# Disorder Driven Melting of the Vortex Line Lattice

P. Olsson[1] and S. Teitel[2]

[1]*Department of Theoretical Physics, Umeå University, 901 87 Umeå, Sweden*
[2]*Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627*
(Received 11 December 2000; published 5 September 2001)

The 3D *XY* model with random in-plane couplings is simulated to model the phase diagram of a disordered type II superconductor as a function of temperature $T$ and randomness strength $p$ for fixed applied magnetic field. As $p$ increases to a critical $p_c$, the first order vortex lattice melting line turns parallel to the $T$ axis, continuing down to low temperatures, rather than ending at a critical point. Above $p_c$ preliminary results suggest the absence of a phase coherent vortex glass.

DOI: 10.1103/PhysRevLett.87.137001 PACS numbers: 74.60.Ge, 64.60.–i

Experimental [1–3], theoretical [4–6], and numerical [7,8] studies have argued that the effect of intrinsic point impurities on otherwise clean single crystal samples of high $T_c$ superconductors leads to a $H$-$T$ phase diagram with the following generic form. At low magnetic fields $H$, an elastically distorted vortex lattice (the "Bragg glass" [4]) undergoes a first order melting transition to a vortex liquid as temperature $T$ is increased. This melting line $T_c(H)$ continues as $H$ is increased, until an "upper critical point," $T_{\rm ucp}$, is reached above which sharp discontinuities in measured quantities become smeared. Increasing $H$ at lower temperatures, the vortex lattice transforms to a disordered vortex state along the "second magnetization peak" line, $H_{\rm sp}(T)$, where critical currents show a sharp increase. As $T$ increases, the $H_{\rm sp}(T)$ line continues to the vicinity of $T_{\rm ucp}$. In $Bi_2Sr_2CaCu_2O_8$ (BSCCO), $H_{\rm sp}(T)$ is only weakly dependent on $T$ [2], and recent experiments [9] suggest that it is associated with a thermodynamic first order phase transition. Whether the disordered state above $H_{\rm sp}(T)$ is a "vortex glass" [5], characterized by true superconducting phase coherence and separated from the vortex liquid by a sharp phase transition, or whether it is a dynamically frozen state that smoothly crosses over to the vortex liquid, remains a topic of controversy [10].

Since many of the experimental and numerical studies focus on dynamical probes, from which it can sometimes be difficult to infer a true equilibrium phase transition, and analytical models must resort to Lindemann or other simplifying approximations, it is important to establish the true equilibrium phase diagram within a realistic model system. Towards this end we have carried out Monte Carlo (MC) studies of the uniformly frustrated three dimensional (3D) *XY* model [11], with uncorrelated quenched random couplings. For a fixed magnetic field $B$ we map out the phase diagram as a function of disorder strength $p$ and temperature $T$. Increasing $p$ at fixed $B$ is believed to play a similar role as the more physical case of increasing $B$ at fixed $p$. We find in our model a single first order phase boundary, $T_c(p)$. At small $p$, $T_c(p)$ is a thermally driven melting of the vortex lattice. Increasing $p$, there is a maximum $p_c$ above which disorder destroys the vortex lattice; near $p_c$, the line $T_c(p)$ turns parallel to the $T$ axis and continues down to low $T$. No critical point separates the thermal from the disorder driven sections of the phase boundary. Recent experiments on BSCCO [12] are in complete agreement with this result. For $p > p_c$, our preliminary results suggest the absence of a true phase coherent vortex glass.

The model we study is given by the Hamiltonian

$$\mathcal{H}[\theta_i] = -\sum_{\text{bonds } i\mu} J_{i\mu}\cos(\theta_i - \theta_{i+\hat{\mu}} - A_{i\mu}), \quad (1)$$

where $\theta_i$ is the phase of the superconducting wave function on site $i$ of a 3D periodic cubic grid of sites, the sum is over all bonds in directions $\hat{\mu} = \hat{x}, \hat{y}, \hat{z}$, and $A_{i\mu} = (2\pi/\phi_0)\int_i^{i+\hat{\mu}} \mathbf{A}\cdot\mathbf{d}\ell$ is the integral of the magnetic vector potential across bond $i\mu$, where $\boldsymbol{\nabla}\times\mathbf{A} = B\hat{z}$ is a fixed uniform magnetic field in the $\hat{z}$ direction. To model random vortex pins in the $xy$ planes we take [13]

$$\begin{aligned} J_{i\mu} &= J_z, \qquad \mu = z, \\ J_{i\mu} &= J_\perp(1 + p\epsilon_{i\mu}), \qquad \mu = x, y. \end{aligned} \quad (2)$$

