Features of the surface tension for the metal–insulator boundary in the vicinity of MI phase transition in the presence of external magnetic field

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The self-consistent equations for MI phase transition are formulated. We assume two order parameters which describe the phase transition. The first one is the density distribution at MI boundary \( \rho(\vec{r}) \). The second one is a two component complex vector in spin space \( \Psi(\vec{r}) \). It determines electron density in metallic or semimetallic phase in the presence of external magnetic field. Two different components of the vector describe possible spin states of electrons inserted in the external magnetic field.

The first order type MI phase transition determined by the variation of the density distribution is considered by means of the gradient expansion of Cahn and Hillard type \([1]\). The second order type transition of electron density beside MI boundary is described by Ginzburg–Landau expansion \([2]\). The obtained nonlinear equations are exactly solved in the case of MI boundary in the presence of parallel to the boundary uniform magnetic field. The surface tension \( \Sigma_{mi} \) at the MI boundary is calculated. It is shown that \( \Sigma_{mi} \) is singular. In particular, \( \Sigma_{mi} \sim n^{3/2} \) as \( n \to 0 \) and \( \Sigma_{mi} \sim (T - T_c(\hat{h}))^{3/2} \). \( T_c(\hat{h}) \) is the transition temperature in the presence of external magnetic field at MI phase transition.

The singular behavior of \( \Sigma_{mi} \) leads to an emphasized hysteresis at MI transition.

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I. INTRODUCTION.

It is well known \([4]\) that the values of surface tension of isolators are more than ten times less than those of metals. The reason of this phenomenon is that the value of surface tension of a metal is determined by outflow of conduction electrons besides the boundary of the metal with vacuum at the distances of the order of interplanar spacing of the metal \([5]\). In addition, the values of surface tension of semimetals are of the same order as in common metals \([4]\). It should be emphasized that the volume electron density in semimetals is of the order of \( 10^{-5} \) from the density of the metals \([4]\).

Any MI transition in a crystalline material, at any rate at zero temperature, must be a transition from a situation in which bands overlap to a situation when they do not \([6]\). Small band-crossing leads to a metallic state with a small number of electron carriers per atomic cell like in semimetals.

II. THE SELF-CONSISTENT EQUATIONS OF MI TRANSITION IN EXTERNAL MAGNETIC FIELD.

Our starting point is two-parameters equation of Ginzburg–Landau type (cf. \([3]\)). One of the order parameters of the transition is the density \( \rho(\vec{r}) \) of metallic and isolator phases. The second order parameter is the electron carriers density which is described as a column with two complex components of electron wave function with different spin components:

\[
\Psi(\vec{r}) = \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_2(\vec{r}) \end{pmatrix}, \quad \Psi^+(\vec{r}) = (\psi_1^*(\vec{r}), \psi_2^*(\vec{r}))
\]

Generally, \( \psi_1(\vec{r}) \) and \( \psi_2(\vec{r}) \) are two complex valued functions for two components of spin. We put the following invariant scalar quantity:

\[
n(\vec{r}) = |\psi_1(\vec{r})|^2 + |\psi_2(\vec{r})|^2 \equiv (\Psi^+ \Psi)
\]

which is electron density in the metallic phase and becomes identically zero in the insulator phase at \( T = 0 \).

There are two additional invariant scalar quantities in the presence of magnetic field: 1) the energy of the magnetic field \( (\vec{h})^2 / 8\pi \) and 2) the convolution made by \( \Psi^+ \) and \( \Psi \) of scalar product consisting from two vectors. One of the vectors is the magnetic field vector \( \vec{h} \). The second is Pauli vector matrix \( \vec{\sigma} = i\sigma_x + j\sigma_y + k\sigma_z \).

So, the Ginzburg-Landau functional may be assumed:

\[
\Phi = \Phi(\rho, \Psi, \Psi^+) = \int d\vec{r} F(\rho, \Psi, \Psi^+).
\]

The functional for \( \rho(\vec{r}) \) is expanded according to Cahn–Hillard \([1]\), see also \([7]\), and the Ginzburg-Landau expansion \([2]\) is used for electron density. The result is:

\[
F(\rho, \Psi, \Psi^+) = \varphi(\rho) + \lambda(\rho)(\nabla \rho)^2 + (\alpha + g(\rho))(\Psi^+ \Psi) + (\Psi^+ \Psi) + (\Psi^+ \Psi)
\]

