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LETTER TO THE EDITOR

Order of the vortex lattice melting transition in a type-II superconductor as a function of magnetic field

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Abstract. Monte Carlo simulations of a lattice London model have been performed to study the order of the vortex lattice melting transition in a pure type-II superconductor for two different values of the total magnetic induction, using the histogram technique and Lee–Kosterlitz finite-size scaling analysis. The results suggest that the melting transition is a first order at low fields and may become second order above some critical field in the absence of any disorder.

A type-II superconductor in the mixed state undergoes a melting transition of its solid vortex lattice into a (disentangled or entangled) liquid state. Theoretical calculations [1], numerical simulations [2] and experiments [3] have yielded strong support in favour of a first-order melting transition in pure bulk materials. However, experiments by Safar *et al* [4] on clean, untwinned YBCCO single crystals seem to show that the first-order melting transition transforms into a continuous one at high fields (about 10 T). These observations were argued to result from disorder, which becomes relevant at large field because the melting temperature gets lower, and smears the first-order transition. An alternative explanation relies on the possible existence of a polymer-like glass, the relaxation timescales of which would prevent the transition from being observed. Recent results reported by Zeldov *et al* [5], who were able to probe the local induction in high-quality BSCCO crystals, while they clearly show a first-order transition at low field, suggest the existence of a critical point at 380 G where melting becomes continuous. The aim of this paper is to explore whether it is possible to account for the transformation of the first-order melting transition into a continuous one with a simple lattice model of superconductors, the behaviour of which at the melting point is investigated by means of Monte Carlo (MC) simulations.

We use a weakly anisotropic (effective mass ratio $\gamma^2 = 10$) lattice London model, the derivation and properties of which are thoroughly described in [6]. The model is defined on a cubic lattice of size $L \times L \times L$ with periodic conditions in all directions (surface effects are therefore removed). Unit cells are of size d, that we take equal to the bare correlation length ξ. We use a finite penetration length orthogonal to the c-axis (z-direction) λ_1 such that $d/\lambda_1 = 0.05$. Simulations at any L start with a density $f = n_1/(Ld)^2$ of straight vortex lines along the c-axis, arranged in an approximate Abrikosov lattice. New configurations, generated following the prescription of [6], are accepted or rejected according to a standard Metropolis procedure. The update procedure conserves the total magnetic induction $B = \phi_0 f z$. Spontaneous nucleations and subsequent fluctuations of closed loops are neglected. The cases $f = 1/(3d)^2 \equiv f_1$ and $f = 1/(6d)^2 \equiv f_2$ are explored. In

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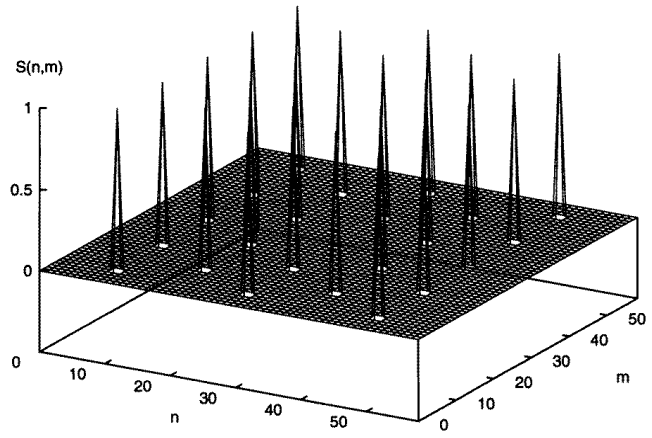

Figure 1. Normalized in-plane structure factor $S(k) = (n_1 L_\perp)^{-2} \langle | \sum_j q_3(r_j) e^{ikr_j} | \rangle$ for the q_3 elements, with $k = (k_1, k_2, 0) = (2\pi/L_\parallel)(n = L_\parallel/2, m - L_\parallel/2, 0)$ $(n, m = 0, 1, \ldots, L_\parallel)$ for an Abrikosov lattice ($T = 0$).

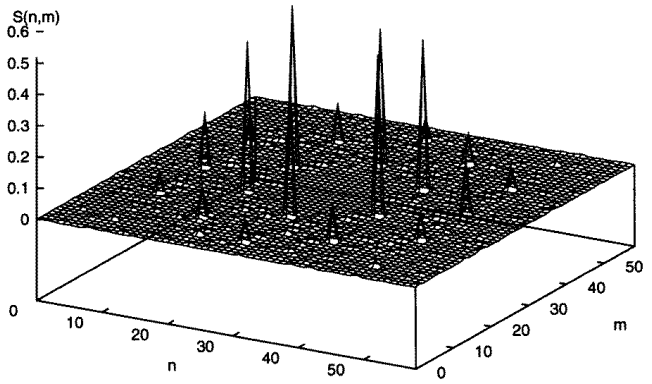

Figure 2. The same as figure 1 at $T \leqslant T_m$.

both cases, we find a melting point from rough temperature sweeps, characterized by a peak in the heat capacity, an abrupt change in slopes of various thermodynamic quantities, and the disappearance of Bragg peaks exhibited by the structure factor of the system in the low-T phase (see, e.g., the structure factor below and above T_m for a $60 \times 60 \times 15$ system at $f = 1/(30d^2)$, represented in figures 1, 2, and 3). For each value of f, the simulations were performed at $L = 6$, 9 (f_1 only), 12, 15 (f_1 only), 18, and 24 (f_2 only). Following a temperature sweep, an optimized histogram method was first used to locate the 'transition' point $T_m(f, L)$ accurately, and a single histogram simulation was run right at that point for 5×10^5 MC steps for $L = 6$, 9, 12 and 2×10^6 MC steps for $L = 15$, 18 and 24. Let us recall that the histogram method (see, e.g., [7]) consists of running a MC simulation at a temperature $T_0 = -1/k_B K_0$ to generate configurations of energy E with a weight $\propto e^{K_0 E}$; the probability of observing the system in a state of energy E is $P_{K_0}(E) = Z_{K_0}^{-1} N(E) e^{K_0 E}$, where $N(E)$ is the number of states of energy E. $P_{K_0}(E)$ is approximated by $H(E)/n$ where $H(E)$ is the histogram obtained during the simulation and