The coupling between planes $J_z$ is uniform, while each bond in the $xy$ plane is randomly perturbed about the constant value $J_\perp$; the $\epsilon_{i\mu}$ are independent Gaussian random variables with $\langle\epsilon_{i\mu}\rangle = 0$, $\langle\epsilon_{i\mu}^2\rangle = 1$, and $p$ controls the strength of the disorder. For computational convenience we choose $J_z/J_\perp = 1/40$, with a vortex line density of $f = a_\perp^2 B/\phi_0 = 1/20$, where $a_\perp$ is the grid spacing in the $xy$ plane, and $\phi_0 = hc/2e$ is the flux quantum. Our system size is $L_x = L_y = 40$, with $L_z = 16$. To check finite size effects, we also considered $L_z = 24$ and 32 for certain cases. Our runs are typically $1-10\times 10^7$ MC sweeps through the entire lattice near transitions. Results below are for a single realization of the disorder only. The extremely time consuming nature of our simulations excluded any serious disorder averaging or finite size scaling. We have, however, considered two other realizations of the disorder and have found qualitatively the same behavior.

In the pure model, $p = 0$, the vortex line lattice has a first order melting transition to a vortex line liquid [14]. To map out this melting transition line in the $p$-$T$ plane we fix the disorder strength $p$, and cool from high $T$,

  

until we reach a temperature $T_c(p)$ at which we observe repeated hopping between coexisting vortex liquid and lattice phases. To detect the vortex lattice, we measure the in-plane vortex structure function [normalized so that $S(0) = 1$],

$$S(\mathbf{k}_\perp) = \frac{1}{f^2 N} \sum_{\mathbf{r}_\perp, z} \langle n_z(\mathbf{r}_\perp, z) n_z(0, z) \rangle e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp}, \quad (3)$$

where $n_z$ is the vorticity in the $xy$ plane, and $N = L_x L_y L_z$. $S(\mathbf{k}_\perp)$ will have Bragg peaks at the reciprocal lattice vectors $\{\mathbf{K}\}$ of the vortex lattice. We find that the vortex lattice always orders into the same periodicity as that of the pure $p = 0$ case, where there are two possible lattice orientations related by a 90° rotation. Defining $S_1$ as the average of $S(\mathbf{K})$ over the six smallest nonzero $\{\mathbf{K}\}$ for one lattice orientation, and $S_1'$ as that for the other orientation, we identify the vortex lattice as states in which either $S_1$ *or* $S_1'$ is large, according to which of the two lattice orientations has formed; in contrast, in the vortex liquid, both $S_1$ and $S_1'$ are small. In Fig. 1 we plot $S_1$ and $S_1'$ vs MC simulation time $t$ at $T_c(p)$ for two disorder strengths. For the weaker disorder, $p = 0.06$, we see both orientations of lattice coexisting with the liquid. For the stronger $p = 0.09$, the disorder induced breaking of the grid's rotational symmetry, which in principle exists for any value of $p$ in any specific sample, becomes strong enough that we see only coexistence between one particular lattice orientation and the liquid [15]. The repeated hopping between lattice and liquid in Fig. 1 verifies that we are well equilibrated. Varying $p$, we thus determine the melting line $T_c(p)$ shown in Fig. 2. Comparing $L_z = 16$ with $L_z = 24$, we found only a small shift in the phase boundary as $L_z$ increased [16].

We now determine if the transition $T_c(p)$ remains first order, as $p$ increases. First order transitions are characterized by discontinuous jumps in thermodynamic quantities. Here we consider the average energy per site $E$, and a variable $Q$ defined to be conjugate to the disorder strength $p$,

$$E = -\frac{1}{N} \sum_{i\mu} J_{i\mu} \langle \cos(\theta_i - \theta_{i+\hat{\mu}} - A_{i\mu}) \rangle, \quad (4)$$

$$Q \equiv \frac{1}{N} \frac{\partial F}{\partial p} = -\frac{J_\perp}{N} \sum_{i,\mu=x,y} \epsilon_{i\mu} \langle \cos(\theta_i - \theta_{i+\hat{\mu}} - A_{i\mu}) \rangle, \quad (5)$$

where $F$ is the total free energy.

