Friedel transition in a modified XY model

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Abstract

Weakly coupled superconducting layers are described by the three-dimensional XY model with strong coupling in two directions and weak coupling in the third direction. For the usual Josephson-type interplane coupling the coherence between the layers is lost at the same temperature as that within the layers. Thus a low-temperature layer decoupling due to a proliferation of fluxons between planes, as proposed by Friedel, does not occur in this case. However, for a modified interplane coupling there are two phase transitions, one of a Kosterlitz-Thouless type from a disordered high-temperature phase to an intermediate phase with phase coherence only parallel to the layers, the second from this effectively two-dimensional phase to a three-dimensional phase with coherence in all directions and a finite "n-state" order parameter. Thus we do find a "Friedel transition" for this special class of models.

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The Berezinskii-Kosterlitz-Thouless (BKT) transition\textsuperscript{,} mediated by the unbinding of vortex pairs, has been clearly observed in superfluid films\textsuperscript{.} More recently, nonlinear transport experiments in layered high-temperature superconductors\textsuperscript{,} have also shown typical signatures of vortex unbinding slightly below the critical temperature $T_c$. This is surprising, since the Josephson coupling between the layers renders the system three-dimensional, in particular close to $T_c$. Specific heat experiments for YBCO single crystals indeed give evidence for three-dimensional critical behavior\textsuperscript{.}

Some time ago Friedel\textsuperscript{,} has argued that the interlayer coupling could be effectively suppressed by a proliferation of Josephson vortex loops or fluxons between the layers. A simple estimate for the fluxon energy suggests that the layers are decoupled at a temperature $T^* < T_c$, so that there would be a two-dimensional regime for $T^* < T < T_c$, with a BKT transition at $T_c$. Unfortunately, a closer look at the problem\textsuperscript{,} indicates that this “Friedel transition” does not occur below $T_c$\textsuperscript{.} Therefore the question arises why nevertheless in nonlinear transport experiments BKT signatures are clearly observed. A way out of this dilemma has been offered by Jensen and Minnhagen\textsuperscript{,} who realized that the Lorentz force acting on the vortices can overcome the interlayer confinement of vortex pairs.

In this Letter we study again the possible existence of a two-dimensional regime below the critical temperature, starting from the classical XY model with strong intralayer coupling $J_\parallel$ and weak interlayer coupling $J_\perp$. A simple criterion for the decoupling transition together with Monte Carlo simulations shows that a layer decoupling below $T_c$ does not occur, in agreement with previous studies\textsuperscript{.} We attribute this negative result to a strong increase of the fluxon energy as a function of temperature. We turn then to the question whether a decoupling can be excluded on general grounds, by considering two modified XY models. For the first model, representing a superlattice of high and low $T_c$ layers\textsuperscript{,} a decoupling seems to occur around the low $T_c$, but a closer look shows that this apparent transition is in reality a crossover from strong to weak interplane coherence. In the second model a modified interlayer coupling is considered, allowing for $n$ equivalent phase differences for the superconducting order parameters of adjacent layers\textsuperscript{.} In this case a decoupling at $T^* < T_c$
is clearly observed for \( n > 2 \).

Incidentally, the problem is of more general relevance, as the question of long-range coherence arises also in other quantum systems. One can for instance ask whether a disordered layered system of electrons, with a large difference between the masses for the motion parallel and perpendicular to the layers, can be metallic in one and insulating in another direction. Anderson has argued that this can happen, if electron-electron interactions are taken into account\(^\text{[12]}\). A measure for quantum coherence in the case of electronic transport is the Drude weight or charge stiffness, while in the context of superfluidity the relevant quantity is the superfluid density \( \rho_s \) (or the helicity modulus, in the language of the XY model).

We consider the classical XY model on a cubic lattice

\[
H = -\sum_{i,\mu} J_\mu \cos(\varphi_i - \varphi_{i+\mu}),
\]

where \( \mu = x, y, z \), \( J_x = J_y = J_\parallel \), \( J_z = J_\perp \), and the phases are restricted to \( 0 \leq \varphi_i < 2\pi \). This model can be derived from the anisotropic Ginzburg-Landau or the Lawrence-Doniach model by neglecting both the fluctuations of the electromagnetic field and the amplitude fluctuations of the order parameter. There are good arguments for doing this, although these degrees of freedom may become relevant within the critical region\(^\text{[13,14]}\). The helicity modulus \( \Upsilon_\mu \) is defined as the second derivative of the free energy with respect to a constant phase gradient in the direction \( \mu \), and can be written as

\[
\Upsilon_\mu = \frac{J_\mu}{N} \left\langle \sum_i \cos(\varphi_i - \varphi_{i+\mu}) \right\rangle - \frac{\beta J_\mu^2}{N} \left\langle \left( \sum_i \sin(\varphi_i - \varphi_{i+\mu}) \right)^2 \right\rangle.
\]

