

LOCALIZED STATES AT THE HELICOIDAL PHASE TRANSITION

A.Buzdin, Y.Meurdesoif

*CPTMB-LPT, University Bordeaux I
33175 Gradignan Cedex, France*

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The appearance of new type of localized states at the helicoidal transition is predicted. The order parameter decays with the oscillation in the vicinity of the defect provoking localized transition. The cases of point-like, linear and planar defects are considered and the specific heat jumps are calculated.

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1. Introduction. The presence of different defects and inhomogeneities may strongly influence the phase transition in bulk materials. One of examples are the surface defects. If near the surface, the local transition temperature is somewhat higher than in the volume, then the localized near-the-surface state appears at temperature T_{CL} slightly above the volume critical temperature T_{C0} . This situation is characteristic for surface magnetism [1], superconductivity localized near twinning plane [2] and local structure transition [3].

If the Landau functional approach is used to describe the phase transition, the local increase of transition temperature can be modelled by a δ -functional contribution to the free energy density $-\gamma\delta(r)\psi^2$ where ψ is the order parameter. The problem of critical temperature of the localized transition is then reduced to the determination of the eigenvalue of a corresponding equation for the order parameter $\psi(r)$. This equation, when the gradient term in the Landau free energy functional has the usual form $\sim(\nabla\psi)^2$, is just the Schrödinger equation with δ -functional potential and self energy $E \sim (T_{CL} - T_{C0})$ (see for example [1,2]). The one dimensional potential well always has a localized state with negative energy [4] (note that local increase of transition temperature corresponds to weak negative δ -functional potential). Then near the surface (or plane defect) the temperature of localized transition will be higher than the volume one $T_{CL} - T_{C0} \sim \gamma^2$. For the linear defect the difference is exponentially small [4] and eventually non-observable. In the case of a point-like defect the local transition is absent, as there is no localized state for weak three dimensional δ -functional potential [4].

The situation however occurs to be quite different in the case of phase transition into a helicoidal state. To be more specific, we will consider the magnetic helicoidal transition like that the one observed for example in MnSi [5] and FeGe [6]. In the absence of the center of symmetry in the crystalline structure, the magnetic free energy functional contains the terms $\sim \lambda \mathbf{M} \cdot \text{rot} \mathbf{M}$ (where \mathbf{M} is the local magnetization) which leads to formation of the helicoidal magnetic structure [7]. The same is true also for cholesteric liquid crystal [8].

In the present article, we demonstrate for helicoidal-type transition that even the point-like increase of transition temperature leads to the formation of a very specific localized state above the bulk critical temperature. We calculate the

structure and thermodynamical characteristics of such unusual localized states near the point-like, linear defects and plane defect.

2. Localized state near a point defect. We consider the problem using the Landau-type functional for magnetic free energy:

$$F = \frac{n\theta}{M_s^2} \int \left[\tau M^2 + \frac{b}{2} M^4 + a^2 (\nabla M_x)^2 + a^2 (\nabla M_y)^2 + a^2 (\nabla M_z)^2 + \lambda \mathbf{M} \cdot \text{rot} \mathbf{M} - \gamma M^2 \delta(\mathbf{r}) \right] d^3 \mathbf{r}. \quad (1)$$

where θ is of the order of magnetic transition temperature T_{C0} , n the density of magnetic atoms, M_s - the saturated magnetization at $T = 0$, and $\tau = (T - T_{C0})/T_{C0}$. Note that T_{C0} is the critical temperature of ferromagnetic transition which occurs in the absence of the term $\lambda \mathbf{M} \cdot \text{rot} \mathbf{M}$. In the presence of this term (the case of the crystalline lattice without center of symmetry), the transition into helicoidal magnetic structure occurs at some temperature T_C higher than ferromagnetic transition temperature ($(T_C - T_{C0})/T_{C0} = \tau_0 = (\lambda/2a)^2$). The term $-\gamma M^2 \delta(\mathbf{r})$ describes the local increase of transition temperature near the point like defect, magnetic stiffness coefficient a is of the order of interatomic distance, and coefficient b has the usual sense. For simplicity, and bearing in mind MnSi, we consider a functional for the cubic crystal symmetry.

