Kosterlitz-Thouless Signatures from 3D Vortex Loops in Layered Superconductors

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Layered 3D high-T_c superconductors exhibit Kosterlitz-Thouless- (KT-) like quasi-2D signatures, and a decoupling of layers for $T > T_c$ has been suggested. A vortex-loop scaling approach to the layered 3D XY model, with bare anisotropic coupling ratio $\gamma_0^{-2} \equiv \mathcal{J}_\perp/\mathcal{J}_\parallel$, shows layer fluctuations are indeed effectively decoupled, but only at *finite* scales $a \lesssim r_0 \sim \gamma_0 \gg 1$, where rectangular loops cutting single layers dominate. Finite-scale KT-like unbinding at "T_{KT}"$(\gamma_0) \lesssim T_c(\gamma_0)$ yields quasi-2D signatures outside a 3D critical region $|(T-T_c)/T_c| \equiv |\varepsilon| = |\varepsilon_c| < \gamma_0^{-1/\nu}$, where multilayer, elliptical tumbling loops dominate, correlated over scales $\xi \sim |\varepsilon|^{-\nu} \gg r_0$.

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Layered high-T_c superconductors show quasi-two-dimensional behavior [1], including strictly 2D Kosterlitz-Thouless (KT) signatures of vortex-point unbinding [2]. It has been suggested, therefore, that the layers decouple [3] above the transition temperature, $T > T_c$. On the other hand, 3D critical scaling behavior has recently been reported [4]. It is clearly of central importance to understand, in a unified picture, both effective layer decoupling and the coexistence of 2D and 3D signatures in layered superconductors.

The prototypical KT system is the 2D planar spin or XY model [2], physically realized in a 2D Josephson junction array (JJA), that has vortex-point topological excitations. A 3D vortex-loop scaling approach has been developed in the isotropic case [5,6], going beyond 2D interlayer perturbations [7].

In this Letter we present a generalization [8] of vortex-loop scaling to the anisotropic 3D XY JJA case, and also calculate quantities related to experimental measurement [1] and Monte Carlo simulations [3,9,10]. These include the transition temperature, the superfluid density (related to the vortex coupling at large scales), the phase slip resistance (defined in terms of the vortex loop fugacity), and the nonlinear current-voltage exponent (related to the finite-scale vortex coupling). We find that, for nonzero bare interlayer coupling, the fixed point is not 2D but [7] (isotropic) 3D: layers do not decouple asymptotically. However, for strong anisotropies, there is an effective *finite-scale* layer decoupling that can produce observable quasi-2D behavior outside a 3D critical temperature region $|(T-T_c)/T_c| \equiv |\varepsilon| < |\varepsilon_c|$.

Vortex-loop blowouts at T_c, suggested by Feynman and Onsager in superfluid helium [5(a),6(a)], have been seen in 3D XY Monte Carlo (MC) simulations [9,10]. T_c is raised [6(b),11] by imposition of an external vorticity-suppressing chemical potential [11]. Thermally activated, tumbling vortex loops of mean diameter $a \sim \xi_-(T) \sim |\varepsilon|^{-\nu}$ and renormalized fugacity $y_l \sim e^{-a/\xi_-}$ increase in size on warming. The vortex intersegment potential is of the Biot-Savart ($\sim 1/R$) type. Loops can nest and screen, and blow out [5,6] for $T \to T_c^+$ ($\xi_-, y_l \to \infty$), with loop segments for $T > T_c$, correlated only over a length $\xi_+ \sim |\varepsilon|^{-\nu}$.

For the anisotropic case, a new [12,13] "Hikami-Tsuneto" (HT) vortex length scale r_0 appears, defined by the inter$(\mathcal{J}_\perp)$/intra$(\mathcal{J}_\parallel)$-plane coupling ratio,

$$r_0 = a_0\gamma_0, \quad \gamma_0^{-2} \equiv \mathcal{J}_\perp/\mathcal{J}_\parallel , \tag{1}$$

where a_0 is the in-plane lattice constant. A strong anisotropy regime is defined by $r_0 \gg 2a_0$, i.e., $\gamma_0^{-1} \ll 0.5$. For $a > r_0$, closed elliptical Biot-Savart interaction loops of major axis a dominate, crossing multiple layers. For $a < r_0$, quasi-2D rectangular loops with log-plus-linear in-plane interaction dominate, crossing single layers.