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Here prime means derivative on $x$. We consider the solution of the equation (10) for $g \equiv 0$ when order parameters $\rho(x)$ and $\Psi(x)$ are not connected. The equation (11) can be easily integrated:

$$x = \int_{\rho_{min}}^{\rho_{max}} \lambda(\rho') d\rho' \left( \int_{\rho_{min}}^{\rho'} \varphi'(\kappa) \lambda(\kappa) d\kappa \right)^{-1/2} \quad (11)$$

If the value $\lambda(\rho)$ does not depend on $\rho$, the equation (11) becomes as follows [7]:

$$x = \int_{0}^{\rho_{max}} d\rho \sqrt{\varphi(\rho)} \sqrt{\varphi(\rho) \lambda(\rho)} \quad (12)$$

It is important to take into account the dependence $\lambda(\rho)$ from $\rho$ as the value $\lambda$ in metallic phase can differ significantly from that in isolator phase.

Let dimension $|\varphi| = \varepsilon$ is the density of energy. In this case the value of $\lambda$ has dimension $|\lambda| \approx c\varepsilon l^2 \rho^{-2}$ and proportional to $l^2$, where $l$ is the length of the variation of density $\rho$. The value of surface tension $\Sigma_\rho$ of MI interface reads as follows [2]:

$$\Sigma_\rho = 2 \int_{\rho_{min}}^{\rho_{max}} d\rho \sqrt{\varphi(\rho) \lambda(\rho)} \quad (13)$$

Here we use only two first terms of (4). The value of the surface tension is $\Sigma_\rho \approx c\varepsilon l$. So, it has the dimension of energy attributed to unit of area. If $\lambda \Rightarrow 0$, the surface tension becomes zero. If $l$ grows, the surface tension will grow as well.

We assume the magnetic field is a function only of one coordinate $x$ perpendicular to MI boundary. In addition, we assume the magnetic field has a component $h_x(x)$ in the plane of the MI boundary and a component $h_z(x)$ perpendicular to it. So, the magnetic field and the vector potential in Landau gauge [5] are as follows: $\vec{h} = (h_x(x), 0, h_z(x))$; $\vec{A}(\vec{r}) = \left(0, \int_{-\infty}^{x} h_z(x') dx'$, $-zh_x(x), 0\right)$.

For simplicity, we assume that MI transition is not accompanied by magnetic phase transition. In this case, we take $h_x$ and $h_z$ do not depend on $x$ and the equation (11) becomes:

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2 \Psi}{\partial x^2} + \left( \frac{\partial}{\partial y} - \frac{e}{\hbar c} (xh_z - zh_x) \right)^2 \Psi + \frac{\partial^2 \Psi}{\partial z^2} \right) +$$

$$+ \hat{\alpha} \Psi + \beta (\Psi^+ \Psi) \Psi + \mu \left(\frac{h_z}{h_x} \Psi \right) = 0$$

$$\hat{\alpha} = (\alpha + g(\rho))$$

We take $\vec{A}(\vec{r}) \equiv 0$. It means we neglect the orbital motion of electrons in magnetic field in the metal. It is
correct if electron free path $l_c$ is less than the radius of the electron orbit in magnetic field $r_h$:

$$l_c < 2\pi r_h, \quad r_h = \frac{q_F}{e\hbar}, \quad p_F - \text{Fermi momentum.} \quad (15)$$

The magnetic field does not influence the motion of an electron between successive collisions. It means the influence of magnetic field cannot be seen during electron mean free time. Really, an electron moves straight line trajectory between successive collisions. The inequality $15$ corresponds exactly to Dingle factor $10$ which determines the absence of de Haas – van Alpen oscillations due to impurity scattering. In addition, it is assumed diffuse reflection at MI boundary.

The other possibility when $\tilde{A}(\vec{r}) \equiv 0$ corresponds the following inequality:

$$\xi_F < 2\pi r_h, \quad (16)$$

$\xi_F$ is the correlation length in the electron Fermi gas in metal. Due to $9$, $\xi_F = h\nu_F/\pi T$. The substitution of the last equation into (16) gives the inequality for the temperatures for which $\tilde{A}(\vec{r})$ can be neglected:

$$2\pi^2 T > h\Omega_h, \quad \Omega_h = \frac{e\hbar}{mc} \quad (17)$$

The inequality $17$ coincides with the condition of the absence of de Haas – van Alpen effect due to the low value of the magnetic field as compared with the temperature $13$.