To reduce the number of coefficients, it is convenient to change the variable introducing $\mathbf{r}' \rightarrow \mathbf{r}/a$, and further we omit the prime. First we consider the question of the temperature of the localized transition and the appearing magnetic structure. For that we may neglect the term $\sim M^4$ in functional (1) and write it in Fourier-representation as:

$$F = \frac{n\theta}{M_s^2} V \sum_{\mathbf{q}} \left[(\tau + q^2) \mathbf{M}_{\mathbf{q}} \cdot \mathbf{M}_{-\mathbf{q}} + i \tilde{\lambda} \mathbf{M}_{-\mathbf{q}} (\mathbf{q} \times \mathbf{M}_{\mathbf{q}}) - \tilde{\gamma} \sum_{\mathbf{q}} \mathbf{M}_{\mathbf{q}} \cdot \mathbf{M}_{\mathbf{q}}' \right]. \quad (2)$$

where $\tilde{\lambda} = \lambda/a$ and $\tilde{\gamma} = \gamma a^3$.

Minimizing the energy over $\mathbf{M}_{\mathbf{q}}$ after some algebra we obtain

$$\begin{aligned} \mathbf{M}_{\mathbf{q}} \left[\tilde{\lambda}^2 q^2 - (\tau + q^2)^2 \right] &= i \tilde{\gamma} \tilde{\lambda} (\mathbf{q} \times \mathbf{M}_0) + \frac{\tilde{\gamma} \mathbf{M}_0 \left[\tilde{\lambda}^2 q^2 - (\tau + q^2)^2 \right]}{(\tau + q^2)} + \\ &+ \frac{\tilde{\gamma} \tilde{\lambda}^2 [\mathbf{q} (\mathbf{q} \cdot \mathbf{M}_0) - q^2 \mathbf{M}_0]}{(\tau + q^2)}, \end{aligned} \quad (3)$$

where $\mathbf{M}_0 = \mathbf{M}(\mathbf{r}=0)$ is the magnetization at the localized defect. In the absence of defect, for $\tilde{\gamma} = 0$, we have from (3) $\tau = \tilde{\lambda} q - q^2$. The actual wavevector of the helicoidal state corresponds to the maximum temperature over q . This maximum is realized for $q = q_0 = \tilde{\lambda}/2$, and the transition temperature is $\tau_0 = \tilde{\lambda}^2/4$ which is naturally higher than ferromagnetic critical temperature ($\tau = 0$). If we are interested in the formation of the localized state just above the bulk transition at $\delta\tau = \tau - \tau_0 \ll \tau_0$, the singular part of $\mathbf{M}_{\mathbf{q}}$ will be related with the wavevector $|\mathbf{q}| \simeq q_0$, and we obtain from (3) the following expressions for $\mathbf{M}_{\mathbf{q}}$

$$\mathbf{M}_{\mathbf{q}} = -\frac{i \tilde{\gamma} (\mathbf{q} \times \mathbf{M}_0)}{\tilde{\lambda} [\delta\tau + (q - q_0)^2]} - \frac{2 \tilde{\gamma} [\mathbf{q} (\mathbf{q} \cdot \mathbf{M}_0) - q^2 \mathbf{M}_0]}{\tilde{\lambda}^2 [\delta\tau + (q - q_0)^2]}. \quad (4)$$

The critical temperature for the appearance of the localized solution is given by the "self-consistent" equation

$$M_0 = M(0) = \int M_q \frac{d^3 q}{(2\pi)^3}. \quad (5)$$

The main contribution to the integral (5) comes from the region $|q| \simeq q_0$. Taking this into account we obtain for the shift of transition temperature $\delta\tau_C = \tau_{CL} - \tau_0$, (where τ_{CL} is the critical temperature for the localized state): $\delta\tau_C = (\tilde{\gamma}\tau_0/6\pi)^2$. Then even a small local increase of "bare" transition temperature gives rise to localized state appearance. This property is a characteristic of the helicoidal transition and is absent for the ferromagnetic one.