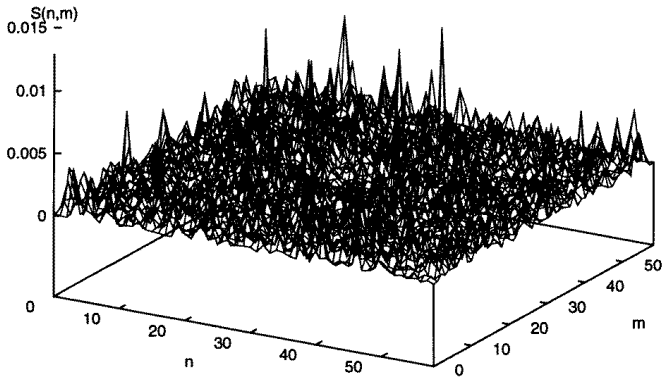

Figure 3. The same as figure 1 at $T > T_m$.

n the number of measurements. The distribution of energies at another value $T = -1/k_B K$ is given by $P_K(E) = Z_K^{-1} N(E) \mathrm{e}^{KE}$, that is, $P_K(E) = (Z_K^{-1}/Z_{K_0}^{-1}) \mathrm{e}^{[K-K_0]E} P_{K_0}(E)$. An approximation of $P_K(E)$ is then

$$\tilde{P}_K(E) = \frac{H(E)\mathrm{e}^{[K-K_0]E}}{\sum_E H(E)\mathrm{e}^{[K-K_0]E}}.$$

This expression makes it possible in principle to compute $P_K(E)$ and associated thermodynamic quantities to locate possible phase transitions, not too far from K_0. Additional simulations performed at other values of K allow for an optimized approximation of $P_K(E)$ with an appropriate combination of histograms that reduces statistical errors [8]. In the course of simulations, equilibration is checked for by running two replicas of the system in parallel and waiting for a reasonably good superposition of, say, both energy histograms (this procedure is very time consuming for large systems) [9]. When this is the case, only one of the two simulations keeps running. Let $K(f, L) = -1/k_B T_m(f, L)$. At a phase transition, the free energy $F(e; K(f, L)) \equiv [K(f, L)]^{-1} \ln P_{K(f,L)}(e)$, where $e = EL^{-3}$ is the internal energy per lattice site, clearly exhibits two minima separated by a barrier of height $\Delta F(L)$ corresponding to the two coexisting phases. If $\Delta F(L)$ increases with system size L for large L (more precisely, $\Delta F(L) = aL^{d-1} + \mathrm{O}(L^{d-2})$, where d is the dimensionality of the system), the transition is first order [10]. This method has been used by Hetzel *et al* [2] to determine the order of the melting transition from a uniformly frustrated 3D XY model, and they found it to be first order. Their simulations were performed with a model that represents an extreme type-II superconductor in a strong magnetic field, in the absence of screening. This result does not really agree with experiments, which all suggest that the first-order melting transition transforms into a second-order one at high enough fields. Note that screening has recently been shown to be a crucial ingredient in a related model of a strongly disordered superconductor, the gauge-glass model [11], where it destroys the finite-temperature glass transition [12].

Our results on the lattice London model are summarized in figure 4, where $\Delta F(L)$ is represented as a function of L^{-1}, for $f = f_1$ and $f = f_2$. For $f = f_2$, $\Delta F(L)$ unambiguously increases with L, thereby suggesting a first-order transition. How ΔF varies with L for $f = f_1$ is not so clear: it is impossible to say, within error bars, whether ΔF is increasing, decreasing, or stable as L increases. But the behaviour at $f = f_1$ is drastically different from the one observed at $f = f_2$, and leaves open the possibility of

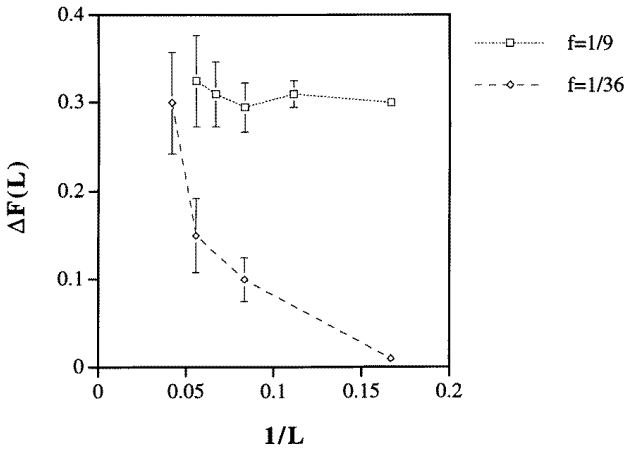

Figure 4. $\Delta F(L)$ as a function of L^{-1} for $f = f_1$ and $f = f_2$.

a continuous transition. More simulations are required to study this question (to explore larger sizes and reduce error bars) and possibly confirm the change in nature of the melting transition; note however that the present simulations are already very heavy, especially for large systems, which are quite difficult to equilibrate and require many more simulation steps (each such step taking more time to compute because of long-range interactions) to obtain reliable histograms.

Finally, let us mention that the question of whether the transition is first or second order in this model may be related to the absence or existence of an intermediate disentangled phase, a controversial problem that has recently received attention [13, 14].

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