To see if there is a discrete jump in $E$ or $Q$ at $T_c(p)$, we use the values of $S_1$ and $S_1'$ to sort microscopic states as either vortex lattice or liquid. We then compute the properties of each phase separately. In Figs. 3a and 3b we show semilog plots of the histograms $P(\Delta S_1)$ of values of $\Delta S_1 \equiv S_1 - S_1'$ encountered during our simulation at $T_c(p)$, for the two cases of Fig. 1. In Fig. 3a, for $p = 0.06$, we see separated peaks for the liquid at $\Delta S_1 = 0$, and for the two lattice orientations at finite positive and negative values of $\Delta S_1$. In Fig. 3b, for the stronger $p = 0.09$, we see only peaks for the liquid and one of the two lattice orientations. Fitting these peaks to empirical forms (Gaussian for the lattice, exponential for the liquid; these are the solid lines in Figs. 3a and 3b), we determine the relative probability for a state with a given value of $\Delta S_1$ to belong to the liquid phase, or either of the two orientations of the lattice phases. Sorting through our microscopic states we probabilistically assign each to one of these three phases. We then plot the histograms of $E$ and $Q$ separately for each phase.

In Fig. 3c we show the histograms $P(E)$ for $p = 0.06$. While the two lattice orientations have the same energy distribution, there is a clear difference between the liquid and the lattice. This results in a finite energy jump $\Delta E$ at the melting transition, which is thus first order. The histograms $P(Q)$ for $p = 0.06$ are shown in Fig. 3e, where we also see a finite jump $\Delta Q$ between liquid and lattice; for $Q$ the disorder couples differently to the two lattice orientations.

In Fig. 3d we show the histograms $P(E)$ for the more strongly disordered $p = 0.09$. In contrast to Fig. 3c, we find that the energy distributions of the liquid and the lattice are now *identical*. Thus there is no energy jump, and

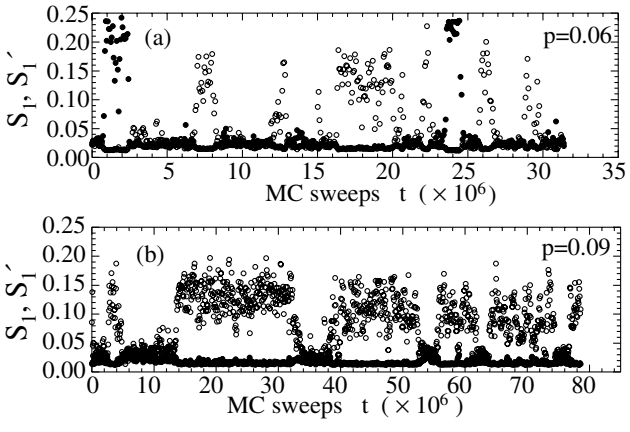


FIG. 1. $S_1$ (●) and $S_1'$ (○) vs the number of Monte Carlo sweeps $t$ for disorder strengths (a) $p = 0.06$, $T_c = 0.255$, and (b) $p = 0.09$, $T_c = 0.200$. The system width is $L_z = 16$. Each data point is an average over $2^{16}$ sweeps.

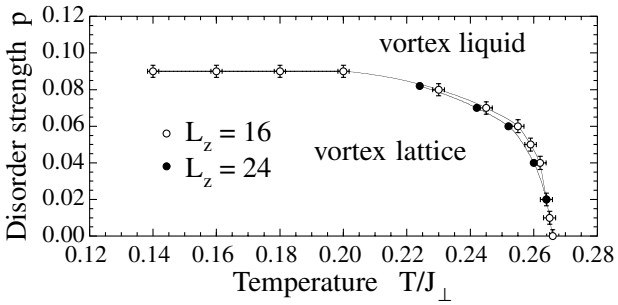


FIG. 2. Vortex lattice melting phase boundary in the $p$-$T$ plane, for $L_z = 16$ (○) and $L_z = 24$ (●).