The anisotropic 3D XY JJA Hamiltonian is [$\beta = (k_B T)^{-1}$]

$$\beta H = -\sum_{\mu,i} \beta \mathcal{J}_\mu (\cos\Delta_\mu \vartheta_i - 1) , \tag{2}$$

with Δ_μ discrete derivatives in directions $\mu = x,y,z$, couplings $\boldsymbol{\mathcal{J}} = (\mathcal{J}_\parallel, \mathcal{J}_\parallel, \mathcal{J}_\perp)$, and angular variables $\pi \geq \vartheta_i > -\pi$ on a cubic lattice of constants $a_\parallel = a_\perp = a_0 = 1$. For the 3D JJA, ϑ_i are the superconductor-grain phases. $\mathcal{J}_\mu$ are the intergrain Josephson couplings $\propto 1 - T/T_{c0}$ where T_{c0} is the superconducting (grain) transition temperature. Superconductor magnitude $|\psi|$ fluctuations at T_{c0} are irrelevant for the intergrain phase coherence at $T_c \ll T_{c0}$. Equation (1) can also be regarded as a weakly $(\mathcal{J}_\perp)$ coupled Ginzburg-Landau (GL) Lawrence-Doniach [13] model, with in-plane coherent regions $\sim a_0$ coupled by $\mathcal{J}_\parallel$ and locked magnitudes $|\psi|^2 \propto 1 - T/T_{\mathrm{GL}}$. Then $\gamma_0^{-2} = \mathcal{J}_\perp/\mathcal{J}_\parallel = M_\parallel/M_\perp$, the ratio of the GL masses [13]. High-T_c compounds are strongly anisotropic, with [1,3,7] $\gamma_0^{-1} \simeq 1.4 \times 10^{-2}$ (thallium) and $\simeq 0.2$ (yttrium).

A standard dual transformation [14] casts the partition function in terms of dual-lattice vortex segments $J_\mu^{(L)}(\mathbf{r}) = 0, \pm 1$, that form closed loops, $\{L\}$:

$$\sum_\mu \Delta_\mu J_\mu^{(L)}(\mathbf{r}) = 0 , \quad \forall L . \tag{3}$$

The vortex-loop [5,6,10,14] partition function, summing over loop configurations, is [8]

$$Z = \sum_{\substack{\{\mathbf{J}(\mathbf{r})\} \\ \text{config}}} \prod_L y_0^{(L)} \exp\left[-\sum_{L \neq L'} \beta H^{(L,L')} \right] . \tag{4}$$

The interloop segment-segment interaction is

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$$\beta H^{(L,L')} = \frac{\pi}{2}\sum_{\mathbf{r}\neq\mathbf{r}'}[K_\perp \mathbf{J}_\parallel^{(L)}(\mathbf{r})\cdot\mathbf{J}_\parallel^{(L')}(\mathbf{r}') + K_\parallel J_\perp^{(L)}(\mathbf{r})J_\perp^{(L')}(\mathbf{r}')]U(\mathbf{r}-\mathbf{r}'), \tag{5}$$

with the $\mathbf{J}_\parallel$ ($J_\perp$) vortex segments coupling through interlayer (intralayer) couplings $K_\perp$ ($K_\parallel$). The vortex and cosine couplings are taken to be proportional [6,8] $K_\mu \simeq \beta\mathcal{J}_\mu a_0$, with a length scale absorbed in the coupling. Spin wave corrections in 3D should be small for low temperatures ($\sim T$), and near transition [$\sim(T_c-T)$]. The bare fugacity of a loop L is determined by the intraloop segment interactions ($\sim H^{(L,L)}$) and segment self-energies [$\sim U(0)$]:

$$y_0^{(L)} = \exp\left[-\beta H^{(L,L)} - \frac{\pi}{2}U(0)\sum_{\mathbf{r}}\{K_\perp(\mathbf{J}_\parallel^{(L)}(\mathbf{r}))^2 + K_\parallel(\mathbf{J}_\perp^{(L)}(\mathbf{r}))^2\}\right]. \tag{6}$$

