Superfluid transition in a correlated defect network

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Motivated by recent experiments on the possible supersolid behavior of ^{4}He solids at low temperature, we consider a model of superfluidity in a defected solid containing a system spanning network of correlated linear dislocations, or planar grain boundaries. Using arguments based on the Harris criterion, as well as numerical simulations, we find that such correlated quenched disorder shifts the familiar superfluid lambda transition to a new disordered universality class in which the correlation length exponent $\nu \geqslant 1$. This results in the temperature derivatives for the superfluid density $d\rho_s/dT$ and for the heat capacity dc/dT remaining finite at the transition T_c, and thus a less singular transition, profoundly different from the usual lambda transition.

Considerable excitement has been generated by the observation by Kim and Chan[1,2] that the period of oscillation of a torsional oscillator (TO) containing solid ^{4}He decreases as the system is cooled below roughly ~ 250 mK. Initially, it was suggested that this effect was due to a transition to a *supersolid* state. The reduction of the mass viscously coupled to the oscillator walls at the supersolid transition would lead to a nonclassical rotational inertia (NCRI), and hence the TO period shift. Subsequent experiments showed this effect was closely tied to the presence of defects in the ^{4}He crystal: the slower the crystal was annealed, the smaller was the resulting signal.[3] Numerous theoretical calculations and simulations followed, supporting the idea that a supersolid should not exist for a pure ^{4}He crystalline state,[4–6] however, superfluidity could exist in the cores of crystalline defects.[7,8] A system spanning network of pinned defects could then lead to an effective supersolid. However experiments failed to see the characteristic features expected for the bulk lambda transition of three-dimensional ($d = 3$) superfluid ^{4}He (Ref. 9). In particular, (1) the TO period shift varies rather smoothly with temperature,[1,2,10,11] with no sign of the sharp singularity expected if some part of this shift was due to a superfluid density $\rho_s \sim |T - T_c|^\nu$, with $\nu \approx 0.67$; and (2) equilibrium measurements of heat capacity[12,13] show a smooth bump rather than the sharp lambda-shaped cusp characteristic of a bulk superfluid transition with $c \sim |T - T_c|^{-\alpha}, \alpha = 2 - d\nu \approx -0.01$ (Ref. 14).

Since this initial excitement, however, there has been increasing evidence that the apparent NCRI effect discussed above is most likely not a consequence of supersolidity.[15–21] The NCRI onset shows nearly identical temperature dependence as the classical mechanical effect due to a stiffening of the shear modulus of the ^{4}He upon cooling.[15] In this scenario the mobility of crystalline defects at high temperatures makes a fraction of the ^{4}He lag the driving oscillation. The pinning of these defects upon cooling changes the effective stiffness of the oscillator and gives rise to the apparent period drop.[17,18] While superfluidity in a pinned defect network could in principle still contribute to an NCRI effect, it seems likely that such a superfluid transition would only occur at temperatures well below the onset of the experimentally observed TO period shift, unless the dislocation density were several orders of magnitude larger than is usually estimated.[7] Experimental

estimates of the dislocation density in helium solids have reported a wide range of densities, $n_d \sim 10^4 - 10^9$ cm^{-2} (Refs. 22 and 23). This corresponds to an onset of superfluidity in a dislocation network of about $T_c \sim T_\lambda a \sqrt{n_d} \sim 0.01 - 1$ mK, where $T_\lambda \sim 2$ K is the bulk superfluid transition temperature, and $a \sim 4$ Å is the solid He lattice constant.[7,24]

Nevertheless, it is still interesting theoretically to consider superfluidity in such a disordered, pinned, defect network, and to ask what would be the signal at the onset of the superfluid transition. Would it be the same as the bulk lambda transition, as has generally been assumed in the literature,[25–27] or is a different, less singular, behavior also possible? Here we address this question by large-scale Monte Carlo simulations of an effective model of superfluidity in a correlated random network.

