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LETTER TO THE EDITOR

Monte Carlo simulations of intrinsically pinned vortices in layered superconductors

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Abstract. Monte Carlo simulations of a lattice London model have been performed to investigate the thermodynamic properties of a vortex lattice, intrinsically pinned by the layered structure of a three-dimensional type-II superconductor. Two successive transitions, evidenced by measurements of the structure factor, are observed: a low-temperature transition that results from the melting of the flux line lattice into a smectic phase where flux lines are confined between *ab*-planes, and a high-temperature transition to a vortex liquid phase.

When a sufficiently strong magnetic field is applied perpendicular to the *c*-axis of a layered high-temperature superconductor, such as YBCO or BSCCO, flux lines can penetrate the material and become 'trapped' between two *ab*-layers. This is due to the modulation of the superconducting order parameter along the *c*-axis which induces a periodic pinning potential; this potential localizes vortices between layers at low temperatures T [1]. In order for such a pinning mechanism to be effective, vortices should run parallel to, or at a small angle with, the *ab*-planes [2]. One question of interest is whether or not there exists a smectic phase [3, 4] where layers would be decoupled. If there now seems to be some agreement about the low-field case, where it has been argued quite convincingly by Mikheev and Kolomeisky [5] that no such phase can exist, the problem remains unsettled as regards the high-field case because interactions among vortices are hard to evaluate (because of the compression modulus due to entropic repulsion). Efetov [6] suggested that there might be a decoupling transition for fields $H > H^* = (\Phi_0/d\Lambda)$, where d is the interlayer distance and $\Lambda = d\gamma^{-1}$ is the Josephson penetration length, $\gamma^2 = \lambda_{ab}^2/\lambda_c^2 = m_{ab}/m_c$ being the superpair effective mass ratio. Korshunov and Larkin [7] suggested that the corresponding decoupling temperature can only be greater than the superconducting transition temperature and that therefore no smectic phase can be observed; they based their discussion on the Lawrence–Doniach model and obtained a lower bound for the decoupling temperature within the Coulomb gas formalism. On the other hand, the renormalization group arguments of Mikheev and Kolomeisky [5], when generalized to higher densities of vortices, suggest the possible existence of a finite T decoupling transition [4]. In this letter, we study the behaviour of a parallel field vortex system in high magnetic fields by means of Monte Carlo simulations of an anisotropic lattice London model [8]. Our simulations suggest the existence of two successive transitions, one at low T from a solid vortex lattice to a smectic phase with a loss of correlations among vortices in neighbouring planes and long-range

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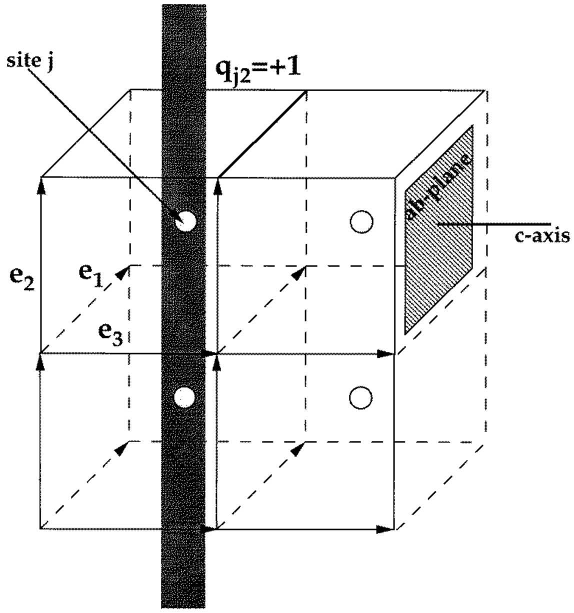

Figure 1. Four plaquettes and two-segment vortex line parallel to the *ab*-planes; circles are lattice sites (i.e. plaquette centres).

vortex-density correlations along the c-axis, and another one at higher T from the smectic phase to a regular 3D liquid phase.