In (5) the interaction U is essentially the 3D lattice Green's function [8,10(a)] [$\mathbf{R}\equiv(\mathbf{R}_\parallel, Z)$]:

$$U(\mathbf{R}) = a_0^2\int\frac{d^3q}{(2\pi)^3}\frac{4\pi e^{i\mathbf{q}\cdot\mathbf{R}}}{[(4-2\cos q_x a_0 - 2\cos q_y a_0) + \gamma_0^{-2}(2-2\cos q_z a_0)]} \simeq \frac{1}{[(R_\parallel/r_0)^2+Z^2]^{1/2}}. \tag{7}$$

From the coordinate space form (7), it is clear that "equipotential" loop configurations are elliptical. (See inset, Fig. 1; $a > r_0$.) The bare ellipse fugacity, for in-plane major axis a_L and minor axis $a_L[1-e^2(\alpha_L)]^{1/2}$ making an angle α_L with the Z axis, is [8]

$$y_0^{(L)}(\alpha_L) \approx \exp\left[-\left\{\pi^2 K_\parallel \frac{a_L}{a_0}\ln\left(\frac{a_L}{a_c}\right)\right\}(1-\delta_0\sin^2\alpha_L)^{1/2}\right]. \tag{8}$$

The ellipse eccentricity is $e(\alpha) \equiv [\delta_0\cos^2\alpha/(1-\delta_0\sin^2\alpha)]^{1/2}$ with $\delta_0 \equiv 1-\gamma_0^{-2}$, and a_c is a core region cutoff containing hairpinlike transverse excursions of the loop from its average geometry [15]. The fugacity is peaked at $\alpha = \pi/2$, consistent with the high-T_c ideas of Friedel [16].

The nested loops tumble freely for scales $a > r_0$, progressively screening the coupling anisotropy seen by the largest $\sim\xi_-(T)$ loops. A detailed scaling analysis [8] shows that the renormalized anisotropy ratio ($\gamma_0^{-1} \to \gamma_l^{-1}$) is asymptotically driven to unity, $1-\gamma_l^{-1} \simeq (1-\gamma_0^{-1})e^{-(l-l_0)} \to 0$. (Asymptotic layer decoupling, by contrast, would imply $\gamma_l^{-1} \to 0$.) The critical behavior is that of an *isotropic* 3D XY model.

The partition function at general minimum scale $a \equiv a_0 e^l$ is then

$$Z \simeq \sum_{\substack{\{\mathbf{J}\}\\ \text{config}}}\prod_L \bar{y}_l^{(L)}\exp\left[-\frac{\pi}{2}K_l\sum_{L\neq L'}\sum_{\mathbf{r}\neq\mathbf{r}'}\mathbf{J}^{(L)}(\mathbf{r})\cdot\mathbf{J}^{(L')}(\mathbf{r}')U(\mathbf{r}-\mathbf{r}')\right], \tag{9}$$

with a geometric mean as the bare initial coupling $K_0 = \sqrt{K_\perp K_\parallel} = K_\parallel\gamma_0^{-1}$, and (dropped) differences between (9) and (5) going [8] as $\sim(1-\gamma_l^{-1}) \to 0$. Scaling equations, derived as in the isotropic case [5,6], involve the angularly averaged loop fugacity $\bar{y}_l$, where $\bar{y}_0 = \int_0^\pi d\alpha\, y_0(\alpha)/\pi$. They are of the isotropic form, to $O((1-\gamma_l^{-1}))$:

$$\frac{dK_l}{dl} \simeq K_l - A_0\bar{y}_l K_l^2, \quad \frac{d\bar{y}_l}{dl} \simeq (6-\pi^2 K_l L_l)\bar{y}_l, \tag{10}$$