According to Friedel’s original suggestion\(^\text{[6]}\), for very weak interlayer coupling \( \Upsilon_\perp \) would vanish at a lower temperature than \( \Upsilon_\parallel \), leaving an intermediate temperature region of essentially 2\textit{d} character.

We present now a simple argument against a layer decoupling below the critical temperature, by expanding \( \Upsilon_\perp \) in powers of \( J_\perp \). The leading order coefficient (\( \sim J_\perp^2 \)) turns out to be the difference of two equal contributions, each of them given by \( S = \int d^2r c^2(r) \). The 2\textit{d} correlation function \( c(r) = \left\langle \cos(\varphi_i - \varphi_{i+r}) \right\rangle \) decays exponentially as a function of distance \( r \)
for $T > T_{KT}$. Therefore the leading term in the expansion of $\Upsilon_\perp$ vanishes identically above the BKT transition (and the same can be shown for all higher order terms). For $T < T_{KT}$ $c(r) \sim r^{-\eta(T)}$, where $\eta(T) \approx 1/4$, which implies that the quantity $S$ is infinite below the BKT transition. We tentatively associate the temperature where $S$ diverges with the transition from an effectively 2$d$ phase of decoupled layers to a 3$d$ phase with finite $\Upsilon_\perp$. According to this criterion the decoupling transition temperature $T^*$ coincides with the critical temperature $T_c = T_{KT}$ in the limit $J_\perp \rightarrow 0$.

In order to gain a qualitative understanding of the temperature dependent helicity modulus, we first use the renormalized harmonic approximation (RHA), where the Hamiltonian (1) is replaced by an effective harmonic term

$$\tilde{H} = \frac{1}{2} \sum_{i,\mu} \tilde{J}_\mu (\varphi_i - \varphi_{i+\mu})^2$$

with variational parameters $\tilde{J}_\mu$. These parameters turn out to be identical to the helicity moduli, $\tilde{J}_\mu = \Upsilon_\mu$. The anisotropy $\Upsilon_\perp/\Upsilon_\parallel$ diminishes with increasing temperature, but remains finite up to the critical temperature, where both $\Upsilon_\perp$ and $\Upsilon_\parallel$ drop to zero discontinuously (Fig.1). We have also performed Monte Carlo simulations using the standard Metropolis algorithm. The results presented in Fig.1 show that the jumps obtained in the RHA are artifacts and that the helicity moduli tend to zero continuously. We note the excellent agreement between the two methods at low temperatures, as expected. Our numerical results for $J_\perp = 0.1J_\parallel$ are consistent with a simultaneous loss of coherence parallel and perpendicular to the layers at $T_c \approx 1.33J_\parallel$. Therefore the temperatures $T^*$ and $T_c$ coincide, in agreement with the simple criterion discussed above.

We focus now our attention on the role of fluxons by considering an approximate version of the XY model, where the nonlinearity is retained only for the interlayer coupling,

$$H = \frac{J_\parallel}{2} \sum_{i,\mu=x,y} (\varphi_i - \varphi_{i+\mu})^2 - J_\perp \sum_i \cos(\varphi_i - \varphi_{i+z}).$$

This is an excellent approximation for the original XY model for $T \ll J_\parallel$. The helicity modulus parallel to the layers is constant and given by $\Upsilon_\parallel = J_\parallel$. In order to calculate $\Upsilon_\perp$
we treat the nonlinear term using the Villain approximation\textsuperscript{17}, which is very accurate both at low \((T \ll J_\perp)\) and at high temperatures \((T \gg J_\perp)\textsuperscript{18}\). The partition function is factorized into a term representing the in-plane harmonic fluctuations and the "fluxon contribution"

\[
Z_{fl} = \sum_{\{m_i\}} e^{-2\pi^2 \beta \sum_{i,j} m_i V_{ij} m_j},
\]

where the variables \(m_i\) are integers. The interaction \(V_{ij}\) is the Fourier transform of