The effect of disorder on a continuous phase transition is usually discussed in terms of the Harris criterion.[28] The Harris criterion[28] argues that uncorrelated point-like disorder is irrelevant whenever $2 < d\nu$, with d the spatial dimension of the system, and ν the correlation length critical exponent. For bulk superfluidity in $d = 3$, the pure system has $\nu_{\text{pure}} \approx 0.67$ and the Harris criterion is satisfied. It has therefore been argued[25–27] that the superfluid onset in a random dislocation network should show the same lambda singularity as in bulk superfluid helium. However, since the dislocation cores are continuous one-dimensional objects, the assumption of uncorrelated *point-like* disorder might not be appropriate. In this work we consider the case when disorder is correlated along a network of intersecting lines or planes. In all cases we argue that the effects of such correlated disorder is to lessen the sharpness of the critical singularity, removing the divergent temperature derivatives at T_c that are characteristic of the usual bulk lambda transition.

To model superfluidity in the pinned dislocation cores of a defected ^{4}He crystal, we start with a three-dimensional (3D) lattice XY model. Neglecting amplitude fluctuations of the condensate order parameter $\Psi(\mathbf{r}) = |\Psi|e^{i\theta(\mathbf{r})}$, the fluctuations in the phase angle θ that drive the superfluid transition can be modeled by the Hamiltonian

$$\mathcal{H} = -\sum_{i,\mu} J_\mu(\mathbf{r}_i) \cos\left[\theta\left(\mathbf{r}_i + \hat{\mu}\right) - \theta(\mathbf{r}_i)\right], \qquad (1)$$

where i labels the discrete sites $\mathbf{r}_i$ of a simple cubic lattice of length L with periodic boundary conditions in all directions, and $J_\mu(\mathbf{r}_i)$ is the quenched coupling on the bond connecting site $\mathbf{r}_i$ to $\mathbf{r}_i + \hat{\mu}$, with $\mu = x,y,z$ the lattice axis directions. We will choose spatially inhomogeneous random couplings $J_\mu(\mathbf{r}_i)$ according to several different schemes.

According to Harris,[28] the effect of disorder is controlled by the mean square fluctuation of the local coupling ΔJ, disorder averaged over a subvolume $V = R^d$ of the system

$$\left[(\Delta J)_R^2\right] \equiv \left[\left\{R^{-d}\sum_\mu \sum_{\mathbf{r}_i \in V}(J_\mu(\mathbf{r}_i) - [J_\mu])\right\}^2\right], \quad (2)$$

where $[\ldots]$ denotes the average over different realizations of quenched disorder. For a continuous transition with diverging correlation length $\xi \sim |T - T_c|^{-\nu}$, the Harris criterion argues that disorder is irrelevant at T_c when the coupling fluctuation averaged over a correlation volume ξ^d satisfies $\sqrt{[(\Delta J)_\xi^2]} < |T - T_c|$ as $T \to T_c$. For future use, we note that $[(\Delta J)_R^2]$ can be rewritten in terms of the coupling correlation averaged over the subvolume V

$$\left[(\Delta J)_R^2\right] = C(R) \equiv R^{-d}\sum_{\mu,\mu'}\sum_{\mathbf{r}_i \in V}[\delta J_\mu(\mathbf{r}_i)\delta J_{\mu'}(0)], \quad (3)$$

where $\delta J_\mu(\mathbf{r}_i) \equiv J_\mu(\mathbf{r}_i) - [J_\mu]$. For uncorrelated point disorder, with $[\delta J_\mu(\mathbf{r}_i)\delta J_{\mu'}(0)] \propto \delta_{\mu,\mu'}\delta_{\mathbf{r}_i,0}$, Eq. (3) yields $C(\xi) \sim \xi^{-d} \sim |T - T_c|^{d\nu}$. The Harris criterion for the irrelevance of such point disorder then becomes $|T - T_c|^{d\nu/2} < |T - T_c|$ or the familiar $2 < d\nu$.