with $A_0 = 4\pi^3/3$, $L_l \equiv 1+\ln[a/a_c(l)]$, and unchanged [6] "fixed points" $(K_{l_-}, y_{l_-}) \equiv (K^*, y^*) = (0.3875, 0.062)$ at $l = l_- \equiv \ln(\xi_-/a_0) \to \infty$. In a model for a scale dependent core $a_c(l)$ (partially supported by numerical simulations [15]), both diameter and core size (for $a \sim \xi_- \sim |\varepsilon|^{-\nu}$) diverge with a constant ratio $a_c(l)/a \approx K_l^x$, where $x = 0.6$ is a self-avoiding random walk exponent. [Loop self-energies $\sim a\ln(a/a_c(l))$ then scale as $\sim a$.] One finds [6] $\nu \approx 0.67$.

Since the minor axis $a[1-e^2(\alpha)]^{1/2} > a_0$, the tumbling ellipse picture of (10) breaks down for $a \lesssim r_0$ for strong anisotropies. Loops are then of two types: (i) fluxonlike [17] loops not crossing planes (α constrained around $\alpha \approx \pi/2$) and (ii) quasi-2D, rectangular loops crossing single planes [3(b)] by vertical unit sides. See inset, Fig. 1, $a < r_0$. The vertical segments $J_\perp(\mathbf{r}_\parallel, z) = +1$, $J_\perp(\mathbf{r}'_\parallel, z) = -1$ have $\mathbf{J}_\parallel$ sides of length $\mathbf{R}_\parallel \equiv |\mathbf{r}_\parallel - \mathbf{r}'_\parallel|$ with $r_0 > R_\parallel > 2a_0$. From (5), (6), and (7) the $\gamma_0^{-1} \to 0$ or KT limit yields [6(c)] an in-plane logarithmic interaction $U(\mathbf{R}) - U(0) \to -2U^{(2D)}(\mathbf{R}_\parallel)\delta_{Z,0}$ with

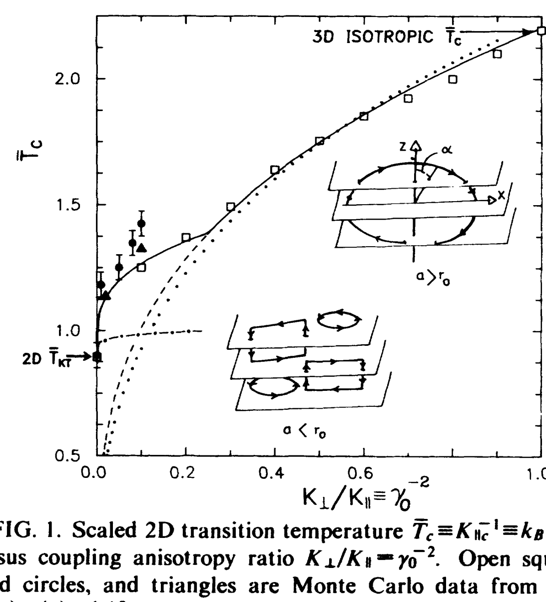

FIG. 1. Scaled 2D transition temperature $\bar{T}_c \equiv K_{\parallel c}^{-1} \equiv k_B T_c/\mathcal{J}_\parallel$ versus coupling anisotropy ratio $K_\perp/K_\parallel = \gamma_0^{-2}$. Open squares, solid circles, and triangles are Monte Carlo data from Refs. [3(b),9(a),9(b)]. Dashed and dotted lines as in text. (Inset: Single-plane quasi-2D excitations for scales $a < r_0 = a_0\gamma_0$, and multiplane elliptical loop at tilt angle α for $a > r_0$.)

$$U^{(2D)}(\mathbf{R}_{\parallel}) \simeq \ln(R_{\parallel}/a_0) + \pi/2 + O((R_{\parallel}/r_0)^2) .$$

