $E_c = -e_3 + e_2$ the value of the energy at which the Fermi surface opens at the boundary of the Brillouin zone be orthogonal to the axis k_z . Enter the parameter t_0 .

1. When $0 \leq \varepsilon < \varepsilon_c$ we put

$$\varepsilon + e_3 = \wp(t_0 + \omega'), \text{ then } \frac{dt_0}{d\varepsilon} = \frac{1}{\wp'(t_0 + \omega')}.$$

2. When $\varepsilon > \varepsilon_c$ we put $t_0 = \omega$.

Using the parameter, we find the expression for the number of states

$$\begin{aligned} N(\varepsilon) &= \frac{2V}{(2\pi)^3} \int dk_x dk_y dk_z = \frac{2V}{(2\pi)^3} \int (k_x^2 + k_y^2) dk_z = \\ &= \frac{V}{2\pi^2} \int_0^{t_0} [\varepsilon + e_3 - \wp(t + \omega')] \left(-\wp'(t + \omega') - \frac{\eta'}{\omega'} \right) dt \end{aligned}$$

After calculations we receive expressions

$$\begin{aligned} N(\varepsilon) &= \frac{V}{(2\pi)^3} \left[\left(\frac{g_2}{12} - \frac{\eta'}{\omega'} (\varepsilon + e_3) \right) t_0 + \right. \\ &\quad \left. + (\zeta(t_0 + \omega') - \eta') \left(\varepsilon + e_3 - \frac{\eta'}{\omega'} \right) + \frac{1}{6} \wp'(t_0 + \omega') \right] \end{aligned}$$

The density of electronic states is determined by the ratio:

$$v(\varepsilon) = \frac{dN(\varepsilon)}{d\varepsilon} = \frac{V}{2\pi^2} \left(\zeta(t_0 + \omega') - \frac{\eta'}{\omega'} (t_0 + \omega') \right)$$

Directly from the definition parameter t_0 follows

$$v(\varepsilon) = \begin{cases} \frac{V}{2\pi^2} |\mathbf{k}(\varepsilon)|, & \varepsilon < \varepsilon_c, \\ \frac{V}{2\pi} \cdot \frac{1}{2|\omega'|}, & \varepsilon > \varepsilon_c. \end{cases}$$

This expression remains valid in the case of the I Lamé zone potential.

Find the derivative of the density of states.

When $0 \leq \varepsilon < \varepsilon_c$ we receive

$$\frac{dv(\varepsilon)}{d\varepsilon} = -\frac{V}{4\pi^2} \cdot \frac{(\eta'/\omega') + e_3 + \varepsilon}{\varepsilon^{1/2}(e_1 - e_3 - \varepsilon)^{1/2}} \cdot \frac{1}{(\varepsilon_c - \varepsilon)^{1/2}}$$

When $\varepsilon > \varepsilon_c$ we receive $\frac{dv(\varepsilon)}{d\varepsilon} = 0$.

The singularity at the point $\varepsilon = e_1 - e_3$ corresponds to the appearance of the Fermi surface in the second zone. The singularity at the point $\varepsilon = 0$ corresponds to the minimum ε (the origin of the Fermi surface in the center of the Brillouin zone). The singularity at the point $\varepsilon = \varepsilon_c$ corresponds to the saddle point (opening of the Fermi surface at the boundary of the Brillouin zone) [11].

Enter the notation

$$\frac{\alpha}{2} = \frac{V}{4\pi^2} \cdot \frac{|\eta'/\omega' + e_2|}{(e_2 - e_3)^{1/2}(e_1 - e_2)^{1/2}}$$

$$A = \frac{V}{2\pi^2} \cdot \left(\frac{g_2}{12} \omega + \frac{\pi}{2|\omega'|} e_3 - \frac{\eta\eta'}{\omega'} \right),$$

$$B = \frac{V}{2\pi} \cdot \frac{1}{2|\omega'|}$$

$$C = -\frac{V}{2\pi^2} \cdot \left[\frac{e_2^2}{2} \cdot \frac{\pi}{2|\omega'|} + e_2 \left(\frac{g_2}{12} \omega - \frac{\eta'}{\omega'} \eta \right) + \frac{3}{40} g_2 \eta - \omega \left(\frac{\eta'}{\omega'} \cdot \frac{g_2}{12} + \frac{1}{20} g_3 \right) \right].$$

Decompose $\frac{dv(\varepsilon)}{d\varepsilon}$, $v(\varepsilon)$ in a series of powers $(\varepsilon_c - \varepsilon)^{1/2}$, we obtain

$$\frac{dv(\varepsilon)}{d\varepsilon} = \begin{cases} \frac{\alpha}{2} \cdot \frac{1}{(\varepsilon_c - \varepsilon)^{1/2}} + O((\varepsilon_c - \varepsilon)^{1/2}), & \varepsilon < \varepsilon_c, \\ 0, & \varepsilon > \varepsilon_c, \end{cases} \quad (5)$$

$$v(\varepsilon) = \begin{cases} B - \alpha(\varepsilon_c - \varepsilon)^{1/2} + O((\varepsilon_c - \varepsilon)^{3/2}), & \varepsilon < \varepsilon_c, \\ B, & \varepsilon > \varepsilon_c, \end{cases} \quad (6)$$