We now wish to consider models of correlated disorder. One such case was considered many years ago in a seminal work by Weinrib and Halperin.[29] They noted that when spatial disorder is introduced as a set of straight *randomly oriented* lines, the resulting disorder-averaged coupling correlation decays algebraically as $[\delta J(\mathbf{r})\delta J(0)] \sim r^{-a}$, with $a = d - 1$. In this case, Eq. (3) gives $C(\xi) \sim \xi^{-a}$ and the Harris criterion argues that disorder is irrelevant when $2 < a\nu$. Using a renormalization group expansion for weak Gaussian disorder, Weinrib and Halperin showed that this is indeed the case: when $a < d$, disorder is irrelevant whenever $2 < a\nu_{\text{pure}}$. They further found that when this criterion fails, the correlation length exponent at the new disordered critical point satisfies $\nu_{\text{disor}} = 2/a$. Applying this conclusion to a 3D superfluid, we see that such linear disorder with $a = 2$ is relevant, resulting in a superfluid density that vanishes linearly as $\rho_s \sim |T - T_c|^{\nu_{\text{disor}}}$, with $\nu_{\text{disor}} = 1$, and a heat capacity $c \sim |T - T_c|^{-\alpha}$ with exponent $\alpha = 2 - d\nu_{\text{disor}} = -1$. In particular, dc/dT scales as $|T - T_c|^{-\alpha-1}$, with $-\alpha - 1 = 0$, and thus remains finite at T_c in contrast to its divergence in the pure model. Thus for such linearly correlated disorder, we expect that the superfluid density vanishes less sharply than for the pure model, while the heat capacity has a far less singular cusp. For planar disorder, as might be the case if superfluidity is carried on randomly oriented twin grain boundaries, $a = d - 2 = 1$ in 3D, and the superfluid singularities are even less sharp.

We next consider a slightly different model of linearly correlated disorder. Motivated by the notion that dislocation lines in solid ^{4}He may preferentially align parallel to crystalline axes, we consider a 3D XY model in which correlated disorder

enters along straight lines oriented only along the three lattice directions. We choose quenched couplings as follows. Within the plane at $r_\mu = 0$, we randomly choose equal numbers of bonds J_μ from the bivalued distribution $J = 1 \pm \delta$. We then continue these couplings in correlated straight lines by requiring $J_\mu(\mathbf{r}_i + \hat{\mu}) = J_\mu(\mathbf{r}_i)$. We follow this procedure for all three directions $\mu = x,y,z$. For the results presented below we use $\delta = 1$; superfluidity is strictly confined to the dislocation cores and the three dimensionality of the superflow results solely from the intersections of these cores to form an interconnected network. This choice corresponds to an average defect density of $n_d = 1/2$ defects per lattice bond. We also performed simulations at other values of n_d. For $n_d = 1/2$ we have also considered the case $\delta = 0.95$, as a model in which superfluid particles may tunnel through the bulk between dislocation cores. We find the critical behavior to be the same in both cases. The coupling correlation for this disorder is $[\delta J_\mu(\mathbf{r})\delta J_{\mu'}(0)] \propto [\delta(x)\delta(y) + \delta(y)\delta(z) + \delta(z)\delta(x)]\delta_{\mu,\mu'}$. However, the volume-averaged correlation is $C(R) \sim R^{-a}$ with $a = d - 1$, just as for randomly oriented lines. We thus expect this disorder to be relevant; applying the Harris criterion at the new disordered critical point then requires $\nu_{\text{disor}} \geqslant 2/a = 1$.

To confirm this behavior, we carry out extensive numerical simulations. The superfluid density is proportional to the XY helicity modulus, which (in units where $m/\hbar = 1$) is given by[30]

$$\rho_s = L^{-3}\left[\left\langle \sum_i J_z(\mathbf{r}_i)\cos[\theta(\mathbf{r}_i + \hat{z}) - \theta(\mathbf{r}_i)]\right\rangle - T^{-1}\left\langle\left(\sum_i J_z(\mathbf{r}_i)\sin[\theta(\mathbf{r}_i + \hat{z}) - \theta(\mathbf{r}_i)]\right)^2\right\rangle\right]. \quad (4)$$

The XY magnetization is $M = |\sum_i e^{i\theta(\mathbf{r}_i)}|$, and its Binder cumulant U is given by

$$U \equiv 2 - \left[\frac{\langle M^4\rangle}{\langle M^2\rangle^2}\right]. \quad (5)$$

We also consider the heat capacity c,

$$c = L^{-3}T^{-2}[\langle\mathcal{H}^2\rangle - \langle\mathcal{H}\rangle^2], \quad (6)$$

and the XY spin susceptibility χ,

$$\chi = L^{-3}T^{-1}[\langle M^2\rangle - \langle M\rangle^2]. \quad (7)$$

To analyze the critical properties of the transition at T_c we apply finite-size-scaling (FSS) methods.[31] We expect ρ_s, U, and χ as a function of T and system length L to obey the usual FSS relations

$$\rho_s(T,L) = L^{-1}\mathcal{R}(tL^{1/\nu}), \quad U(T,L) = \mathcal{U}(tL^{1/\nu}),$$
$$\chi(T,L) = L^{\gamma/\nu}\mathcal{X}(tL^{1/\nu}), \quad (8)$$

where $\mathcal{R}(\cdot)$, $\mathcal{U}(\cdot)$, and $\mathcal{X}(\cdot)$ are scaling functions, and $t \equiv (T - T_c)/T_c$.

