The surface tension at the metal-insulator phase transition in the magnetic field.

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Abstract. Any metal-insulator transition in a crystalline matter must be the transition from a situation in which the electronic bands overlap to that when they do not [1]. On the basis of the phenomenological theory [2], various singularities are considered in the magnetic field for the surface tension at the metal-insulator contact. The surface tension displays also the quantum magnetic oscillations at low temperatures [3]. The consideration is applied to the Mott insulator in the magnetic field.

1. Introduction.
It is well known [4, 5] that the characteristic magnitudes for the surface tension in insulators are one order of magnitude lower than those in metals. The physical mechanism underlying this difference is related to the conduction electrons penetrating outside from the interface to vacuum at a distance of order of about atomic layer spacing in the metal bulk [6, 7]. At the same time, the surface tension of semimetals with the characteristic electron density differing from that of usual metals by the factor $10^{-6} - 10^{-5}$ is about the same order of that of usual metals [5].

The metal-insulator transitions (MIT) in crystals are (at least at zero temperature) transitions from the state where the electron bands overlap to the state with no overlapping [1]. The weak overlapping is responsible for the transition to the metallic semimetal-type state with the number of charge carriers per unit cell being far below unity and typical for the case of semimetals.

We consider the self-consistent equations of MIT in the external magnetic field. The MIT belongs to the first-order phase transition with the order parameter corresponding to the transition of matter density $\rho(\vec{r})$ for two different phases, metallic and isolating. The MIT is accompanied by appearing the second-order parameter, namely, electron density vanishing in the insulator phase.

The new order parameter is the electron and holes densities in two bands. The density of electrons and holes can be described by a vector in the Hilbert space with electronic and hole components $\Upsilon(\vec{r})$. Here $\Upsilon(\vec{r})$ is a vertical column and $\Upsilon^+(\vec{r})$ is a horizontal row:

$$\Upsilon(\vec{r}) = (u^+ \uparrow(\vec{r}), v^+ \uparrow(\vec{r}), u^\downarrow(\vec{r}), v^\downarrow(\vec{r}), u^\downarrow(\vec{r}), v^\downarrow(\vec{r})).$$

The components of vector $\Upsilon(\vec{r})$ are the functions of electrons and holes for the up and down spins. In the absence of magnetic field all these components of the vector $\Upsilon(\vec{r})$ are real functions.
2. The Phenomenological Theory of Metal-Insulator phase transition.

The role of these two order parameters \(\rho(\vec{r})\) and \(\Upsilon(\vec{r})\) is quite different. The density \(\rho(\vec{r})\) governs a position of the MIT as a function of pressure and temperature \((p, T)\). The order parameter \(\Upsilon(\vec{r})\) becomes nonzero just in the point \(\rho = \rho_c(p, T)\). However, the physical properties of the system depend weakly on \(\rho\) alone. On the other hand, the value of \(\Upsilon(\vec{r})\) can drastically change the physical properties of the system. In particular, the surface tension \(\Sigma\) of the MI interface depends only weakly on \(\rho\) and is determined to a great extent by the variation of \(\Upsilon(\vec{r})\).

The physical reason of the phenomenon is an outflow of conduction electrons to the MI interface \(\rho(\vec{r})\) at a fixed temperature, say, at \(T = 0\). We expand the functional \(F(\rho, \Upsilon, \Upsilon^+)\) in the vicinity of \(\rho(\vec{r})\) and \(\Upsilon(\vec{r})\):

\[
\Phi = \Phi[\rho, \Upsilon, \Upsilon^+] = \int d^2r F(\rho, \Upsilon, \Upsilon^+), \\
F = F_\rho(\rho(\vec{r})) + F_\Upsilon(\Upsilon(\vec{r})) + F_{\text{int}}(\rho(\vec{r}), \Upsilon(\vec{r})).
\]