After Fourier transform of (4), we obtain the distribution of the magnetic moment in the real space. Choosing z axis along $M(0)$, in cylindrical coordinates it may be written as

$$\begin{aligned} M_\rho &= \frac{3}{2}M(0)\sqrt{\frac{\pi}{2}} \frac{(q_0\rho)(q_0z)}{[(q_0\rho)^2 + (q_0z)^2]^{\frac{3}{4}}} J_{\frac{3}{2}} \left(\sqrt{(q_0\rho)^2 + (q_0z)^2} \right), \\ M_\varphi &= \frac{3}{2}M(0)\sqrt{\frac{\pi}{2}} \frac{(q_0\rho)}{[(q_0\rho)^2 + (q_0z)^2]^{\frac{3}{4}}} J_{\frac{3}{2}} \left(\sqrt{(q_0\rho)^2 + (q_0z)^2} \right), \\ M_z &= \frac{3}{2}M(0) \int_0^{\pi/2} \sin^3 \theta J_0(q_0\rho \sin \theta) \cos(q_0z \cos \theta) d\theta \end{aligned} \quad (6)$$

Note that calculating Fourier transform of (4) we have put $q = q_0$ at the nominator, which is justified at the distance $|r|2\pi/(q_0\sqrt{\delta\tau_C})$ around the defect. At larger distances, the magnetic moment decreases exponentially and the effective volume V of the localized state is $V \sim q_0^{-3}(\delta\tau_C)^{-3/2}$. It increases when $\delta\tau_C \rightarrow 0$ which is a general phenomenon for localized states [1-3] and is related with the divergency of the effective coherence length near T_C . Then for smaller $\tilde{\gamma}$ the localized state appears closer to bulk transition temperature but its dimensions becomes larger. The structure (6) of the localized state is rather complicated. In Fig. 1, the distribution of the magnetic moment in the plane $z = 2\pi/q_0$ is presented.

Knowing the magnetic moment distribution, we may obtain the jump of specific heat at such localized transition.

$$\Delta C = \frac{n\theta}{M_S^2 b T_{C0}} \frac{\left[\int M^2 d^3 r \right]^2}{\int M^4 d^3 r} = \frac{n\theta}{M_S^2 b T_{C0}} \frac{2\pi}{I} \left(\frac{2}{3} \right)^2 \frac{1}{q_0 \delta\tau_C}$$

where the factor $I \simeq 1.17$, comes from numerical evaluation of the integral. The divergency of ΔC when $\tilde{\gamma} \rightarrow 0$ can be explained due to the rise of the effective volume when $\tilde{\gamma} \rightarrow 0$, however the density of the specific heat $\Delta C/V \sim (\delta\tau_C)^{1/2}$ goes to zero while $\tilde{\gamma} \rightarrow 0$.

3. Localized state near a line defect. The only change in the initial Landau functional for the magnetic free energy in such case is the local increase of critical

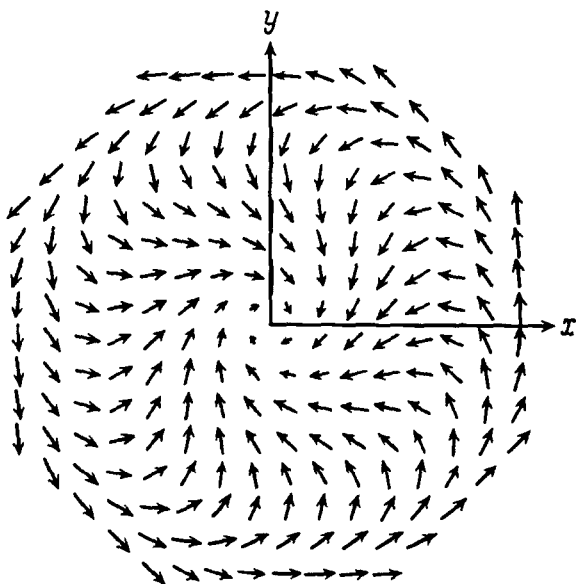


Fig.1. The magnetic structure for point like defect in the plane $z = 2\pi/q_0$. The in-plane M_x and M_y components of magnetization are presented. Note that z axis is chosen along the magnetic moment at $x=y=z=0$

