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Vortex Rings and Phase Transition in Layered-Lattice Superconductors.

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Abstract. – The phase transition temperature of a layered-lattice superconductor (Josephson-junction array) is shown to have a finite limit T_c^0 for arbitrarily small interlayer coupling. T_c^0 is a temperature of a phase transition in the absence of Josephson coupling between layers. In contrast to a single layer for which phase transition (in a strict sense of the word) is smeared due to screening of long-range vortex-vortex interaction, in layered systems the interaction of layers via magnetic field restores the Berezinskii-Kosterlitz-Thouless transition. We show also that phase transition in layered superconductors cannot be associated with proliferation of vortex rings of the most favourable orientation (*i.e.* lying between the layers) as was recently suggested by Friedel. The temperature of the hypothetical phase transition in the subsystem of such vortex rings turns out to be much higher than T_c^0. The results obtained are also applicable for layered planar magnets. We expect them to be qualitatively valid to all layered superconductors, *e.g.*, high-T_c crystals.

As is well known the phase transition in two-dimensional (2D) systems with planar symmetry (*XY*-magnets, superfluid films, etc.) consists in dissociation of neutral molecules formed by pointlike singularities (vortices) of opposite sign. In 3D systems the phase transition also manifests itself in the behaviour of topological excitations which in this case are linear singularities, *i.e.* vortex lines. In a low-temperature (ordered) phase only closed vortex rings are thermodynamically stable, whereas in a disordered one vortex lines of infinite length are also present.

Recently Friedel has put forward a conjecture [1] that in case of 3D systems with planar symmetry formed by weakly coupled layers the phase transition should be associated with proliferation at low-energy plane vortex rings lying between the neighbouring layers. According to Friedel the temperature of this transition T_c should diminish down to zero with decrease of the strength of interlayer coupling and thus could be even much lower than the temperature of the phase transition in the system of noninteracting layers T_c^0. This conclusion was based on estimates of typical energy scales characterizing the vortex rings of the appropriate orientation.

In this paper we use a more rigorous approach taking into account the interaction of different vortex rings to study such layered systems as lattice superconductors (Josephson-junction arrays) and XY-magnets. We show that the phase transition in the subsystem of interlayer vortex rings could take place only at temperatures that are substantially higher than T_c^0. This means that the proposed interpretation [1] of the phase transition in layered systems cannot be considered as adequate. Actual phase transition takes place in the vicinity of T_c^0 and cannot be accounted for exclusively by the proliferation of the vortex rings of the most favourable orientation.

In what follows we shall describe a lattice superconductor by a model partition function of the form

$$Z = \int D\{\theta\} \sum_{\{m\}} \int D\{A\} \exp[-H\{\theta, m, A\}/T], \tag{1a}$$

where

$$H\{\theta, m, A\} = \sum_{r,\alpha} \left\{ \frac{J_\alpha}{2} (\nabla_\alpha \theta - 2\pi m_\alpha - A_\alpha)^2 + \frac{D_\alpha}{2} (\mathrm{rot}\, A)_\alpha^2 \right\}. \tag{1b}$$

Here phase variables $\theta \equiv \theta(\boldsymbol{r})$ defined on the sites $\boldsymbol{r}$ of a simple cubic lattice stand for the phases of the order parameter of superconducting grains forming the array. The cosine form of the Josephson coupling of neighbouring grains is substituted in eq. (1) by the periodicized Gaussian one. It emerges after the summation over integer variables $m_\alpha(\boldsymbol{r}) \equiv m(\boldsymbol{r}, \boldsymbol{r} + \boldsymbol{e}_\alpha)$ that can be considered as defined on the links of the lattice. The last term in eq. (1b) stands for the energy of fluctuating magnetic field. It is expressed via auxiliary variables $A_\alpha(\boldsymbol{r})$ that are related to the vector potential $A(\boldsymbol{R})$ as

$$A_\alpha(\boldsymbol{r}) \equiv A(\boldsymbol{r}, \boldsymbol{r} + \boldsymbol{e}_\alpha) = \frac{2\pi}{\phi_0} \int_{r}^{r+e_\alpha} \mathrm{d}\boldsymbol{R}\, \boldsymbol{A}(\boldsymbol{R}), \qquad \phi_0 = \pi\hbar c/e. \tag{2}$$

