Monte Carlo simulation of layered high-temperature superconductors

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We present results from Monte Carlo simulations of the vortex state in layered high temperature superconductors. We use a set of potentials derived from the Lawrence-Doniach free-energy functional which incorporates (i) intra-layer coupling (ii) inter-layer Josephson and electromagnetic interactions. We have employed a novel technique for performing an in-plane infinite lattice summation for the intra-layer interactions. This provides a minimum 50,000 times faster speed-up in the simulations over previous naïve methods which add periodic images in shells of increasing radius. We present results of the numerical B-T phase diagram in the pure system and obtain good agreement with available experimental/theoretical results.

1. INTRODUCTION

The nature of the vortex state in high temperature superconductors is not yet fully understood. The competition between the ordering forces of the elastic lattice and the disordering influence of thermal energy and material pinning leads to a number of possible vortex phases including a Bragg glass, a vortex glass and liquid states. We report some preliminary results from Monte Carlo simulations of the vortex state in a model three-dimensional system.

2. MODEL

We perform particle-particle simulations using a model derived from the Lawrence-Doniach free energy functional. We consider N_z superconducting layers separated by a distance s and each containing N_{xy} point-like vortex pancakes. Each vortex is described by its position vector $r_{i,k}$ within the plane and vortex lines are defined by connecting each vortex to a unique neighbour in the layers above and below. Periodic boundary conditions are applied in all directions. Each layer has an oblique geometry commensurate with the hexatic nature of the solid phase. The vortex density is fixed such that $N_{xy}/A_{xy} = \Phi_0/B$ giving a trigonal lattice spacing of $a_0^2 = (4/3)^{1/2}(\Phi_0/B)$, where $\Phi_0 = hc/2e$ is the flux quantum.

We apply an intra-layer interaction potential acting between all vortices in the same layer. This takes the form of a modified Bessel function appropriate to line-like interactions in the vortex state [1]. In contrast to previous numerical simulations we apply a full set of potentials between the pancakes that define a single line, including Josephson pairwise, three and four body interactions and electromagnetic contributions. These are derived in [2].

The scaling length λ for the intra-layer interaction is large and yields a long-range potential. We have developed a new summation method to determine the system energy summed over infinite periodic repeats of the unit cell. The Bessel function is expanded using the Gegenbauer addition formulae [3]. The potential between a pair of particles is expressed as:

$$K_0^*\left(\frac{w}{\lambda}\right) = K_0\left(\frac{z}{\lambda}\right) + \sum_{k=-\infty}^{\infty} I_k\left(\frac{z}{\lambda}\right)[c_k \cos(k\theta) - s_k \sin(k\theta)] \quad (1)$$

where c_k and s_k are coefficients determining the energy contribution from the infinite lattice, which can be pre-computed. z and θ refer to unit cell separations and I_k is a modified Bessel function. The resulting calculation is a minimum of 50,000 times faster than the naïve summation of image cells at increasing radius (see Figure 1).

Various observables are used to determine the phase of the vortex system. These include Delaunay triangulation, hexatic order parameter, and number of topological defects (definitions as in e.g. [4]). To probe the translational properties of the system
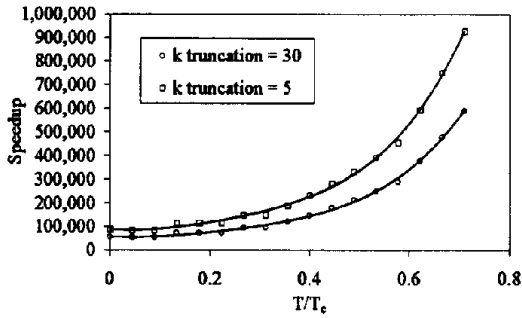
Figure 1. Speedup achieved by infinite lattice summation over naïve summation method as a function of temperature in the simulation and the number of coefficients used in (1).
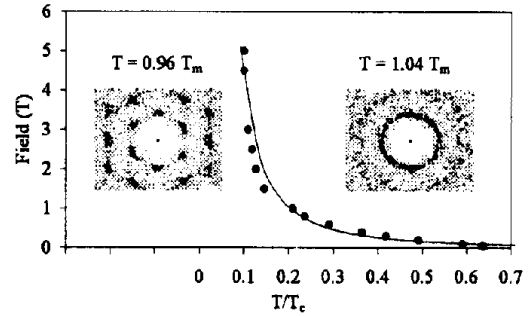

Figure 2. Numerical phase diagram obtained from annealing data. Trend line is fitted from equation (2) *Inset*: Structure factors observed just above and below the melting temperature T_m.

we calculate the structure factor from the two-dimensional Fourier transform of the ensemble average of the vortex positions at a given temperature.

3. RESULTS

With material parameters appropriate to BSCCO compounds (λ_{ab} = 1500Å, s = 10Å, Γ = 500) we have performed Monte Carlo simulations on systems of size N_{xy} = 192 and N_z = 10. Using 1×10^4 sweeps to equilibrate and 5×10^4 sweeps for observations we have determined the phase diagram of the pure three dimensional system using field cooled annealing. The relatively low number of sweeps employed leads to some hysteretic effects in the melting properties of the system and for consistency we present results from annealing runs only.

Starting from a melted state we have reduced the temperature in 0.25K steps through the freezing point. We identify a solid phase through a sharp increase in hexatic order, a decrease in the number of topological defects and the onset of Bragg peaks in the structure factor. By monitoring the specific heat capacity of the system energy we identify the temperature at which freezing occurs. The results are presented in figure 2. A theoretical melting line based on nearest neighbour interactions is given by [1]:

$$B_m = \frac{c_L^4 \Phi_0^5}{(\mu_0 \pi)^2 \Gamma^2 (k_B T)^2 \lambda_{ab}^4}.$$ (2)

The line in figure 2 is fitted using an optimal value of c_L = 0.27. This is similar to empirical results [5].

Pinning is introduced into the model system as a periodic disordering energy surface superposed over the simulation cell. Qualitatively the surface is generated such that typically five maxima and minima occur within each vortex spacing of the lattice at 1T. At constant field, the freezing point of the vortex system is observed to reduce in the presence of pinning and decreases as the average pinning strength increases as expected.

Our simulations indicate that use of the full set of interaction potentials yields results similar to those obtained with simplified potentials. Further, as discussed in [3], our infinitely summed potential does not introduce unphysical defects into the annealed state and therefore pinned systems can be simulated more reliably. We will report on further results of such simulations elsewhere.

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