temperature along the line defect is described by the term $-\tilde{\gamma} M^2(0,0,z)\delta(x)\delta(y)$, with the z axis chosen along the line. We obtain the self-consistent equation similar to (5) for $M_0(q_z)$, where $M_0(q_z)$ is Fourier harmonic of $M(\rho=0,z)$.

Using equation (4), we find the following system of equations giving the relation between $\delta\tau$ and the free parameter q_z , where q_z is a modulation vector along the defect.

$$\begin{aligned} M_0^x &= \frac{\tilde{\gamma}}{\tilde{\lambda}^2} \int \frac{i\tilde{\lambda}q_z M_0^y + (q_y^2 + q_z^2) M_0^x}{\delta\tau + (\delta q)^2} \frac{dq_{\perp}}{(2\pi)^2} \\ M_0^y &= \frac{\tilde{\gamma}}{\tilde{\lambda}^2} \int \frac{i\tilde{\lambda}q_z M_0^x + (q_x^2 + q_z^2) M_0^y}{\delta\tau + (\delta q)^2} \frac{dq_{\perp}}{(2\pi)^2} \\ M_0^z &= \frac{2\tilde{\gamma}}{\tilde{\lambda}^2} \int \frac{q_{\perp}^2 M_0^z}{\delta\tau + (\delta q)^2} \frac{dq_{\perp}}{(2\pi)^2} \end{aligned} \quad (7)$$

The critical temperature $\delta\tau_c$ must be obtained by maximization of $\delta\tau$ with respect to q_z . One solution with $M_0^x = M_0^y = 0$ can be easily found. For this solution maximum transition temperature is reached at $q_z = 0$ and $\delta\tau_c = (\tilde{\gamma}\tilde{\lambda}/8)^2$.

However there exist another solution of the type $M_0^x + iM_0^y$ and $M_0^z = 0$ which gives a higher transition temperature. For this solution, the maximum temperature $\delta\tau$ corresponds to wavevector q_z near q_0 . We obtain for

$$\epsilon = \frac{q_0}{q_z} - 1 = \left(\frac{2}{3\pi}\right)^{1/4} \left(\frac{\delta\tau}{q_0^2}\right)^{3/8} \approx \left(\frac{2}{3\pi}\right)^{1/4} \left(\frac{\tilde{\gamma}}{2}\right)^{3/4}$$

the transition temperature

$$\delta\tau_c \approx \left(\frac{\tilde{\gamma}\tilde{\lambda}}{4}\right)^2 \left(1 - 2\left(\frac{4}{3\pi}\right)^{3/4} \tilde{\gamma}^{1/4}\right) \quad (8)$$

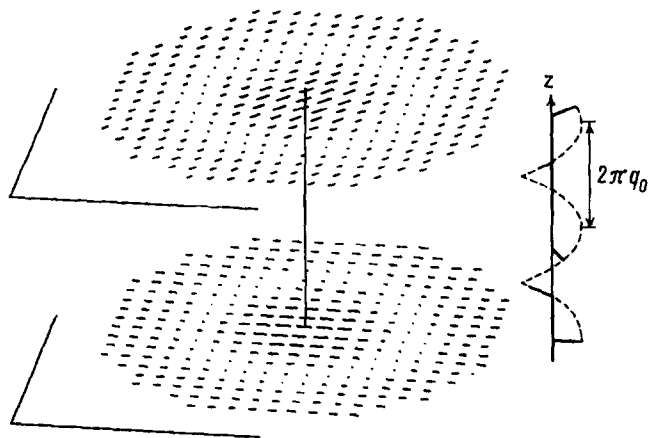


Fig.2 The magnetic structure for the line-defect, z axis is chosen along the defect and we present the magnetic moment for two planes. The moment is oriented in xy plane and the unit along z axis corresponds to $\sqrt{2\epsilon}$ unit in xy plane. It means that real structure is obtained by the contraction $\sqrt{2\epsilon}$ along z axis