The parameter \(\rho(\vec{r})\) describes the first-order phase transition between the insulating and metal phases whereas the vector function \(\Upsilon(\vec{r})\) describes the second-order phase transition. We expand the functional \(F_\rho(\rho(\vec{r}))\) according to the Cahn–Hilliard approximation [9], see also [10]:

\[
F_\rho(\rho(\vec{r})) = \varphi(\rho) + \frac{1}{2}\lambda(\rho)(\nabla \rho)^2.
\]

We use the Ginzburg-Landau expansion [11] for \(\Upsilon(\vec{r})\):

\[
F_\Upsilon(\Upsilon(\vec{r})) = \alpha(\Upsilon^+)\Upsilon + \frac{1}{2}\beta(\Upsilon^+)^2 + \frac{\hbar^2}{2m} (\nabla \Upsilon^+) \nabla \Upsilon(\vec{r}) ;
\]

\[
\alpha = \alpha_0 - \rho_c.
\]

Here we have expanded coefficient \(\alpha\) linearly in \(\rho\) in the vicinity of \(\rho_c\). It is analogous to the well-known expansion of the appropriate parameter in temperature \(T\) [11] for the Landau theory of the second-order phase transition. The expansion proposed is convenient for investigating the MIT at a fixed temperature, say, at \(T = 0\). The interaction term \(F_{\text{int}}(\rho(\vec{r}), \Upsilon(\vec{r}))\) is taken as a linear function of \(n(\vec{r})\) (cf. [2]):

\[
F_{\text{int}}(\rho(\vec{r}), \Upsilon(\vec{r})) = g(\rho) (\Upsilon^+ \Upsilon).
\]

The variation of \(\Phi = \Phi[\rho, \Upsilon, \Upsilon^+]\) in \(\rho(\vec{r})\) and \(\Upsilon^+(\vec{r})\) gives the self-consistent equations of the Ginzburg-Landau type for the MI phase transition:

\[
\lambda^{1/2}(\rho) \nabla \left( \lambda^{1/2}(\rho) \nabla \rho(\vec{r}) \right) = \frac{d\varphi}{d\rho}(\rho) + \frac{dg}{d\rho}(\Upsilon^+) \Upsilon,
\]

\[
-\frac{\hbar^2}{2m} \nabla^2 (\Upsilon + \beta (\Upsilon^+) \Upsilon) = 0.
\]
In the case $g \equiv 0$, the parameters $\rho$ and $\Upsilon$ are independent and the surface tension $\Sigma$ at the interface between the metallic and the insulating phases can be calculated separately for $\rho$ and $\Upsilon$, correspondingly $\Sigma_\rho$ and $\Sigma_\Upsilon$. The surface tension $\Sigma_\rho$ can readily be calculated as [2, 10]:

$$
\Sigma_\rho = \int_{\rho_{\text{ins}}}^{\rho_{\text{met}}} d\rho \sqrt{\varphi(\rho)\lambda(\rho)/2} .
$$

(8)

3. The surface tension at the MI interface in the magnetic field

We consider the surface tension in the external magnetic field. In the functional (5) we should include the energy of the magnetic field, namely $H^2/8\pi$. Also we should involve $[\nabla - e/\hbar c \vec{A}]$ instead of nabla $\nabla$ and also $[\mu(\Upsilon^+ \vec{H} \sigma \Upsilon)]$ [2]. Here $\sigma$ is the Pauli matrix. So, we arrive to the following equation, where $x$ is the coordinate perpendicular to the interface:

$$
-\frac{\hbar^2}{2m} \left( \frac{d^2 \Upsilon}{dx^2} \right) + (\alpha + g \rho) \Upsilon + \beta (\Upsilon^+ \Upsilon) \Upsilon + \hat{\Lambda}(\vec{H}) \Upsilon = 0 .
$$

(9)