Simulations are performed on a cubic lattice, the unit cell of which is of size d, which we take to be equal to the bare correlation length ξ. Vortex lines are constructed from finite elements e_μ, where $|e_\mu| = d$ and $\mu = 1, 2, 3$, located at the centre of each cell. The vorticity $q_{j\mu} = 0, \pm 1, \pm 2, \ldots$ indicates the number of flux quanta carried by cell j in the μ-direction. Solving the lattice London equation without disorder, and with periodic conditions in all directions [8], yields the energy $E = \sum_{i,j} \sum_{\mu=1}^{3} G(r_i - r_j) q_\mu(r_i) q_\mu(r_j)$. In this expression, the anisotropic couplings $G(r_i - r_j)$ are defined through their Fourier transforms

$$G_3(p) = \frac{4\pi^2 J(\kappa^2 + \lambda_3^{-2} d^2)}{(\kappa^2 + \lambda_1^{-2} d^2)(\kappa_1^2 + \kappa_2^2 + \gamma^2 \kappa_3^2 + \lambda_3^{-2} d^2)}$$

and

$$G_1(p) = G_2(p) = \frac{4\pi^2 (\gamma^2 J)}{(\kappa_1^2 + \kappa_2^2 + \gamma^2 \kappa_3^2 + \lambda_3^{-2} d^2)}$$

where $\kappa_\mu = 2\sin(p_\mu d/2)$, $\kappa^2 = \sum_{\mu=1,2,3} \kappa_\mu^2$, $\lambda_1 = \lambda_2$ (respectively, λ_3) is the penetration depth for fields perpendicular (respectively, parallel) to the ab-planes and $J = \phi_0^2 d\gamma^2 / 32\pi^3 \lambda_{ab}^2$ sets the energy scale. In the following, $k_B T$ will be defined in units of J. We use a finite penetration depth λ_1 such that $d/\lambda_1 = 0.1$, and moderate anisotropy values given by $\gamma^2 = 1, 2, 10, 20$.

Simulations start with a fixed number n_l of straight vortex lines along the 2-direction ($||ab$), arranged in an approximate anisotropic (Abrikosov) triangular lattice (see in figure 1 the organization of a plaquette with two vortex segments $||ab$). New configurations, generated by adding a randomly selected elementary loop of unit vorticity at a randomly

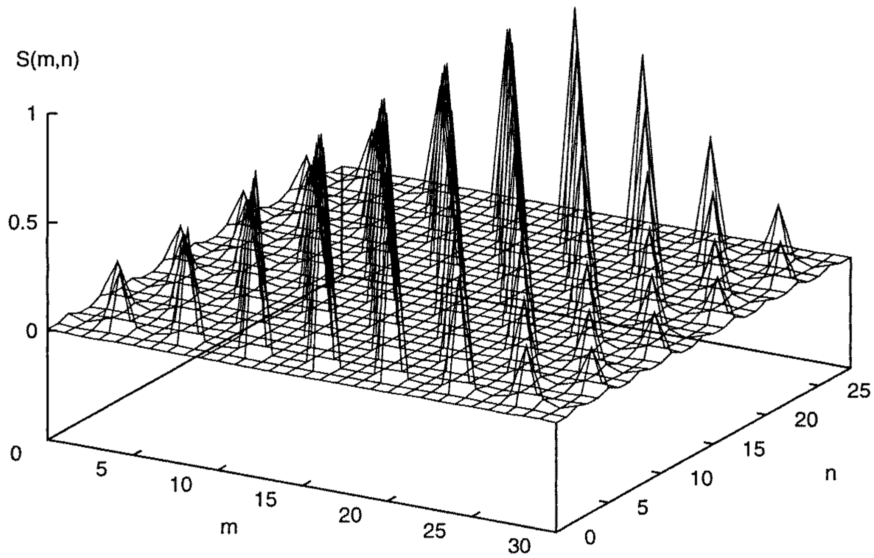

Figure 2. (1,3)-plane structure factor $S(n, m)$ for the q_2 elements at $T = 0.2\ J < T_1 = 0.35\ J$ (with $\gamma^2 = 10$ and $B \approx 0.13\ B_{c2}$).