The lattice gradient is denoted in eq. (16) as $\nabla_\alpha \theta \equiv \theta(\boldsymbol{r} + \boldsymbol{e}_\alpha) - \theta(\boldsymbol{r})$ and the lattice curl as $\mathrm{rot}\, A$:

$$(\mathrm{rot}\, A)_\alpha = A(\boldsymbol{r} + \boldsymbol{e}_\beta, \boldsymbol{r} + \boldsymbol{e}_\beta + \boldsymbol{e}_\gamma) - A(\boldsymbol{r} + \boldsymbol{e}_\gamma, \boldsymbol{r} + \boldsymbol{e}_\beta + \boldsymbol{e}_\gamma) - A(\boldsymbol{r}, \boldsymbol{r} + \boldsymbol{e}_\gamma) + A(\boldsymbol{r}, \boldsymbol{r} + \boldsymbol{e}_\beta), \tag{3}$$

with $\boldsymbol{e}_\alpha$, $\boldsymbol{e}_\beta$ and $\boldsymbol{e}_\gamma$ forming the right-hand triad ($\boldsymbol{e}_\alpha[\boldsymbol{e}_\beta \times \boldsymbol{e}_\gamma] = 1$). The r.h.s. of eq. (3) actually is a sum over the perimeter of some elementary plaquette of the original cubic lattice. It will be convenient to consider variable $(\mathrm{rot}\, A)_\alpha$ as defined on the dual lattice link intersecting this plaquette.

Being interested in the layered systems peculiarities we shall consider two directions in the plane of the layers as equivalent and accordingly shall denote: $J_\alpha = J_\parallel(J_\perp)$, $D_\alpha = D_\parallel(D_\perp)$ for $\alpha = x$, $y(z)$. For $D_\alpha \rightarrow \infty$ fluctuations of $A_\alpha(\boldsymbol{r})$ become frozen and the partition function (1) can be also used for describing a planar magnet formed by spins $\sigma(\boldsymbol{r}) = (\cos\theta, \sin\theta)$.

In contrast to the case of genuine cosine interaction the model partition function (1) allows for decoupling of the continuous and discrete degrees of freedom. The former can be integrated out rigorously. Both integrations over θ and over A in eq. (1) are Gaussian and thus can be performed by variation of $H\{\theta, m, A\}$. After tedious but straightforward calculations one then obtains the Hamiltonian

$$H\{m\} = \sum_{r,r',\alpha} \frac{1}{2} (\mathrm{rot}\, m)_\alpha(\boldsymbol{r})\, G_\alpha(\boldsymbol{r} - \boldsymbol{r}')\, (\mathrm{rot}\, m)_\alpha(\boldsymbol{r}') \tag{4}$$

describing a system of closed loops on the dual lattice. The interaction function $G_\alpha(\boldsymbol{r})$ is defined via its Fourier transform:

$$G_\parallel(\boldsymbol{q}) = \frac{4\pi^2 J_\parallel J_\perp D_\parallel}{J_\parallel J_\perp + D_\parallel (J_\parallel k_\parallel^2 + J_\perp k_\perp^2)}, \tag{5a}$$

$$G_\perp(\boldsymbol{q}) = \frac{4\pi^2 J_\parallel^2 [J_\perp D_\perp + D_\parallel (D_\perp k_\parallel^2 + D_\parallel k_\perp^2)]}{[J_\parallel J_\perp + D_\parallel (J_\parallel k_\parallel^2 + J_\perp k_\perp^2)][J_\parallel + D_\perp k^2 + D_\parallel k_\perp^2]} \tag{5b}$$

with $k_\parallel^2 = k_x^2 + k_y^2$; $k_\alpha^2 = 2(1 - \cos q_\alpha)$. For an isotropic system (with J_α and D_α not dependent on α) an analogous transformation has been performed by Thomas and Stone [2].

The integer variable $(\operatorname{rot} m)_\alpha$ in eq. (4) can be identified with the vortex line topological charge whose conservation is ensured by the relation: $\sum_\alpha \nabla_\alpha (\operatorname{rot} m)_\alpha = 0$. Thus all vortex lines either form closed rings or go to infinity. For $D_\alpha \to \infty$ the interaction of vortex lines described by eqs. (5) is currentlike (and thus long-range), whereas for finite D_α's this interaction becomes screened by magnetic field at large distances.

As we have intention of studying the layered systems, we shall be interested exclusively in the case $J_\perp \ll J_\parallel$. Note that for $J_\perp \to 0$, $G_\parallel(\boldsymbol{q})$ in contrast to $G_\perp(\boldsymbol{q})$ also tends to zero. This means that both energy and interaction of plane vortex rings oriented in the plane of the layers decrease unrestrictedly. This is what has led Friedel to his conclusion that in such systems weakening of the interlayer coupling $J_\perp$ is accompanied by the unbounded decrease of T_c [1]. Friedel assumed that the phase transition will occur when the typical distance between the interlayer vortex rings will become comparable with their typical size, the merging of different rings leading to formation of arbitrarily large rings. This estimate does not take into account the interaction between rings.