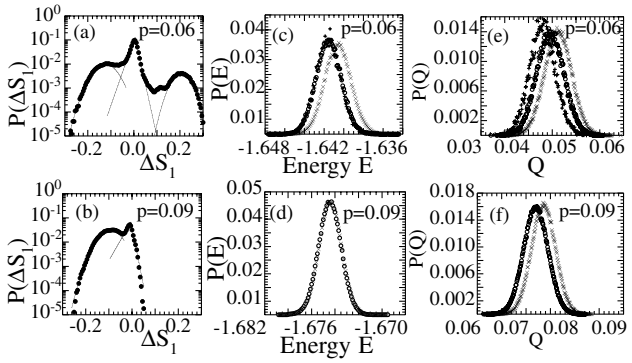


FIG. 3. Histograms of $\Delta S_1 \equiv S_1 - S_1'$, energy $E$, and disorder conjugate $Q$ for $p = 0.06$, $T_c = 0.255$ and $p = 0.09$, $T_c = 0.200$, for $L_z = 16$, at the melting temperature $T_c(p)$. (○) and (+) are for the two lattice orientations; (×) is for the liquid.

moreover no specific heat jump, in going from liquid to lattice. However the histograms of $P(Q)$, shown in Fig. 3f, remain clearly different for liquid and lattice. Thus there is a finite jump $\Delta Q$ at the melting transition, and the transition remains first order. Combining $\Delta E = 0$ with the Clausius-Clapeyron relation, we conclude that the melting line must now be perfectly parallel to the temperature axis [17], and the transition becomes disorder, rather than thermally, driven. As shown in Fig. 2, we have been able to follow the melting line from where it first turns parallel to the $T$ axis, down to several lower temperatures.

In Fig. 4 we plot $\Delta E$ and $\Delta Q$ vs $p$ along the melting line for $L_z = 16$ and 24. That $\Delta E$ and $\Delta Q$ never simultaneously vanish indicates that no critical point exists along the melting line. Our measured jumps in $\Delta E$ and $\Delta Q$ increase somewhat for increasing $L_z$, indicating the presence of finite size effects in our system (see further discussion later on). The fact that the jumps *increase,* however, supports the conclusion of a first order transition in the thermodynamic limit.

Although our simulations are for a specific value of $B$, if we assume that the above result continues to hold for general values of $B$, then it must be true that the phase diagram in the $B$-$T$ plane at fixed $p$ similarly turns parallel to the $T$ axis at low temperatures. The point where the melting line first turns parallel to the $T$ axis has many features in common with an upper critical point; discontinuities as $T$ varies across the melting line below this point will cease to exist as $T$ varies above this point, yet there is no true critical end point and the first order melting line extends continuously down to lower temperatures.

Next, we investigate the superconducting phase coherence in our model, by computing the helicity modulus [11], $\Upsilon_z$, parallel to the applied magnetic field. $\Upsilon_z = 0$ indicates the absence of phase coherence. In Fig. 5a we show $\Upsilon_z$ vs $T$, for two different disorder strengths $p < p_c = 0.09$, comparing systems with $L_z = 16$ and $L_z = 24$. In both cases we see a discontinuous jump in $\Upsilon_z$ at the melting transition. As $L_z$ is increased, we see that $\Upsilon_z$ vanishes in the vortex liquid; the vortex lattice melting thus marks the loss of superconducting phase coherence.

We now consider $p > p_c$. In Fig. 5b we show $\Upsilon_z$ vs $T$ for $p = 0.12$ and system sizes $L_z = 16$ and $L_z = 32$. We see a dramatic finite size effect, suggesting that $\Upsilon_z$ decreases to zero as $L_z \to \infty$ and so there is no phase coherent vortex glass. The difficulty in equilibrating our $L_z = 32$ system at low $T$, however, makes this conclusion still preliminary. Similar results were found in dynamical simulations by Reichhardt *et al.* [8]. Kawamura [18], however, found a finite vortex glass $T_c$ in studies of a model similar to Eq. (1), but at a much higher field and disorder. A vortex glass transition has also recently been found for an interacting vortex line model with $f = 1/2$ and very strong pinning [19].