To carry out our Monte Carlo (MC) simulations to high accuracy we used an effective Wolff collective update algorithm, which minimizes the effects of critical slowing down at the transition.[32] As the Wolff algorithm is not so efficient
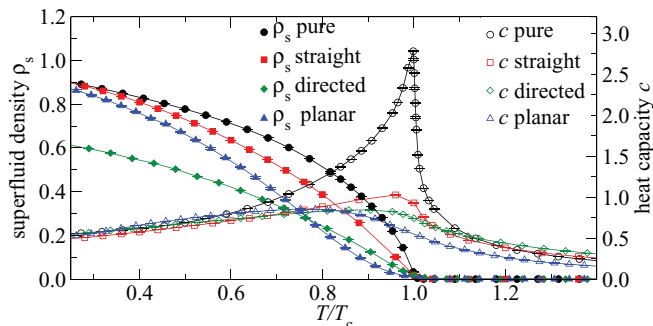
FIG. 1. (Color online) Superfluid density ρ_s (solid symbols) and heat capacity c (open symbols), vs T/T_c, for several model systems on a lattice of length $L = 40$. Black circles: pure 3D XY model; red squares: straight line disorder; green diamonds: directed random line disorder; blue triangles: random planar disorder. For the disordered models, results are averaged over several hundred to more than a thousand random coupling configurations.

at lower temperatures, we add one ordinary Metropolis sweep through the system for each 100 Wolff updates. Data for the averages were accumulated during 4–16×10^3 Monte Carlo steps (MCS), after equally many initial MCS were discarded to reach equilibrium. One MCS is defined as L^3 single site update attempts. We tested for equilibration by increasing the number of discarded initial MCS until stable results were obtained. For our FSS analysis, quenched disorder averages were computed over 10^3–10^4 independent realizations of the random couplings $J_\mu(\mathbf{r}_i)$.

The main qualitative results of this work are shown in Fig. 1, where we plot the superfluid density ρ_s and heat capacity c versus T/T_c of a system of fixed length $L = 40$, for both the pure 3D XY model ($T_c = 2.203$ in units of J/k_B) and for our model of Eq. (1) with linearly correlated disorder ($T_c = 2.501$ in units of $[J]/k_B$, as determined below). The results for the disordered case are averaged over several hundred realizations of the quenched random couplings. We see that the presence of the disorder dramatically softens the singularities of the pure system, removing the sharp singularities of the lambda transition. Derivatives with respect to temperature that diverge as $T \rightarrow T_c$ in the pure model appear to become finite in the disordered model.

To verify this conclusion, and to demonstrate that the model with linearly correlated defects belongs to a new disordered universality class, we perform a FSS analysis to determine critical exponents.[31] In Figs. 2(a) and 2(c) we plot, respectively, $L\rho_s$ and U versus T for different system sizes $L = 10$–80. Equations (8) predict that the curves for different L should all intersect at the common point $t = 0$, i.e., when $T = T_c$. We see that as L increases, the curves do indeed seem to be approaching a common intersection point, yielding $T_c \approx 2.5$. The temperature for the models with disorder is given in units of $[J]/k_B$. The deviations from a perfect common intersection are due to corrections to scaling, which can be noticeable when L is insufficiently large.[14]