A more rigorous approach to the problem of calculating the phase transition temperature for the subsystem of plane interlayer vortex rings requires that the Hamiltonian (4) should be considered for the case when $m_\parallel$ is put down to zero in accordance with $(\operatorname{rot} m)_\perp = 0$. Introducing delta-functional factors that allow for substitution of summation over $m_\perp(\boldsymbol{r})$ by integration:

$$Z = \sum_{\{m_\perp\}} \exp[-H\{m\}/T] \to \sum_{\{s\}} \int D\{m_\perp\} \exp\left[\sum_r 2\pi i m_\perp(\boldsymbol{r})\, s(\boldsymbol{r}) - \frac{H\{m\}}{T}\right] \tag{6}$$

and performing Gaussian integration over $m_\perp$, one obtains a partition function expressed via conjugate variables $s(\boldsymbol{r})$:

$$Z \sum_{\{s\}} \exp\left[-\frac{1}{2}\sum_{r,r'} s(\boldsymbol{r})\, V(\boldsymbol{r}-\boldsymbol{r}')\, s(\boldsymbol{r}')\right], \tag{7a}$$

with $V(\boldsymbol{r})$ defined via its Fourier-transform

$$V(\boldsymbol{q}) = \frac{4\pi^2 T}{k_\parallel^2 G_\parallel(\boldsymbol{q})} = \frac{T}{J_\perp} + \frac{T}{D_\parallel k_\parallel^2} + \frac{T k_\perp^2}{J_\parallel k_\parallel^2}. \tag{7b}$$

The partition function (7a) with interaction (7b) has the form of the partition function of the layered system consisting of 2D lattice Coulomb gases (with logarithmical interaction) in which charges belonging to neighbouring layers also interact logarithmically. The renorm-group equations for such a system practically coincide with the Kosterlitz equations [3] for a pure 2D Coulomb gas. This means that the phase transition in such systems belongs to the same Berezinskii-Kosterlitz-Thouless universality class and takes place when the renormalized prelogarithmic factor in the interaction of elementary charges (belonging to the same layer) becomes equal to four. For the transition temperature T_* this gives

$$\left(\frac{2}{J_\parallel}+\frac{1}{D_\parallel}\right)\frac{T_*}{2\pi}-4\sim\exp\left[-\frac{T_*}{J_\perp}\right]. \tag{8}$$

Equation (8) describes the renormalization shift of the transition point due to finite fugacity Y on the layered Coulomb gas. The value of fugacity $Y\sim\exp[-T/2J_\perp]$ is related to the first term in eq. (7*b*). The smaller is the fugacity (the smaller is $J_\perp$) the more exact is eq. (8).

From the form of eq. (8) it becomes evident that for $J_\perp\to 0$ T_* has the finite limit

$$T_*\to T_*^{\min}=\frac{8\pi J_\parallel D_\parallel}{2D_\parallel+J_\parallel}\sim 4\pi\min[J_\parallel, 2D_\parallel], \tag{9}$$

which disagrees with Friedel conclusions. However, such a behaviour does not contradict the possibility of two-stage disordering with the interlayer correlations being destroyed at lower temperatures than the intralayer correlations. To make sure whether this interesting scenario could be brought into life, one should compare T_* with the phase transition temperature in the system with no direct interlayer coupling (*i.e.* with $J_\perp$ renormalized down to zero).

For $J_\perp=0$ all terms containing $(\mathrm{rot}\, m)_\perp$ disappear from eq. (4) which permits to consider $(\mathrm{rot}\, m)_\perp$ as an independent integer variable l:

$$H\{l\}=\frac{1}{2}\sum_{r,r'\alpha} l(\boldsymbol{r})\,G_\perp(\boldsymbol{r}-\boldsymbol{r}')\,l(\boldsymbol{r}'). \tag{10}$$

Charges l can be identified with topological charges of 2D vortices in this or that layer, whose interaction described by eq. (5*b*) for $J_\perp=0$ is logarithmic. It is noteworthy that in case of a single layer (2D Josephson junction array) the magnetic field screens the logarithmic interaction of the vortices destroying thus the phase transition in a strict sense of the word [4], whereas in case of a layered system formed by uncoupled layers only the strength of the logarithmic interaction is renormalized.

As in the previously studied case the phase transition in such layered Coulomb gas belongs to the Berezinskii-Kosterlitz-Thouless universality class. Calculating the prelogarithmic factor of interlayer interaction of pointlike vortices for $J_\perp=0$ the temperature of vortex molecules dissociation T_c^0 can be estimated as

$$T_c^0\sim\frac{1}{8\pi}\int\frac{\mathrm{d}q_z}{2\pi}G_\perp(q)=\frac{2\pi J_\parallel D_\parallel}{J_\parallel+\sqrt{J_\parallel(J_\parallel+4D_\parallel)}+4D_\parallel}\sim\frac{\pi}{2}\min(J_\parallel, 2D_\parallel) \tag{11}$$

and for any relation between the parameters is much lower than T_*.