The $\mathbf{J}_{\parallel}$ energy in the fugacity (6) yields a linear effective potential, $\sim 2\pi Q_0(R_{\parallel}/a_0 - 1)$, between the $J_{\perp} = \pm 1$ sides. The coefficient Q_0 can be estimated in two opposite limits. For $\gamma_0^{-1} \to 0$, the $U(R)$ interaction of $J_{\parallel} - J_{\parallel}$ segments on quasi-2D loops is strongly screened by (in-plane) fluxon loops [17] that are well above their own [8] KT transition at $K_{\parallel c}^{-1} \sim \gamma_0^{-2} \ll \bar{T}_c$. Thus from (6), $Q_0 \approx \frac{1}{2} K_0^{(2D)} \gamma_0^{-2} U(0)$. Neglecting $J_{\parallel}$ screening, the $1/R$ interaction gives [8]

$$Q_0 \approx \tfrac{1}{2} K_0^{(2D)} \gamma_0^{-1} \ln(K^*)^{-x} \approx 0.284 K_0^{(2D)} \gamma_0^{-1} .$$

Similar linear potentials, $\sim \gamma_0^{-1} R_{\parallel}$ but for all scales, arise in modified 3D XY models [3] with alternate-plane vorticity suppression [11] that suppresses multiple-plane loops.

Scaling equations for rectangular loops of scales $a < r_0$ are obtained [8] in the usual [2(b)] way from the partition function for single-plane ($z' = z$) variables $J_{\perp}(\mathbf{r},z) \times J_{\perp}(\mathbf{r}',z)$, with log-plus-linear interaction. They are of KT-like form

$$\frac{dK_l^{(2D)}}{dl} = -3A_0 y_l^{(2D)} (K_l^{(2D)})^2 ,$$
$$\frac{dy_l^{(2D)}}{dl} = [4 - 2\pi(K_l^{(2D)} + Q_0 e^l)] y_l^{(2D)} . \qquad (11)$$

Including effects of 2D spin waves [18] (stiff up to $T \sim T_{\mathrm{KT}}$), the bare $a = a_0$ inputs are the coupling $K_0^{(2D)} \approx K_{\parallel}/[1 + 1/(2K_{\parallel})]$, $J_{\perp} = \pm 1$ *pair* fugacity $y_0^{(2D)} \approx \exp(-\pi^2 K_0^{(2D)})$ and (say) $Q_0 \simeq \frac{1}{2} K_0^{(2D)} \gamma_0^{-2} U(0)$. The renormalized pair fugacity (i.e., rectangle population) is found to vanish rapidly, $y_l^{(2D)} \to 0$, beyond $l = l_0 \equiv \ln(r_0/a_0)$.

In the strong anisotropy regime $\gamma_0^{-1} < 0.5$, (10) is valid for 3D ellipses, $a > r_0$, and (11) is valid for quasi-2D rectangles, $a < r_0$. $K_{l_0}^{(2D)}, y_{l_0}^{(2D)}$ from (11) are therefore handed over at $l = l_0$ to (10) as the inputs $K_{l_0}, \bar{y}_{l_0}$. (The $a < r_0$ quasi-2D T dependences that are thus fed in can control noncritical T dependences of fugacities for $a > r_0$.) In the weak anisotropy regime $\gamma_0^{-1} > 0.5$, (10) is used throughout, since elliptical loops of all scales tumble freely, and quasi-2D excitations are not well defined ($r_0 < 2a_0$).

T_c is evaluated in all cases from the change in (3D) asymptotic scaling flows (solid line, Fig. 1). The MC data [9] match T_c reasonably well. If the weak anisotropy procedure is erroneously used even for small $\gamma_0^{-1} \to 0$, then T_c is driven to zero (dashed line). The dotted line is from "approximate self-duality" [10(a)]. The dash-dotted line is $T_{\mathrm{KT}}(\gamma_0)$, defined through $\pi K_{l_0}^{(2D)}(T_{\mathrm{KT}}) = 2$ for a fictitious finite-scale ($\lesssim r_0$) "unbinding" of the quasi-2D excitations.

Armed with (10) and (11), one can numerically calculate the layered superconductor/anisotropic JJA quantities.