chosen site of non-zero vorticity, are accepted or rejected according to a standard Metropolis procedure. One MC step corresponds to V such elementary trials, with $V = L_1 L_2 L_3$, where L_μ is the linear size of the lattice in the μ-direction. The update procedure conserves both the local vorticity and the total magnetic induction $B_\mu = (\phi_0 d/V)\sum_j q_\mu(r_j)$. In what follows, $L_1 = L_2 = L_3 \equiv L$, $B_1 = B_2 = 0$ and $B_2 = \phi_0 n_L/L^2$. Spontaneous nucleations and subsequent fluctuations of closed loops are neglected. The normalized (1,3)-plane structure factor $S(k) = (n_l L)^{-1}\langle|\sum_j q_2(r_j)\mathrm{e}^{\mathrm{i}k\cdot r_j}|^2\rangle$ for the q_2 elements, with $k = (k_1,\ 0,\ k_3) = 2\pi/L(n-(L/2),\ 0,\ m-(L/2))$ $(n,\ m = 0,\ 1,\ \ldots,\ L_{||})$, was measured during the simulations, discarding the first 10 000 MC steps used to reach thermal equilibrium. $\langle\ldots\rangle$ denotes thermal averaging. Simulation were run for 20 000 MC steps with $n_l = 120$ vortices in a $32 \times 15 \times 30$ lattice.

Two successive transitions can be observed: (i) A solid–smectic transition at $T = T_1$, characterized by the disappearance of the Bragg peaks of the solid triangular lattice's reciprocal lattice, which are replaced by the Bragg 'planes' expected in the absence of correlations between flux lines in neighbouring layers and a solid-like modulation of the vortex density along the c-axis. (ii) A smectic–3D liquid transition, at $T = T_2$. At T_2, Bragg peaks completely disappear to yield a characteristic liquid structure factor. Figures 2, 3 and 4 show the (1,3)-plane structure factor for the q_2 elements at fixed anisotropy $\gamma^2 = 10$ and magnetic field $B \approx 0.13\ B_{c2}$, at $T < T_1$ (figure 2), $T_1 < T < T_2$ (figure 3) and $T > T_2$ (figure 4). Figure 5 represents $S(n = 2, m = 15)$ (a wavevector that belongs to the Bragg plane of the smectic phase) and $S(n = 2, m = 7)$ (a wavevector which is a Bragg peak of the solid triangular lattice's reciprocal lattice, but that does not belong to the Bragg plane of the smectic phase) as a function of T/J: T_1 ($\approx$0.35) and T_2 ($\approx$3.3) are clearly seen. These results therefore suggest the existence of an intermediate smectic phase with decoupled layers at large field, even at moderate anisotropy. It is not possible to make any conclusions about the order of these transitions from the simulations. Figure 6

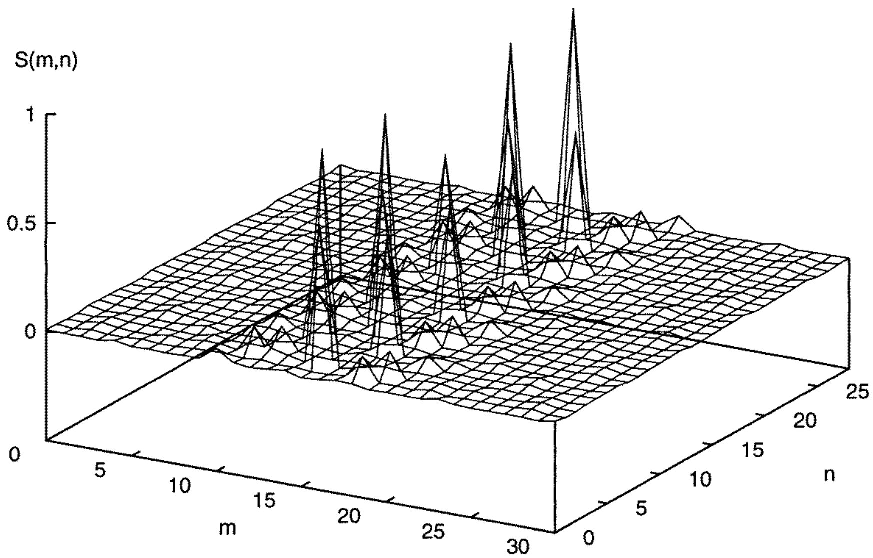

Figure 3. $S(n, m)$ at $T_1 = 0.35\ J < T = 1.8\ J < T_2 = 3.3\ J$ (with $\gamma^2 = 10$ and $B \approx 0.13\ B_{c2}$).