\[
V(q) = J_\perp^* \frac{2 - \cos q_x - \cos q_y}{2 - \cos q_x - \cos q_y + (J_\perp^*/J_\parallel)(1 - \cos q_z)},
\]

where the effective interlayer coupling is given by

\[
J_\perp^* = \left(2\beta \log \frac{2}{\beta J_\perp}\right)^{-1}
\]

for \(\beta J_\perp \ll 1\). We notice that \(V_{ij}\) is exactly equal to the interaction energy of two elementary fluxons calculated in the usual vortex loop representation of the 3d XY model\textsuperscript{19}. The variables \(m_i\) are the quantum numbers of the fluxons, and large loops can be constructed by adding elementary fluxons. Since the energy scale \(J_\perp^*\) increases roughly linearly with temperature the multiplication of fluxons is strongly slowed down. The helicity modulus perpendicular to the layers, \(\Upsilon_\perp\), can be expressed in terms of fluxon variables,

\[
\Upsilon_\perp = J_\perp^* \left\{1 - 4\pi^2 \beta J_\perp^* \frac{1}{N} \left\langle \left(\sum_i m_i\right)^2 \right\rangle\right\}.
\]

This confirms that for this approximate model the proliferation of fluxons is directly related to the loss of interlayer coherence. Eq. (8) could in principle be used for calculating \(\Upsilon_\perp\), but since the couplings \(V_{ij}\) decrease only slowly with distance (like a dipole-dipole interaction) we have calculated \(\Upsilon_\perp\) starting from the original expression (4), using both the RHA and Monte Carlo simulations. The results, shown in Fig.2, demonstrate that even for small couplings \(J_\perp\) the helicity modulus \(\Upsilon_\perp\) vanishes only far above the BKT transition, i.e. in a temperature region where the Hamiltonian (4) is no longer a good approximation for the original XY model. Nevertheless, the model defined by Eq. (4) is interesting, since it does show a layer decoupling without simultaneous loss of intraplane coherence. The transition
temperature $T^*$ for infinitesimal interplane coupling $J_\perp$ can be easily calculated from the perturbation expansion described above. In the present case the correlation function $c(r)$ decays algebraically with an exponent $\eta(T) = T/(2\pi J_\parallel)$, and $T^*$ is simply given by the relation $\eta(T^*) = 1$. Fig.2 shows that the resulting value $T^* = 2\pi J_\parallel$ is consistent with the Monte Carlo data. The vanishing of $\Upsilon_\perp$ for $T > T^*$ implies that also $\langle \cos(\varphi_i) \rangle$ vanishes, although the susceptibility remains infinite up to $2T^*$.

The analysis given above strongly supports the view that the interlayer coherence is not destroyed by thermal fluctuations below the critical temperature in the 3d XY model, even for arbitrarily small interlayer coupling. We now address the question whether this conclusion is generally valid, by studying two modifications of the original XY model. The first represents a stack of layers with periodically varying intralayer couplings. The extensively studied superlattices of low and high $T_c$ layers are nice realizations of such a model. The second modification concerns the interlayer coupling, which is replaced by a different form, namely $J_\perp \cos(\varphi_i - \varphi_{i+z})$ is substituted by $(J_\perp/n^2) \cos[n(\varphi_i - \varphi_{i+z})]$, where $n$ is an arbitrary positive integer ($\geq 2$). Although such a term cannot be excluded within Ginzburg-Landau theory, it would in general be expected to be much smaller than the conventional term with $n = 1$.

We consider first a superlattice consisting of one ”strong” layer with intralayer coupling $J_\parallel^{(1)}$, alternating with $n$ ”weak” layers with $J_\parallel^{(2)} < J_\parallel^{(1)}$, and a constant interlayer coupling $J_\perp$. The Monte Carlo results (Fig.3) show that nothing spectacular happens for $n = 1$. For $n = 3$, however, the helicity modulus $\Upsilon_\parallel$ exhibits a kink slightly above the low $T_c(\approx J_\parallel^{(2)})$, while simultaneously $\Upsilon_\perp$ drops practically to zero. There is apparently a region with vanishing interlayer coherence between this temperature and the critical temperature $T_c \approx J_\parallel^{(1)}$. However, a true decoupling is very unlikely. In the extreme situation where $J_\parallel^{(2)} = 0$, one can integrate out the variables of the weak layers and deduce a model involving only the strong layers with an effective interlayer coupling $J_\perp^{eff} \approx (\beta J_\perp/2)^n J_\perp$. We can then use our previous results for one type of layers and conclude that the helicity modulus $\Upsilon_\perp$ remains finite (though very small) up to $T_c$. Thus a Friedel transition does not occur for
this type of superlattices.