Here the operator $\hat{\Lambda}(\vec{H})$ is the four-row matrix [2] determined by the magnetic field $\vec{H} = i \vec{H}_z + \vec{k} \vec{H}_z$. The vector $\vec{k}$ is directed along the metal-insulator boundary and the vector $\vec{i}$ is parallel to the boundary. The Equation (9) can be reduced to the following one:

$$
-\xi_{\vec{H}}^2(T) \frac{d^2 f}{dx^2} - f + f^3 = 0 , \quad \xi_{\vec{H}}(T) = \sqrt{\frac{\hbar^2}{2m|\alpha|}} , \quad g = 0 .
$$

(10)

Here the dimensionless function $f(x)$ has the following solution $f(x) = \tanh \left[ \frac{x}{\sqrt{2}\xi_{\vec{H}}(T)} \right]$. Here $\xi_{\vec{H}}(T)$ and $f(x)$ are the functions of the magnetic field $\vec{H}$. The calculation of the surface energy $\Sigma_\Upsilon$ is straightforward and gives:

$$
\Sigma_\Upsilon = \frac{2\sqrt{2}}{3} \xi_{\vec{H}}(T) \beta n_0^2 .
$$

(11)

Here $n_0$ is the bulk density of electrons in the metal. If we put $n_0$ to be of the order of unity per crystal cell, for $\Sigma_\Upsilon$ (11) we get the typical magnitude for metals.

In addition, we consider the surface tension oscillations in the external magnetic field. In this case we should replace $\vec{H}$ for $\vec{H} + 4\pi \vec{M}$ in (9)[2, 3]. Here we have [2, 3] to substitute

$$
\hat{\vec{M}} = \vec{H} - (\Upsilon^+ \Upsilon) \frac{\partial \Omega}{(\Upsilon^+ \Upsilon)} .
$$

The quantity $\Omega$ is the thermodynamical potential [11]. The oscillating magnetic moment has the following structure [3]:

$$
\hat{\vec{M}} = \Im \vec{A} \exp[iN(\epsilon_F)] \exp \left( -\frac{2\pi^2 T}{\hbar \omega_c} \right) ,
$$

$$
N(\epsilon_F) = \left( \frac{\epsilon_F}{\hbar \omega_c} \right) , \quad \hbar \omega_c = \frac{eH}{mc} .
$$

The quantity $N(\epsilon_F)$ is the number of Landau levels under the Fermi surface, $N(\epsilon_F) \gg 1$. And $|\vec{A}| \cong |\sqrt{N(\epsilon_F)} \ast M_{mon}|$ [3, 11].
4. Conclusions.
Based on the Ginzburg-Landau expansion, the phenomenological theory of metal-insulator phase transition in the magnetic field is considered.

The surface tension $\Sigma_T$ (7) is investigated for the various situations. It is shown that the typical magnitude of the metal surface tension is much larger than that for insulators. The singularities and the surface tension oscillations in the external magnetic field are considered.

So far, we have considered the system of non-interacting electrons and holes. If we replace the constant $\beta$ (5) with an operator $\hat{\beta}$ that takes the electron-hole interaction into account, we will come to an insulator even for the overlapping bands, namely, to the Mott insulator. However, this approach leads only to an effective description of the phenomenon. The self-consistent approach is to take into account the Coulomb interaction based on the Hubbard interaction [12, 13, 14]. This requires the splitting of the electronic band into two subbands (Hubbard bands [14] based on the consideration in Ref. [12]) and leads to a significant modification of the electronic order parameter $\Upsilon(r)$.

At last, it should be emphasized that the Mott insulator under the influence of magnetic field can turn into a metallic, or more precisely, semi-metallic state. In this case, we are talking about a sufficiently weak Hubbard interaction, so that the magnetic fields of $\sim 10^5$ kOe are sufficiently strong for the transition to the semi-metallic state. This can be compared with the transition of semimetals Bi and Sn to the insulator state (see [15]). In the Mott insulator the surface tension is much less as compared with the case when the system becomes semi-metallic one.

5. References
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