The dimensionless (isotropic case) superfluid density, at finite scales, is the vortex coupling with an absorbed length scale removed [5,6], $\rho_l \equiv K_l/a$. Figure 2 shows, for various γ_0^{-1} values, the infinite scale $\rho_\infty/K_{\parallel}$ versus scaled temperature $\bar{T} \equiv K_{\parallel}^{-1}$. (i) There are rapid roll-offs but not 2D jumps, at (not shown) temperatures $\bar{T}_{\mathrm{KT}}(\gamma_0)$, that are near the (dash-dotted) $2/\pi$ slope KT line. (ii) The only singular behavior is at T_c, $\rho_\infty \sim |\varepsilon|^{\nu}$. (iii) The $\gamma_0^{-2} = 0.02$ 3D XY MC simulations [3(b)] (dashed line) are matched reasonably well.

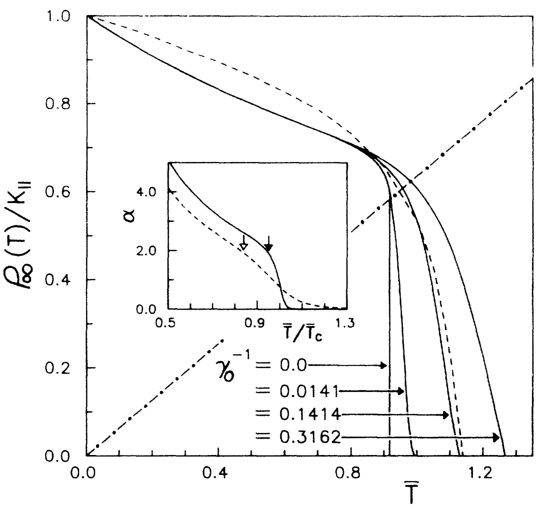

FIG. 2. Scaled superfluid density $\rho_\infty(T)/K_{\parallel}$ versus scaled temperature $\bar{T} \equiv K_{\parallel}^{-1}$ for various anisotropies $\gamma_0^{-1} \equiv (K_{\perp}/K_{\parallel})^{1/2}$. Dashed line is MC result for $\gamma_0^{-1} = 0.14$. [Inset: Current-voltage exponent $\alpha = \pi K_{l_0}^{(2D)}(T)$ versus $\bar{T}/\bar{T}_c(\gamma_0)$ with $l_0 = \ln(\gamma_0)$ for $\gamma_0^{-1} = 1.4 \times 10^{-2}$ (solid) and 0.2 (dashed). Solid and open arrow heads denote $\bar{T}_{\mathrm{KT}}$ in the two cases.]

In strictly 2D, a current drive I unbinds $T < T_{\mathrm{KT}}$ paired vortices, for length scales beyond $r_I \sim 1/I$, yielding power law current-voltage dependences [1], $V \sim I^{1+\alpha}$, where $\alpha = \pi K_\infty^{(2D)} \to 2$ as $T \to T_{\mathrm{KT}}^-$ and $\alpha = 0$ for $T > T_{\mathrm{KT}}$. In 3D, if $r_I < r_0$, a similar current-induced quasi-2D excitation depairing of $J_{\perp} = \pm 1$ should yield a finite-scale exponent $\alpha = \pi K_{l_0}^{(2D)}(T)$, with $\alpha(\bar{T}_{\mathrm{KT}}) \equiv 2$. The inset of Fig. 2 shows this α versus $\bar{T}/\bar{T}_c(\gamma_0) = (T/T_c)(1 - T_c/T_{c0})/(1 - T/T_{c0})$ for $\gamma_0^{-1} = 1.4 \times 10^{-2}, 0.2$. α is smooth through $\bar{T}_{\mathrm{KT}}$, similar to the high-T_c experiments [1].