For a more accurate determination of the critical T_c, as well as the correlation length exponent ν, we expand the scaling functions of Eqs. (8) as third-order polynomials, and fit our data to these scaling forms with T_c, ν, and the polynomial
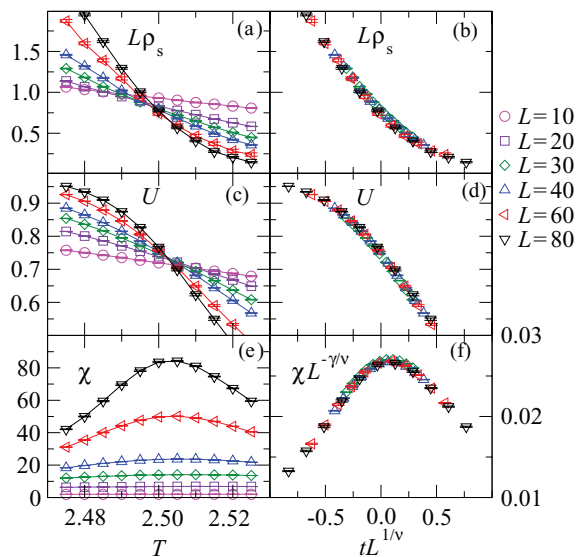

FIG. 2. (Color online) (a) Scaled superfluid density $L\rho_s$, (c) Binder cumulant U, and (e) susceptibility χ vs T for system sizes $L = 10$–80. Scaling collapse of (b) $L\rho_s$, (d) U, and (f) $\chi L^{-\gamma/\nu}$ vs $tL^{1/\nu}$, for system sizes $L = 30$–80, using values $T_c = 2.501$, $\nu = 1$, and $\gamma = 1.84$.

coefficients as free fitting parameters. We restrict our fits to data satisfying $|tL^{1/\nu}| < 0.5$. Using system sizes $L_{\min}$ to $L_{\max} = 80$, we plot the resulting fitted values for T_c and ν versus $1/L_{\min}$ in Figs. 3(a) and 3(b), respectively. We see that as $L_{\min}$ increases, the values of T_c and ν from $L\rho_s$ and U approach each other. A procedure *including* corrections to scaling yields consistent values of $T_c = 2.501 \pm 0.001$ and $\nu = 1.00 \pm 0.05$ from fits to both $L\rho_s$ and U. The errors represent one standard deviation statistical error as estimated using the method of synthetic data sets.[33] Using these common values of T_c and ν, the resulting scaling collapses, plotting $L\rho_s$ and U versus $tL^{1/\nu}$, are shown in Figs. 2(b) and 2(d), for sizes $L = 30$–80. We note that our result $\nu \approx 1$ is identical to the prediction of Weinrib and Halperin for algebraically correlated couplings with $a = d - 1 = 2$, and implies that the new disordered fixed point just marginally satisfies the Harris criterion for stability.

Next we consider the susceptibility χ of Eq. (7). In Fig. 2(e) we plot χ versus T for system sizes $L = 10$–80. The exponent
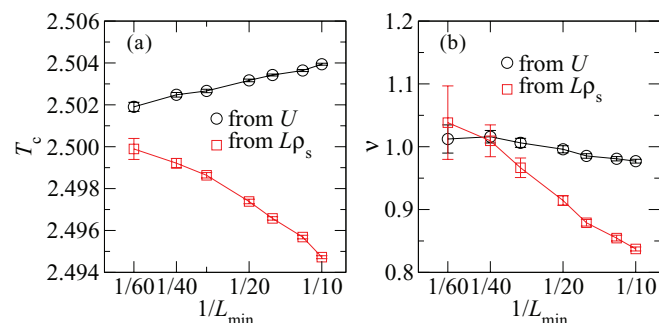

FIG. 3. (Color online) Values of (a) T_c and (b) ν obtained by fitting data with $|tL^{1/\nu}| < 0.5$ to third-order polynomial expansions of the scaling functions of Eqs. (8), using data from system sizes $L_{\min}$ to $L_{\max} = 80$.
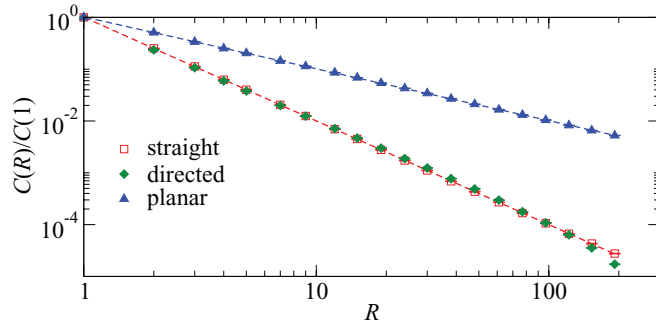
FIG. 4. (Color online) Integrated coupling correlation $C(R)$ of Eq. (3), vs R, for a system of length $L = 200$. Results are normalized by $C(1)$, and shown for the case of straight randomly positioned lines, directed random lines, and random flat planes.