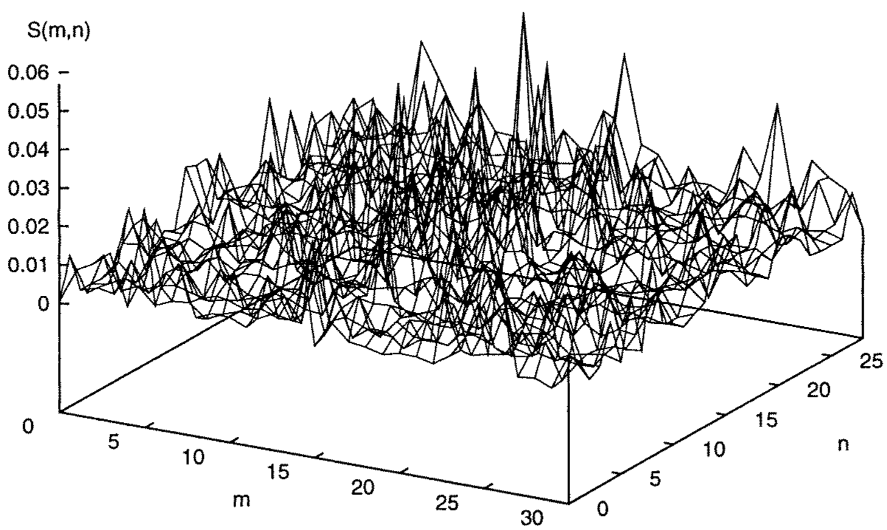

Figure 4. $S(n, m)$ at $T = 3.6\ J > T_2 = 3.3\ J$ (with $\gamma^2 = 10$ and $B \approx 0.13\ B_{c2}$).

represents the two transition temperatures T_1 and T_2 as a function of the anisotropy factor; the temperature range of the smectic phase decreases to 0 as the system becomes isotropic.

In conclusion, we have shown by means of Monte Carlo simulations the existence of a decoupling (3D solid $\rightarrow$ 3D smectic) transition in a model type-II superconductor (anisotropic lattice London model), when a large magnetic field is applied parallel to the layers, as suggested by Efetov [6]. This result is also relevant to 2D bosons in a periodic potential, and suggests the existence of two transitions. Our thermodynamic simulations

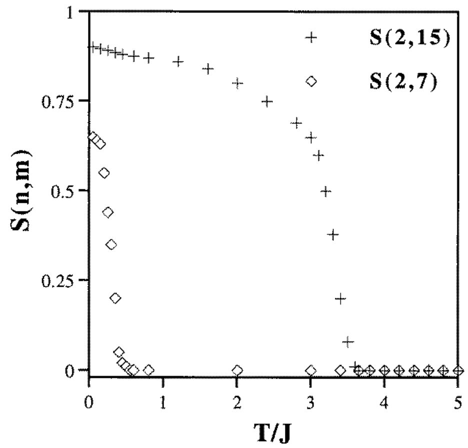

Figure 5. $S(2, 15)$ and $S(2, 7)$ (average over ten simulations of 2×10^5 MC steps each) as a function of T/J for $\gamma^2 = 10$ and $B \approx 0.13\ B_{c2}$.

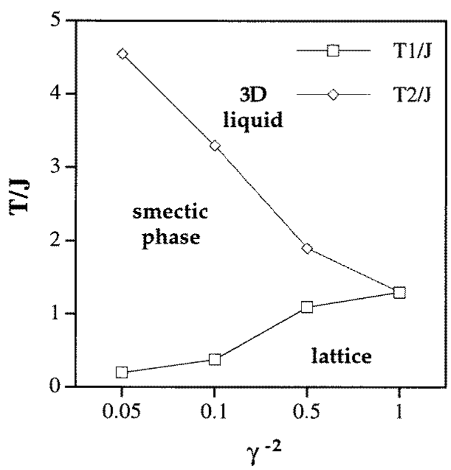

Figure 6. Transition temperatures T_1 and T_2 as a function of the anisotropy factor γ^2.

will be complemented by more 'dynamic' Monte Carlo simulations where the response of the system to an applied current along the c-axis is studied; such simulations will make it possible to compare our results with other theoretical and experimental results (e.g. [3, 9, 10, 11]).

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