If $\tilde{A}(\vec{r}) \equiv 0$, we can write (14) as a system of two connected nonlinear equations for components $\Psi(x)$ [11]:

$$\frac{-\hbar^2}{2m} \frac{d^2}\psi_1 + \tilde{\alpha}\psi_1 + \tilde{\beta}(|\psi_1|^2 + |\psi_2|^2) \psi_1 + \mu(h_x\psi_2 + h_z\psi_1) = 0 \quad (18)$$

$$\frac{-\hbar^2}{2m} \frac{d^2}\psi_2 + \tilde{\alpha}\psi_2 + \tilde{\beta}(|\psi_1|^2 + |\psi_2|^2) \psi_2 + \mu(h_x\psi_1 - h_z\psi_2) = 0 \quad (19)$$

We try to find solutions of the system (18) - (19) in the following way:

$$\psi_2(x) = q\psi_1(x), \quad (20)$$

$q$ is a certain constant determined by $h_x$ and $h_z$. The equations (18) and (19) coincide identically provided the following equation is valid:

$$h_xq + h_z = \frac{h_x}{q} - h_z \quad (21)$$

It is clear that if $q = q_{\pm}$

$$q_{\pm} = \frac{|h_x|}{\sqrt{h_x^2 + h_z^2 + h_z sgn h_x}} \quad \text{and} \quad q_{-} = -\frac{1}{q_{+}} \quad (22)$$

the equations (18) and (19) coincide one with another. We rewrite the equation (18) as follows:

$$-\frac{\hbar^2}{2m} \frac{d^2}\psi_1 + \tilde{\alpha}\psi_1 + \tilde{\beta}(1 + q^2)|\psi_1|^2\psi_1 = 0 \quad (23)$$

$$\tilde{\alpha} = \tilde{\alpha} + \mu(h_xq + h_z), \quad \tilde{\beta} = \tilde{\beta}(1 + q^2); \quad q = q_{\pm}.$$}

The nonlinear equation (23) has two uniform solutions. The first one $\psi_1 \equiv 0$ corresponds to the phase of isolator. The second one $\psi_0$ corresponds to the metallic phase with the following square modulus of the order parameter:

$$|\psi_0|^2 = -\frac{\tilde{\alpha}}{\tilde{\beta}(1 + q^2)} \quad (24)$$

The value $|\psi_0|^2 = q^2|\psi_0|^2$ corresponds to the value $|\psi_0|^2$. The sum of these quantities (see (2)) equals to the bulk electron density of metal $n_0$: $|\psi_1|^2 + |\psi_0|^2 = n_0$,

$$|\psi_1|^2 = \frac{n_0}{1 + q^2}, \quad |\psi_0|^2 = \frac{q^2 n_0}{1 + q^2}.$$}

We introduce the dimensionless function (23) as follows:

$$\psi_1(x) = \psi_0 f(x) \quad (25)$$

The equation (23) becomes:

$$-\xi^2(T) \frac{d^2f}{dx^2} - f + f^3 = 0, \quad \xi(T) = \sqrt{\frac{\hbar^2}{2m|\tilde{\alpha}|}} \quad (26)$$

The function $f(x)$ satisfies the following boundary conditions:

$$f = 0, \quad \text{if} \quad x = 0$$

$$f \to 1, \quad \text{if} \quad x \to \infty$$

The equation (20) has the solution (cf. (11)):

$$f(x) = \tanh\left[\frac{x}{\sqrt{2\xi(T)}}\right] \quad (27)$$

In the vicinity of phase transition $\tilde{\alpha}$ becomes zero. $|\psi_0|^2$ and $|\psi_0|^2$ have square root singularity (see (24)). The function $f(x)$ changes its value at the coherence length $\xi(T)$. The coherence length goes to infinity like square root singularity (26).