We turn now to the second modification where the interlayer interaction is replaced by 
\( (J_\perp/n^2) \cos[n (\varphi_i - \varphi_{i+\perp})] \). Monte Carlo results for \( n = 2, 3, 4 \) are shown in Fig. 4. For \( n > 2 \) the helicity modulus \( \Upsilon_\perp \) drops to zero far below the critical temperature where \( \Upsilon_\parallel \) vanishes, while for \( n = 2 \) both transitions seem to occur at the same temperature. This observation is in agreement with the analysis of perturbation theory. In the present situation we have to consider the correlation function

\[
c_n(r) = \langle \cos[n (\varphi_i - \varphi_{i+r})] \rangle \sim r^{-\eta_n(T)}
\]

For the exponent \( \eta_n \) we use the relation \( \eta_n = n^2 \eta \) together with the numerical values for \( \eta(T) \). The criterion \( \eta_n(T^*) = 1 \) yields decoupling temperatures \( T_n^* \) in good agreement with those found in the Monte Carlo simulations for \( n = 3, 4 \). For \( n = 2 \) the reported value \( \eta(T_{KT}) = 1/4 \) indicates that both transitions – the Friedel and the BKT transition – occur simultaneously.

In summary, our numerical simulations and perturbative arguments confirm that for the layered XY model an intermediate effectively 2\( d \) phase does not exist, even for arbitrarily small interlayer couplings, \( J_\perp \ll J_\parallel \). This absence of a low-temperature decoupling transition is nicely illustrated in a simplified version of the model where the role of fluxons is particularly transparent. The interplane coherence also persists for superlattices of high- and low-\( T_c \) layers, although an apparent decoupling is observed for thick enough low-\( T_c \) layers. In contrast, a low-temperature decoupling transition is found for an interlayer coupling with \( n \)-fold symmetry, at least for \( n > 2 \).

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FIGURES

FIG. 1. Helicity moduli $\Upsilon_{\parallel}$ (full circles) and $\Upsilon_{\perp}$ (open circles) of the anisotropic XY model with $J_{\perp}/J_{\parallel} = 0.1$ as functions of temperature as obtained from Monte Carlo simulations of a $36 \times 36 \times 36$ lattice. The solid curves show the RHA results.

FIG. 2. Helicity modulus $\Upsilon_{\perp}$ of the approximate version (Eq. (4)) of the XY model with $J_{\perp}/J_{\parallel} = 0.1$ (open circles) and $J_{\perp}/J_{\parallel} = 0.5$ (full circles). The symbols are Monte Carlo data and the full lines are RHA results. Arrows indicate the Kosterlitz–Thouless temperature $T_{KT}$ and the layer decoupling temperature $T^* = 2\pi J_{\parallel}$, respectively.

FIG. 3. Helicity moduli $\Upsilon_{\parallel}$ (full symbols) and $\Upsilon_{\perp}$ (open symbols) for the superlattice model (as defined in the text) with $J_{\parallel}/J_{\parallel}^{(1)} = 0.3$ and $J_{\perp}/J_{\parallel}^{(1)} = 0.1$. Monte Carlo data for a $36 \times 36 \times 36$ lattice with one (circles) and three (triangles) weak layers are presented. The inset shows $\Upsilon_{\perp}$ in the crossover region.

FIG. 4. Helicity moduli $\Upsilon_{\parallel}$ (full symbols) and $\Upsilon_{\perp}$ (open symbols) of the XY model with modified interplane interaction $(J_{\perp}/n^2) \cos[n(\varphi_i - \varphi_{i+1})]$ with $J_{\perp}/J_{\parallel} = 0.1$. Monte Carlo data for $n = 2$ (circles), $n = 3$ (triangles) and $n = 4$ (diamonds) are shown. The intersection of the dashed line with slope $2/\pi$ and the $\Upsilon_{\parallel}$ curves locates the BKT transition at $T_{KT}$. Arrows indicate the calculated layer decoupling temperatures $T_{n}^*$ for $n = 3, 4$. 

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$\gamma_{\parallel}(T) / \gamma_{\parallel}(0)$

Fig. 1
Fig. 2
Fig. 3
Fig. 4