Finally, in Fig. 6 we plot the longitudinal phase angle correlation length, $\xi_z$, in the liquid $T \geq T_c(p)$, as determined by fitting the correlation function,

$$C(z) = \sum_j \langle e^{i[\theta_j - \theta_{j+z\hat{z}}]} \rangle, \tag{6}$$

to an exponential decay for $z < L_z/2$. For fixed $T$, $\xi_z$ decreases as $p$ increases. However, since $T_c(p)$ decreases as $p$ increases, the value $\xi_z(T_c(p))$ at melting *increases* as

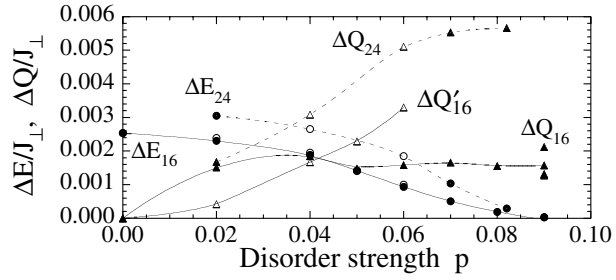


FIG. 4. Jumps $\Delta E$ and $\Delta Q$ vs $p$ along the melting line, $T_c(p)$. Solid lines connect data for $L_z = 16$; dashed lines connect data for $L_z = 24$. Solid and open symbols denote the two possible lattice orientations. Only for $\Delta Q$ in $L_z = 16$ do we see a noticeable difference between lattice orientations.

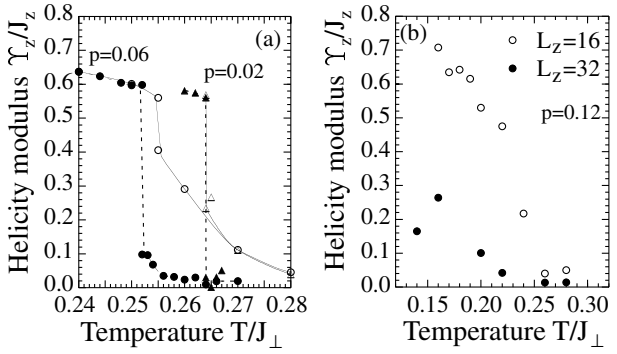


FIG. 5. Longitudinal helicity modulus $\Upsilon_z/J_z$ vs $T$ for disorder strengths (a) $p = 0.02$ and $p = 0.06 < p_c$ (open symbols and solid lines are for $L_z = 16$; solid symbols and dashed lines are for $L_z = 24$); and (b) $p = 0.12 > p_c$.

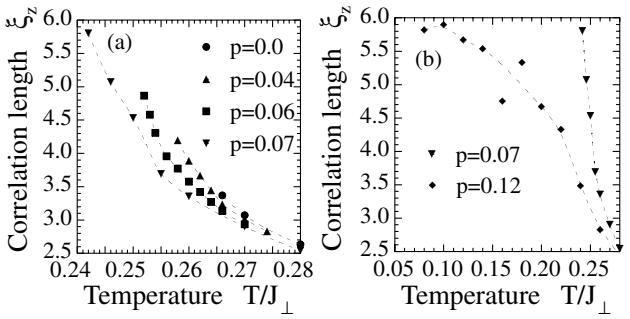


FIG. 6. Longitudinal correlation length $\xi_z$ vs $T$ in the vortex liquid phase for (a) several values of disorder $p < p_c = 0.09$ at $L_z = 24$; and for (b) $p = 0.12 > p_c$ at $L_z = 32$, in comparison to $p = 0.07 < p_c$ from (a).

$p$ increases. Even in the disordered state above $p_c$, $\xi_z$ can be as large as in the liquid just above the thermally driven melting line. Thus the disorder driven melting need not be thought of as a layer decoupling transition.

As we were finishing this work, we learned of similar work by Nonomura and Hu [20], using the same model (1) with a slightly different scheme for the randomness, a much stronger anisotropy $J_z/J_\perp = 1/400$, and a vortex density $f = 1/25$. They too find a first order vortex lattice disordering line nearly parallel to the $T$ axis at low $T$. This agreement with our results suggests the robustness of our conclusions to the particular parameters we have chosen. However Nonomura and Hu also claim to find a first order "vortex slush" to liquid transition extending to higher disorder from the thermally driven melting line, as well as a vortex glass to vortex slush transition at lower $T$. We too find a peak in specific heat for $p > p_c$ that lies at a $T$ in the vicinity of the thermally driven melting line, however we have interpreted this as a smooth crossover rather than a true phase transition. Further work is required to clarify the nature of the phase diagram in this region.

We would like to thank C. Marcenat for valuable discussion. This work was supported by the Engineering Research Program of the Office of Basic Energy Sciences at the Department of Energy Grant No. DE-FG02-89ER14017, the Swedish Natural Science Research Council Contract No. E 5106-1643/1999, and by the resources of the Swedish High Performance Computing Center North (HPC2N). Travel between Rochester and Umeå was supported by Grants No. NSF INT-9901379 and STINT No. 99/976(00).