The calculation of the surface tension for MI boundary is in analogy with that for the metal – superconductor boundary (see (11)) and gives the following equation:

$$\Sigma_\Phi = \tilde{\alpha}\psi_1^2(1 + q^2) \int_0^\infty dx \left(\xi^2(T) \left(\frac{df}{dx}\right)^2 - \frac{1}{2}(1 - f^2)^2\right)$$

We use the first integral of the equation (26):

$$\xi^2(T) \left(\frac{df}{dx}\right)^2 = \frac{1}{2}(1 - f^2)^2$$
and arrive at a goal:

\[ \Sigma_{\Psi} = -\tilde{\alpha}\psi_1^2(1 + q^2) \int_0^\infty dx(1 - f^2)^2 = \]

\[ = -\tilde{\alpha}\psi_1^2(1 + q^2)\sqrt{2\xi(T)} = \beta\sqrt{2n_0^2}\xi(T) \quad (28) \]

It leads to \( \Sigma_{mi} \sim n_0^{3/2} \) in the limit \( n_0 \to 0 \). In the vicinity of the point MI transition in the magnetic field \( T_c(\vec{h}) \) the value \( \Sigma_{mi} \sim (T - T_c(\vec{h}))^{3/2} \).

So, the surface tension at MI boundary becomes as follows:

\[ \Sigma_{mi} = \Sigma_{\rho} + \Sigma_{\Psi} + \Sigma_{\rho\Psi} \quad (29) \]

\( \Sigma_{\rho} \) is determined by \( [13] \), and \( \Sigma_{\Psi} \) by \( [28] \). \( \Sigma_{\rho\Psi} \) is determined by interaction between two order parameters \( \rho(\vec{r}) \) and \( \Psi(\vec{r}) \) and its value is of the order of \( [28] \). However, it contains an additional factor proportional to \( g(\rho) \).

### IV. CONCLUSIONS.

The system of equations formulated in spin space describes MI phase transition in the external magnetic field. The exact solution of this nonlinear system of equations is obtained in the external uniform magnetic field. The magnetic field has an arbitrary direction relative to the MI boundary.

It is shown that the surface tension for MI boundary has a singular behavior. The point of phase transition behaves in different manner for the parallel to the boundary component of the magnetic field and for perpendicular one. We assumed that the orbital motion in the magnetic field is suppressed due to some type of scattering in the system as it usually takes place for MI phase transitions. It can be scattering on impurities or temperature suppression of coherent motion.

The singular behavior manifests itself for other thermodynamic and kinetic features of the system close to MI transition. Probably, it take place in binary compounds with B20 structure like MnSi, FeSi and FeGe, where recently uncommon properties where found. In particular, in the FeSi compound was found MI transition accompanied by anomalies of phonon spectra with a strong temperature dependence \( [12] \). It was discovered significant softening of phonon spectrum by increase of temperature in the vicinity of MI phase transformation \( [13] \).

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[1] J.W. Cahn and J.E. Hillard, J. Chem. Phys. 28 , 258 (1958); ibid. 42 , 93, (1964).
[2] L.P. Pitaevskii, E.M. Lifshitz (1980). Statistical Physics, Part 2. Vol. 9 (1st ed.). Butterworth-Heinemann. ISBN 978-0-7506-2636-1.
[3] Jinwu Ye, Phys. Rev. Lett., 97, 125302 (2005); P. M. Chaikin and T. C. Lubensky, Principles of Condensed Matter Physics, Cambridge university press, 1995.
[4] Tables of physical quantities. Editor I. K. Kikoin. M., Atomizdat, 1976.
[5] M.B. Partensky UFN, 128, 69 (1979)
[6] N. F. Mott, "Metal-Insulator" Second Edition Taylor&Francis London–New York–Philadelphia, 1990.
[7] I. M. Lifshits and Yu. Kagan. Sov. Phys. JETP 35, 206 (1972)
[8] L.D. Landau, E.M. Lifshitz (1977). Quantum Mechanics: Non-Relativistic Theory. Vol. 3 (3rd ed.). Pergamon Press. ISBN 978-0-08-020940-1.
[9] L.D. Landau, E.M. Lifshitz (1980). Statistical Physics. Vol. 5 (3rd ed.). Butterworth-Heinemann. ISBN 978-0-7506-3372-7.
[10] R. B. Dingle, Proc. Roy. Soc. A211, 517 (1952).
[11] P. G. De Gennes Superconductivity of Metals and Alloys, W. A. Benjamin, INC. New York – Amsterdam (1966).
[12] O. Delaire, K. Marty, M.B. Stone, P.R.C. Kent, M.S. Lucas, D.L. Abernathy, D. Mandrus, B.C. Sales, PNAS, 108, 12, 4725 (2011).
[13] P. P. Parshin, P. A. Alekseev, K. S. Nemkovskiy, J. Persson, A. I. Chumakov, R. Rueffer, Sov. Phys. JETP (in print)