Friedel Transition in Layered Superconductors

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Weakly coupled superconducting layers are described by the anisotropic 3D *XY* model. A low-temperature layer decoupling due to a proliferation of fluxons between planes, as proposed by Friedel, does not occur. The same is true for a periodic superlattice of high and low T_c layers, although the interplane coherence can become extremely weak. On the other hand a true layer decoupling is found for a random stack. [S0031-9007(96)01487-1]

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The Berezinskii-Kosterlitz-Thouless (BKT) transition [1,2], mediated by the unbinding of vortex pairs, has been clearly observed in superfluid films [3]. More recently, nonlinear transport experiments in layered high-temperature superconductors [4] 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 [5].

Some time ago Friedel [6] 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 [7] indicates that this "Friedel transition" does not occur below T_c [8]. 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 [9], 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 $J_\|$ 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 [8]. We attribute this negative result to a strong increase of the fluxon energy as a function of temperature. We turn then to question whether a decoupling can be excluded on general grounds, by considering a superlattice of high and low T_c layers [10]. For an ordered array 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. On the other hand, in a disordered array we do find a true layer decoupling.

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. This seems not to occur for noninteracting particles [11], but Anderson has argued that it can happen, if electron-electron interactions are taken into account [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 ρ_s (or the helicity modulus, in the language of the *XY* model).

We consider the classical *XY* model on a cubic lattice

$$H = -\sum_{i,\mu} J_\mu \cos(\varphi_i - \varphi_{i+\mu}), \tag{1}$$

where $\mu = x, y, z$, $J_x = J_y = J_\|$, $J_z = J_\perp$, and the phases are restricted to $0 \le \varphi_i < 2\pi$. 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 [13,14]. The helicity modulus Υ_μ is defined as the second derivative of the free energy with respect to a constant phase gradient in the direction μ, and can be written as

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

According to Friedel's original suggestion [6], for very weak interlayer coupling $\Upsilon_\perp$ would vanish at a lower temperature than $\Upsilon_\|$, leaving an intermediate temperature region of essentially 2D character.

We present first 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 2D correlation function $c(r) = \langle \cos(\varphi_i - \varphi_{i+r}) \rangle$ decays exponentially as a function of distance r for $T > T_{\rm KT}$. 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 $T < T_{\rm KT}$ $c(r) \sim r^{-\eta(T)}$, where $\eta(T) \lesssim 1/4$ [15,16], 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 2D phase of decoupled layers to a 3D phase with finite $\Upsilon_\perp$. According to this criterion the decoupling transition temperature T^* coincides with the critical temperature $T_c = T_{\rm KT}$ in the limit $J_\perp \to 0$.

In order to substantiate this conclusion we consider an approximate version of the XY model, where the nonlinearity is retained only for the interlayer coupling,

$$H = \frac{J_\parallel}{2} \sum_{i,\mu=x,y} (\varphi_i - \varphi_{i+\mu})^2 - J_\perp \sum_i \cos(\varphi_i - \varphi_{i+z})\,. \tag{3}$$

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 [17], which is very accurate both at low ($T \ll J_\perp$) and at high temperatures ($T \gg J_\perp$) [18]. The partition function is factorized into a term representing the in-plane harmonic fluctuations and the "fluxon contribution"

$$Z_{\rm fl} = \sum_{\{m_i\}} e^{-2\pi^2\beta \sum_{i,j} m_i V_{ij} m_j}, \tag{4}$$

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

$$V(\mathbf{q}) = J_\perp^* \times \frac{2 - \cos q_x - \cos q_y}{2 - \cos q_x - \cos q_y + (J_\perp^*/J_\parallel)(1 - \cos q_z)}, \tag{5}$$

where the effective interlayer coupling is given by

$$J_\perp^* = \left(2\beta \ln \frac{2}{\beta J_\perp} \right)^{-1} \tag{6}$$

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 [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,

$$\Upsilon_\perp = J_\perp^* \left\{ 1 - 4\pi^2 \beta J_\perp^* \frac{1}{N} \left\langle \left(\sum_i m_i \right)^2 \right\rangle \right\}. \tag{7}$$

This confirms that for this approximate model the proliferation of fluxons is directly related to the loss of interlayer coherence. Equation (7) could in principle be used for calculating $\Upsilon_\perp$, but since the couplings V_{ij} decrease only slowly with distance (as a dipole-dipole interaction) we have calculated $\Upsilon_\perp$ starting from the original expression (3), using both the renormalized harmonic approximation (RHA) and Monte Carlo simulations. The results, shown in Fig. 1, 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 (3) is no longer a good approximation for the original XY model [20]. We note the excellent agreement between the two methods up to high temperatures.