γ in Eq. (8) is obtained from a power-law fit to the maximum value of $\chi(T)$ versus L. We find $\gamma = 1.84 \pm 0.1$. Using this value of γ, and $T_c = 2.501, \nu = 1.0$ as determined above, we show in Fig. 2(f) the resulting scaling collapse, plotting $\chi L^{-\gamma/\nu}$ versus $t L^{1/\nu}$ for system sizes $L = 30$–80. The collapse is excellent. From the two independent exponents $\nu \approx 1.0, \gamma \approx 1.84$ all the other thermodynamic critical exponents can be obtained from standard scaling laws.[34] Hyperscaling gives the heat capacity exponent $\alpha = 2 - d\nu \approx -1.0$; the Rushbrook equality $\alpha + 2\beta + \gamma = 2$ gives for the order parameter exponent $\beta \approx 0.58$; and the correlation function exponent η is obtained from $\gamma = (2 - \eta)\nu$ giving $\eta \approx 0.16$.

So far, our linear disorder has taken the form of perfectly straight lines. In a solid, however, dislocation cores may wander as they traverse the system. To consider the effect of such wandering, we generalize our model by letting each defect line be a directed random walk. For a walk directed along $\hat{z}$, for example, each step in the $\hat{z}$ direction is allowed to include a random transverse fluctuation $\Delta \mathbf{r}_\perp$, sampled equally from $\Delta \mathbf{r}_\perp = \{0, \pm \hat{x}, \pm \hat{y}\}$. For each walk the $\Delta \mathbf{r}_\perp$ are constrained to sum to zero, so that the line at $z = L$ returns to its starting position at $z = 0$ under the periodic boundary conditions. For each such walk j, a variable $n_j = 1$ is placed on each bond of the walk. The couplings of the corresponding XY model are then set to $J = \sum_j n_j$ on each bond. Finally, all couplings J

are rescaled by a constant factor so that the disorder average $[J_\mu] = 1$. We thus construct such configurations on a lattice of size $L = 200$ and numerically compute the integrated coupling correlation $C(R)$ of Eq. (3), averaging over more than 1000 different realizations of the disorder. Our results are shown in Fig. 4, along with $C(R)$ as computed for our original straight line model. We find a clear algebraic decay in both cases, with $C(R) \sim R^{-a}$, $a = 2$. Thus the directed random line model is expected to be in the same universality class as our straight line model. In Fig. 1 we show results for ρ_s and heat capacity c for this directed random line model, as obtained from simulations on a lattice of size $L = 40$, averaging over several hundreds of disorder configurations. The effect of superfluidity seems slightly suppressed, as compared to the straight line case, but the shapes of the singularities appear to be the same.

We have also considered a random plane model. We select a sequence of flat planes as follows. For planes oriented with normal along $\hat{z}$, each xy plane at height z is randomly selected or not with probability $1/2$. Such random plane sequences are selected in all three directions $\hat{x}, \hat{y}, \hat{z}$ simultaneously. For each such plane j we set $n_j = 1$ for all bonds in the plane; the XY bond couplings are $J = \sum_j n_j$, and then rescaled so that $[J] = 1$. In Fig. 4 we plot the resulting numerically computed correlation $C(R)$. We find an algebraic decay with $C(R) \sim R^{-a}$, $a = 1$. In Fig. 1 we show results for ρ_s and heat capacity c for this random plane model, as obtained from simulations on a lattice of size $L = 40$, averaging over more than 1000 disorder configurations. As expected, the singularity at T_c is now even smoother than for the random line models.

To conclude, we have considered a variety of models for a superfluid with long-range-correlated quenched disorder. In all cases we have argued that the disorder changes the universality class of the superfluid transition to one with $\nu \geqslant 1$. Our results show that superfluidity in such correlated disorder networks would not display the familiar sharp features of the lambda transition of an ordinary bulk superfluid.

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