The experimentally observed features of the superconducting transition temperature under pressure in pure metal are associated with a change in the topology of the Fermi surface as it approaches the critical value of energy. The dependence $T_c(P, c)$ reflects the peculiarities of the density of electronic states $T_c(P, c) \approx v(\varepsilon)$, and the extremum of the dependence $\frac{1}{T_c} \frac{\partial T_c}{\partial P}$ corresponds to the appearance of a new electronic cavity of the Fermi surface. $\frac{\partial T_c}{\partial P} = \frac{\partial T_c}{\partial \varepsilon_f} \frac{\partial \varepsilon_f}{\partial P} \approx$

$\frac{\partial \nu(\epsilon)}{\partial \epsilon_f} \frac{\partial \epsilon_f}{\partial P}$. Where a positive sign $\frac{\partial \nu(\epsilon)}{\partial \epsilon_f}$ corresponds to an electronic cavity and a negative sign corresponds to a hole.

The theoretical calculation of the electron density of conductivity and its derivative for the topological transition with the formation of a new electron cavity is shown in Fig. 3, where the lines show the theoretical dependence $\frac{\partial \nu(\epsilon)}{\partial \epsilon_f}$ and $\nu(\epsilon)$ the points show experimental data on the derivative $\frac{1}{T_c} \frac{\partial T_c}{\partial P}$ and T_c as a function of electron concentration n . For comparison, used experimental data on the system Mo – Re obtained in work [12].

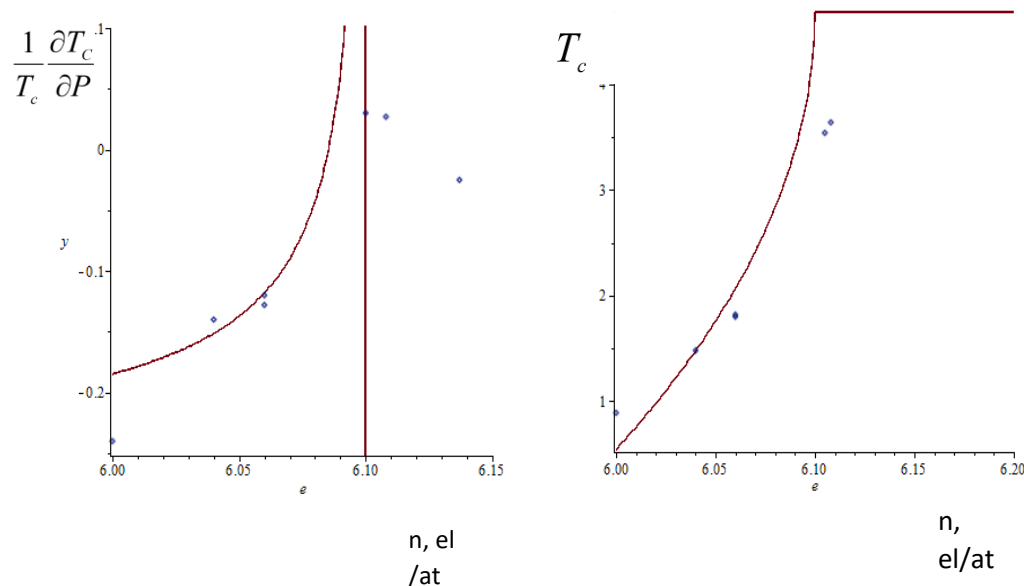


Fig. 3. Dependence $\frac{1}{T_c} \frac{\partial T_c}{\partial P}$ and T_c on the number of valence electrons. Theory (-) and experiment (•).

From fig.3 it is seen that the extremum of the derivative $\frac{1}{T_c} \frac{\partial T_c}{\partial P}$ corresponds to the root feature for $\frac{\partial \nu(\epsilon)}{\partial \epsilon_f}$, which allows to use the obtained formulas to calculate the thin spectrum of most metals. For the system Mo – Re, the value of the energy gap is $\epsilon_c - \epsilon_f = 0.017\text{eV}$ [12].

The following parameters were chosen for the calculations: potential periods $\omega = 1$, $\omega' = 1.52i$, the parameter $\alpha^2 \approx m^*$ has the content of the effective mass at the edge of the Brillouin zone $m^* = -6.25$ [10]. The adjustment parameters are the boundaries of the energy zones e_1, e_2, e_3

To go to the dimensional values, it is necessary $\epsilon, \epsilon_f, \epsilon_c$ to multiply $u_0 = \frac{\hbar^2}{2am}$ by , where the mass of the electron, the characteristic length (lattice parameter ~ 0.314nm), and m^* multiply by \hbar^2/u_0 .

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