The transition temperature T^* of model (3) 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 $\eta(T^*) = 1$. Figure 1 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 2D susceptibility remains infinite up to $2T^*$. Thus for infinitesimal $J_\perp$ we find two transitions, a first at T^* where both the order parameter and the helicity modulus $\Upsilon_\perp$ vanish, and a second at $2T^*$ where the susceptibility diverges. It seems to be this second transition which has been identified by the renormalization group approach [8].

The analysis given above strongly supports the view [8] that the interlayer coherence is not destroyed by

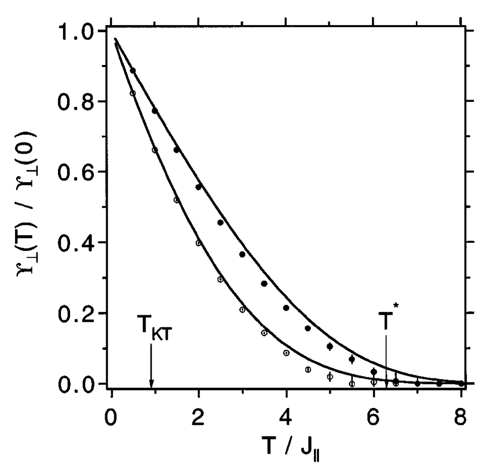

FIG. 1. Helicity modulus $\Upsilon_\perp$ of the approximate version [Eq. (4)] of the XY model with $J_\perp/J_\parallel = 0.1$ (open circles) and $J_\perp/J_\parallel = 0.5$ (full circles). The symbols are Monte Carlo data and the full lines are RHA results. Arrows indicate the Kosterlitz-Thouless temperature $T_{\rm KT}$ and the layer decoupling temperature $T^* = 2\pi J_\parallel$, respectively.

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 remains valid for a stack of layers with periodically varying *intra*layer couplings. The extensively studied superlattices of low and high T_c layers are nice realizations of such a model [10]. We consider a superlattice consisting of one "strong" layer with intralayer coupling $J_\parallel^{(1)}$, alternating with r "weak" layers with $J_\parallel^{(2)} < J_\parallel^{(1)}$, and a constant interlayer coupling $J_\perp$. The Monte Carlo results (Fig. 2) show that nothing spectacular happens for $r = 1$. For $r = 3$, 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 a finite effective interlayer coupling [21]. We can then use our previous results for one type of layer 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 superlattice.

Given the weak interplane coherence in an ordered superlattice it is natural to ask what happens for a random stack of high and low T_c layers, or, in our language, for a random sequence of strong and weak layers with couplings $J_\parallel^{(1)}$ and $J_\parallel^{(2)}$ ($J_\parallel^{(1)} > J_\parallel^{(2)}$), respectively. This problem is quite complicated in general, but the particular case $J_\parallel^{(2)} = 0$ can be analyzed explicitly. In the same way as for an ordered array the weak layers can be eliminated in the partition function, leading to a sequence of layers with intralayer coupling $J_\parallel^{(1)}$ and an effective interlayer interaction decreasing with the number r of consecutive weak layers. For a concentration c of weak layers the numbers r are distributed according to $w(r) = (1 - c)c^r$.

We have calculated the helicity modulus in the limit $\beta J_\parallel^{(1)} \gg 1$ for an infinite number of layers, averaging over the randomness according to the distribution $w(r)$. We find

$$\Upsilon_\perp = \frac{1}{1 - c}\left\{\sum_{r=0}^{\infty} w(r)\,[J_\perp^{\mathrm{eff}}(r)]^{-1}\right\}^{-1}, \tag{8}$$

where the effective couplings can be expressed in terms of modified Bessel functions I_n,

$$J_\perp^{\mathrm{eff}}(r) = \frac{1}{\beta}\,\frac{\sum_{n=-\infty}^{\infty} I_n^{r+1}(\beta J_\perp)n^2}{\sum_{n=-\infty}^{\infty} I_n^{r+1}(\beta J_\perp)}. \tag{9}$$