This critical temperature is higher than the one for the solution $M_0^x = M_0^y = 0$. We conclude that the helicoidal localized state with a modulation vector $\approx q_0$ along z axis must appear at the temperature $\tau_0 + \delta\tau_c$ given by (8).

The structure in the real space is

$$\begin{aligned} M^x &= M(0) \cos(q_0 z) J_0(q_0 \rho \sqrt{2\epsilon}), \\ M^y &= M(0) \sin(q_0 z) J_0(q_0 \rho \sqrt{2\epsilon}). \end{aligned} \quad (9)$$

The range of application of these equations is $\rho \ll 1/(q_0 \tilde{\gamma}^{5/8})$. At larger distances, the magnetization decreases exponentially. We illustrate the distribution of magnetization as presented in Fig.2. The specific heat jump at the transition is

$$\Delta C \simeq \frac{n\theta}{M_S^2 b T_{C0}} \left(\frac{\pi^3}{12} \right)^{1/4} \frac{1}{4\tilde{\lambda}^2 \tilde{\gamma}^{1/4} \ln \tilde{\gamma}}$$

4. Localized state near a planar defect. Considering the case of planar defect, we choose z axis perpendicular to the plane. The local increase of critical temperature in the plane is described by the term $-\tilde{\gamma} M(x, y, 0) \delta(z)$ in the free magnetic energy. The analysis of the system of equations similar to (7) shows that the solution with the highest transition temperature is of the type $M_0^y + iM_0^z$ and $M_0^x = 0$, while the transition temperature is $\delta\tau_c = \frac{3}{16} (2\tilde{\lambda} \tilde{\gamma}^2)^{2/3}$ and the wave vector is directed along z axis and occurs to be close to q_0 ($\epsilon = \frac{q_0}{q_0} - 1 = \frac{1}{q_0} \sqrt{\frac{\delta\tau_c}{3}}$). The magnetic structure of localized state is

$$\begin{aligned} M^y &= M(0) e^{-q_0 |z| \sqrt{\epsilon}} \frac{2}{\sqrt{3}} \sin \left(q_0 |z| \sqrt{\frac{\epsilon}{3}} + \frac{\pi}{3} \right) \cos(q_0 x), \\ M^z &= M(0) e^{-q_0 |z| \sqrt{\epsilon}} \frac{2}{\sqrt{3}} \sin \left(q_0 |z| \sqrt{\frac{\epsilon}{3}} + \frac{\pi}{3} \right) \sin(q_0 x) \end{aligned}$$

and the specific heat jump is

$$\Delta C \simeq \frac{n\theta}{M_S^2 b T_{C0}} \frac{2.12}{q_0 \sqrt{\epsilon}} = 2.12 \frac{n\theta}{M_S^2 b T_{C0}} \left(\frac{16}{\tilde{\gamma} \tilde{\lambda}^2} \right)^{1/3}.$$

5. Conclusion. We have found the structure of the localized states for the systems with helicoidal transitions. It occurs that even a small point-like local increase of the transition temperature gives rise to localized state appearance. The very easy broadening of the helicoidal transitions may be its inherent property. The preliminary data on the specific heat in MnSi [9] approve our conclusions. Apparently in MnSi, the main type of defects are the dislocations. It may be interesting to perform the neutron diffraction studies to verify the predictions concerning the structure (see eq. (8)) of such line defect state. In our analysis we have neglected the fluctuations which could influence the detailed structure of the localized state, but would not change qualitatively our prediction based on Landau functional approach.

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