[1] R. Cubitt *et al.,* Nature (London) **365**, 407 (1993).
[2] B. Khayhovich *et al.,* Phys. Rev. Lett. **76**, 2555 (1996); Phys. Rev. B **56**, R517 (1997).
[3] T. Nishizaki *et al.,* Phys. Rev. B **61**, 3649 (2000).
[4] T. Giamarchi and P. Le Doussal, Phys. Rev. Lett. **72**, 1530 (1994); Phys. Rev. B **52**, 1242 (1995); T. Nattermann, Phys. Rev. Lett. **64**, 2454 (1990); D. S. Fisher, Phys. Rev. Lett. **78**, 1964 (1997); T. Nattermann and S. Scheidl, Adv. Phys. **49**, 607 (2000).
[5] D. S. Fisher, M. P. A. Fisher, and D. A. Huse, Phys. Rev. B **43**, 130 (1991).
[6] D. Ertaş and D. R. Nelson, Physica (Amsterdam) **272C**, 79 (1996); J. Kierfeld, T. Nattermann, and T. Hwa, Phys. Rev. B **55**, 626 (1997); T. Giamarchi and P. Le Doussal, Phys. Rev. B **55**, 6577 (1997); A. E. Koshelev and V. M. Vinokur, Phys. Rev. B **57**, 8026 (1998); B. Horowitz and T. R. Goldin, Phys. Rev. Lett. **80**, 1734 (1998); J. Kierfeld and V. Vinokur, Phys. Rev. B **61**, R14 928 (2000).
[7] S. Ryu, A. Kapitulnik, and S. Doniach, Phys. Rev. Lett. **77**, 2300 (1996); N. K. Wilkin and H. J. Jensen, Phys. Rev. Lett. **79**, 4354 (1997); A. van Otterlo, R. T. Scalettar, and G. T. Zimányi, Phys. Rev. Lett. **81**, 1497 (1998).
[8] C. Reichhardt, A. van Otterlo, and G. T. Zimányi, Phys. Rev. Lett. **84**, 1994 (2000).
[9] M. B. Gaifullin *et al.,* Phys. Rev. Lett. **84**, 2945 (2000); D. Giller *et al.,* Phys. Rev. Lett. **84**, 3698 (2000); C. J. van der Beek *et al.,* Phys. Rev. Lett. **84**, 4196 (2000).
[10] D. López *et al.,* Phys. Rev. Lett. **80**, 1070 (1998); A. M. Petrean *et al.,* Phys. Rev. Lett. **84**, 5852 (2000).
[11] Y.-H. Li and S. Teitel, Phys. Rev. Lett. **66**, 3301 (1991); T. Chen and S. Teitel, Phys. Rev. B **55**, 15 197 (1997).
[12] N. Avraham *et al.,* Nature (London) **411**, 451 (2001).
[13] Note that our random coupling model results in an effective vortex-pin interaction that is not local, as the relation between wave function and vortex is not local. However our randomness is still "pointlike" in that there are no correlations along any particular direction.
[14] X. Hu, S. Miyashita, and M. Tachiki, Phys. Rev. Lett. **79**, 3498 (1997).
[15] In the vortex lattice the random pinning energies of the vortex line segments should add as independent random variables. The splitting of the $p = 0$ degeneracy of the two vortex lattice orientations is then $\Delta \sim p\sqrt{fL^2L_z}$, and is thus significant in the thermodynamic limit for any value of $p$. That we find no changes in behavior whether $\Delta$ is small ($p \leq 0.06$) or large ($p > 0.06$) suggests that this symmetry breaking does not affect the nature of the transition.
[16] The random couplings of our $L_z = 24$ model are identical to those of our $L_z = 16$ model for the first 16 layers; the remaining eight layers are chosen independently.
[17] Considering $dF[T, p_c(T)]/dT = \partial F/\partial T + NQdp_c/dT$ for the free energies of liquid and lattice phases, and noting that along the melting line the values of $F$ and $E \propto \partial F/\partial T$ are equal in the two phases while the values of $Q$ are not, implies that $dp_c(T)/dT = 0$.
[18] H. Kawamura, J. Phys. Soc. Jpn. **69**, 29 (2000).
[19] M. Wallin (private communication).
[20] Y. Nonomura and X. Hu, Phys. Rev. Lett. **28**, 5140 (2001).