Comparison of eq. (11) with eq. (9) shows that even in the limit of small interlayer coupling the disordering cannot possibly take place as two separate transitions. Both inter- and intralayer correlations will disappear simultaneously at temperature T_c lying in the interval: $T_c^0<T_c<T_*$. In order to specify the value of T_c, it is convenient to make use of one more representation of the original partition function (1) in the form of the partition function of the gas of interacting loops. If one introduces in eq. (1) for each lattice link a substitution

of the form

$$\sum_{m_\alpha=-\infty}^{\infty} \exp\left[-\frac{J_\alpha}{2T}(\nabla_\alpha\theta - 2\pi m_\alpha - A_\alpha)^2\right] \to \sum_{n_\alpha=-\infty}^{\infty} \exp\left[i(\nabla_\alpha\theta - A_\alpha)\, n_\alpha - \frac{T}{2J_\alpha} n_\alpha^2\right], \tag{12}$$

then the integration over θ provides a constraint for $n_\alpha : \sum_\alpha \nabla_\alpha n_\alpha = 0$, which makes it possible to consider the integer variable n_α as a curl of some other integer variable p_β defined on the links of the dual lattice. One should perform then a Gaussian integration over A_α for the partition function to acquire the desired form

$$Z \sim \sum_{\{p_\alpha\}} \exp\left[-\frac{T}{2}\sum_{r,r',\alpha} (\operatorname{rot} p)_\alpha(\boldsymbol{r})\, g_\alpha(\boldsymbol{r}-\boldsymbol{r}')\,(\operatorname{rot} p)_\alpha(\boldsymbol{r}')\right]. \tag{13a}$$

Here the interaction function $g_\alpha(\boldsymbol{r})$ defined by its Fourier transform

$$g_\parallel(\boldsymbol{q}) = \frac{1}{J_\parallel} + \frac{1}{D_\perp k_\parallel^2 + D_\parallel k_\perp^2}; \qquad g_\perp(\boldsymbol{q}) = \frac{1}{J_\perp} + \frac{D_\perp/D_\parallel}{D_\perp k_\parallel^2 + D_\parallel k_\perp^2} \tag{13b}$$

decays algebraically for any finite values of D_α in contrast to the vortex rings representation (4), where finite values of D_α lead to the screening of the long-range interaction. These two representations can be considered as dual to each other. For the case of an isotropic system they both were obtained by Thomas and Stone [2].

The partition function (13) describes a system of interacting loops on the original cubic lattice. In the limiting case of $J_\perp \to 0$ only the loops that are oriented in the plane of the layers do survive and all the other loops become frozen out. We already have had an experience with the system of plane loops of exactly this kind. However the application of the previously developed method leads now to the representation (10) which already has been obtained by a different way. Thus for the case of zero $J_\perp$ the dual representation (13) does not provide any new results.

However in this representation it becomes evident when passing from zero to finite $J_\perp$ that any corrections related to loops that comprise links oriented perpendicular to the layers will be exponentially small in the ratio $T/J_\perp$. In particular the shift of the transition temperature with respect to the case of zero interlayer coupling will be also exponentially small:

$$\ln(T_c - T_c^0) \sim T_c^0/J_\perp\,. \tag{14}$$

Returning to the vortex ring representation, one can then conclude that the phase transition in a layered system will take place at a temperature much lower than the temperature of hypothetical phase transition in the subsystem of interlayer vortex rings and thus should be associated with vortex rings perpendicular to the layers. From the two-dimensional point of view the simplest rings of such a kind can be identified with neutral vortex molecule in this or that layer. Precisely these objects were taken into consideration by Hikama and Tsuneta [5] when investigating the layered XY-model. The results of our analyses provide evidence that this approach (neglecting the vortex rings with the most favourable orientation) remains adequate also for the more complex problem of layered-lattice superconductors.

In conclusion we can sum up that our calculation of the phase transition temperature T_c for layered-lattice superconductors and magnets has shown that i) in the limit of small interlayer coupling T_c tends to a finite value and ii) that this phase transition cannot be interpreted as a phase transition in the gas of vortex rings of the most favourable orientation. Truly, the fluctuations of the order parameter modulus were not incorporated in our analyses, but since the formation of topological excitations is associated with the behaviour of the order parameter phase, we do not expect this to make a qualitative difference. Thus our conclusions are to be applicable not only to Josephson junction arrays, but also to real layered superconductors, *e.g.*, high-T_c crystals.

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