Figure 3 shows $\Upsilon_\perp$ as a function of temperature both for a periodic superlattice and a random stack. While coherence persists in the periodic case, for a random stack $\Upsilon_\perp$ is seen to vanish linearly at a temperature T^* of the order of $J_\perp$, i.e., much below the critical temperature where $\Upsilon_\parallel$ vanishes. The decoupling temperature T^* can be calculated from Eq. (8), and we find

$$\frac{I_1(\beta^* J_\perp)}{I_0(\beta^* J_\perp)} = c. \tag{10}$$

The result depicted in the inset of Fig. 3 shows that T^* vanishes for $c = 1$, as it should, and increases strongly for small c. The loss of interplane coherence can be most easily understood for $\beta J_\perp \ll 1$, where the effective couplings (9) are simply given by

$$J_\perp^{\mathrm{eff}}(r) = J_\perp\left(\frac{\beta J_\perp}{2}\right)^r. \tag{11}$$

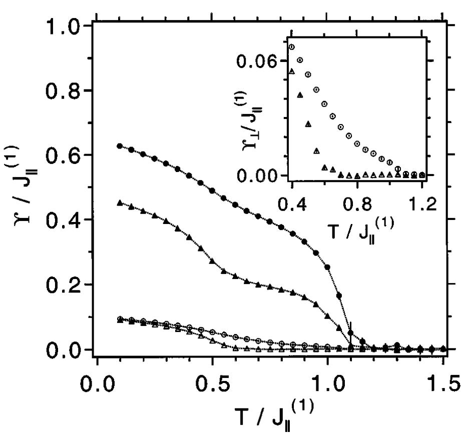

FIG. 2. Helicity moduli $\Upsilon_\parallel$ (full symbols) and $\Upsilon_\perp$ (open symbols) for the superlattice model (as defined in the text) with $J_\parallel^{(2)}/J_\parallel^{(1)} = 0.3$ and $J_\perp/J_\parallel^{(1)} = 0.1$. Monte Carlo data for a $36 \times 36 \times 36$ lattice with one (circles) and three (triangles) weak layers are presented. The inset shows $\Upsilon_\perp$ in the crossover region.

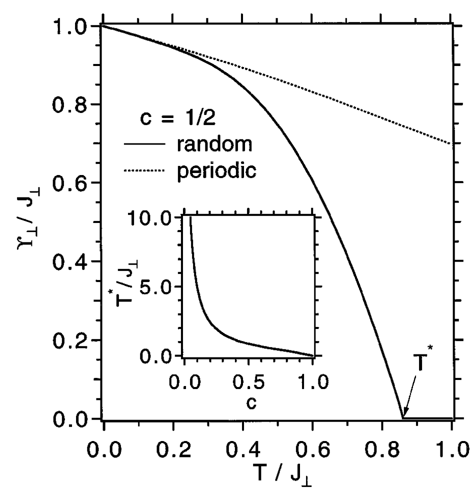

FIG. 3. Helicity modulus $\Upsilon_\perp$ for a random stack with equal numbers of weak ($J_\parallel^{(2)} = 0$) and strong ($\beta J_\parallel^{(1)} \gg 1$) layers (full line), as compared to an alternating array (broken line). The inset shows the decoupling temperature T^* as a function of the concentration c of the weak layers.

It is then straightforward to derive the distribution function $p(J_\perp^{\mathrm{eff}})$ of these couplings, which exhibits a power law for $J_\perp^{\mathrm{eff}} \to 0$ with exponent

$$\nu = \frac{\ln c}{\ln \frac{\beta J_\perp}{2}} - 1 . \tag{12}$$

It follows that p diverges for $T > T^*$ and tends to zero for $T < T^*$, where $T^* = J_\perp/(2c)$ coincides with Eq. (10) in the temperature range considered here.

The extension of our analysis to finite values of $J_\parallel^{(2)}$ is not straightforward. However the Monte Carlo results in Fig. 2 suggest that there is no qualitative change in this case. Thus we expect that for a random stack and $J_\parallel^{(2)} > 0$ the decoupling temperature T^* is merely shifted above $J_\parallel^{(2)}$.

In summary, our numerical simulations and perturbative arguments confirm that for the layered *XY* model an intermediate effectively 2D 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. Interestingly, for a random stack a true layer decoupling occurs at a temperature T^* due to a sharp increase of the weight of small effective Josephson couplings at this temperature. At this stage it is not clear how to observe experimentally the loss of interplane coherence in layered superconductors. The most promising quantitity for measuring the helicity modulus seems to be the complex impedance [22], although it might be difficult to isolate experimentally a specific component of the helicity tensor, in particular, a tiny value of $\Upsilon_\perp$.

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