The 2D resistance due to phase slips across an area is $R^{(2D)} \sim \xi_+^{-2}$, where the intervortex separation $\xi_+ = n_v^{-1/2}$ is related to the single-vortex areal density $n_v = y_l^{1/2}/a^2$ at a suitable, large l scale [1]. The 3D case phase-slip resistance in the plane, including interplane vortex-segment lockings over $\sim \xi_+$, is $R \sim R^{(2D)} \xi_+ \sim \xi_+^{-1}$. Here $\xi_+ = n_v^{-1/3}$ is related to the asymptotic ($l \to \infty$), single-segment volume density $n_v = y_l^{1/2}/a^3$. Figure 3 shows the scaled 3D resistance $\log_{10}[R(\bar{T})/R(\infty)]$ versus scaled temperature $\bar{T}/\bar{T}_{\mathrm{KT}} = 1.09 K_{\parallel}^{-1}(T)$, for widely differing γ_0^{-1} values (where $\bar{T}_{\mathrm{KT}}^{-1} = 1.09$ for the strictly 2D case). All curves fall close to the 2D $\gamma_0^{-1} = 0$ curve. This is similar to "universal resistance scaling" of Minnhagen, found [3] for film and superlattice data. The inset shows

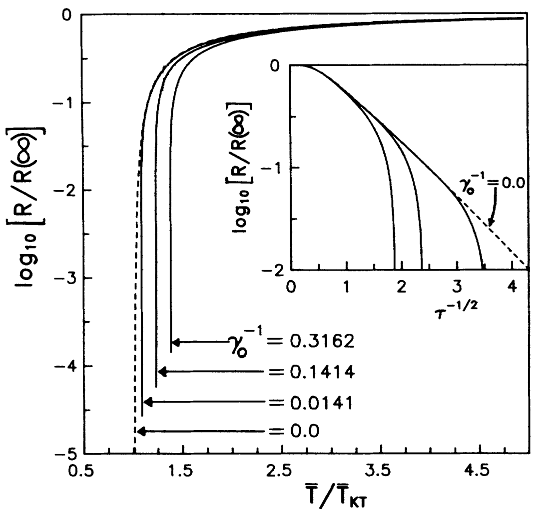

FIG. 3. Scaled phase-slip resistance $\log_{10}[R(\bar{T})/R(\infty)]$ versus scaled temperature variable $\bar{T}/\bar{T}_{KT} \equiv 1.09 K_{\parallel}^{-1}(T)$ for γ_0^{-1} values as shown. (Inset: $\log_{10}[R(\bar{T})/R(\infty)]$ versus $\tau^{-1/2} \equiv [(\bar{T}/\bar{T}_{KT})-1]^{-1/2}$ for $\gamma_0^{-1}=0$, and other values as in main figure.)

a KT-like linearity [1] of $\log_{10}[R(\bar{T})/R(\infty)]$ versus $\tau^{-1/2}-[(\bar{T}/\bar{T}_{KT})-1]^{-1/2}$ before critical behavior [4] $R \sim |\varepsilon|^{\nu}$ sets in for $|\varepsilon| < \varepsilon_c < \gamma_0^{-1/\nu}$, where log-log plots of the resistance curve give $\nu=0.67$.

Thus quasi-2D behavior in layered superconductors is understandable through a 3D vortex-loop scaling, without invoking new nonvortex solitons [1(b)] or complete layer decoupling above T_c. These XY model results should remain essentially unchanged by internal gauge field effects, consistent with (isotropic case) simulations [19]. Since the magnetic flux line generated by circulating vortex currents must follow the topological vortex line, the self-generated net magnetic field of closed-loop quasi-2D excitations is weak, and confined to an interplane London penetration depth.

Further work could include the incorporation of external gauge fields (flux lattice), MC work to detect quasi-2D excitations, comparison of the model results with high-T_c data, experimental search near T_c for 3D exponents, and measurements in micron-scale anisotropic 3D JJA constructed by appropriately stacked 2D arrays. Since the signatures seen are of 3D XY phase vortices, interacting fermion models that naturally generate JJA-like quantum phase coherence variables [20] are worth exploring further.

In conclusion, an anisotropic 3D XY vortex-loop scaling approach shows that 3D critical behavior, induced by multiple-plane 3D loops, can coexist with noncritical quasi-2D KT-like behavior, induced by finite-scale, single-plane loops. Excitations behave as though layers are quasidecoupled at small scales and isotropically coupled at large scales.

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