Using inhomogeneity to raise the superconducting critical temperature in a two-dimensional *XY* model

Y. L. Loh and E. W. Carlson
Department of Physics, Purdue University, West Lafayette, Indiana 47907, USA
(Received 5 February 2007; published 27 April 2007)

Superconductors with low superfluid density are often dominated by phase fluctuations of the order parameter. In this regime, their physics may be described by *XY* models. The transition temperature T_c of such models is of the same order as the zero-temperature phase stiffness (helicity modulus), a long-wavelength property of the system: $T_c = A\Upsilon(0)$. However, the constant A is a nonuniversal number, depending on dimensionality and the degree of inhomogeneity. In this Brief Report, we discuss strategies for maximizing A for two-dimensional *XY* models; that is, how to maximize the transition temperature with respect to the zero-temperature, long-wavelength properties. We find that a framework type of inhomogeneity can increase the transition temperature significantly. For comparison, we present similar results for Ising models.

DOI: 10.1103/PhysRevB.75.132506 PACS number(s): 74.81.−g, 74.62.Yb, 74.81.Fa

There is experimental evidence that many strongly correlated systems such as nickelates, cuprates, and manganites exhibit some degree of inhomogeneity—spatial variations of structure, composition, or local electronic properties.[20] It is important, from both scientific and technological points of view, to understand how such mesoscale variation—whether ordered or disordered—influences macroscopic properties such as superconductivity. That is, does inhomogeneity help or harm superconductivity, or is it a side issue entirely?

Intuition suggests that inhomogeneity should be detrimental to superconductivity through its association with disorder or competing orders. However, there are many counterexamples. The transition temperatures of Al, In, Sn, and other soft metals can be increased by going from bulk samples to grains, films, or layered structures.[21] For attractive-U Hubbard models, T_c can be increased by making U vary in space.[1,2] This is not too surprising: in BCS theory, the critical temperature has a strong nonlinear dependence on the attraction, $T_c \sim e^{-1/\nu U}$; since $\langle e^{-1/\nu U}\rangle \geq e^{-1/\nu\langle U\rangle}$, favorable spatial variations in U, if they exist, are strongly amplified. Even for repulsive-U models, the superconducting gap can be increased by going from a homogeneous two-dimensional (2D) system to an array of two-leg ladders with strong intraladder couplings and weaker interladder couplings.[3]

The microscopic models in Refs. 1–3 deal simultaneously with the effects of spatially modulated pairing strength and spatially modulated phase stiffness. To gain physical insight, it is useful to focus on one effect at a time. Here, we study phenomenological *XY* models, i.e., we assume that the pairing energy scale (and the magnitude of the superconducting gap) are constant in space, and concentrate on the physics of phase fluctuations.

In this Brief Report, we consider superconductors with low superfluid density. For such systems, the transition is dominated by fluctuations of the phase of the superconducting order parameter, described by an *XY* model; the superconducting T_c is the Berezinskii-Kosterlitz-Thouless[4–6] (BKT) transition temperature of the *XY* model. We numerically study 2D *XY* models with inhomogeneous couplings. We find that although most patterns of inhomogeneity reduce T_c, there are "framework" patterns that increase T_c by up to a theoretical maximum of 76%. For comparison, we also study inhomogeneous Ising models; the results support our findings for *XY* models.

The *XY* model has the following classical Hamiltonian:

$$\mathcal{H}_{XY}[\theta] = -\sum_{\langle ij\rangle} J_{ij}\cos(\theta_i - \theta_j), \tag{1}$$

where i,j are site labels, J_{ij} are nearest-neighbor couplings (representing the local phase-coherence energy scale), and θ_i are real-valued phase (angle) variables. We consider here only two-dimensional models. We define a "homogeneous" model as one where all the couplings are equal, $J_{ij}=J_0$. Inhomogeneity is represented by spatial variations in J_{ij}. For a meaningful study, it is necessary to impose some kind of constraint on the inhomogeneity; in contrast to Ref. 1, which fixes the average attractive Hubbard potential $\overline{U(\mathbf{r})}$, we choose to fix the average coupling, $\overline{J_{ij}}=J_0$. Our constraint eliminates the aforementioned increase of T_c due to inhomogeneous pairing strengths, allowing us to isolate the effects of inhomogeneous phase stiffness. It has the further advantage of preserving the values of the helicity modulus $\Upsilon(T=0)$ and energy $U(T=0)$ at zero temperature (for the patterns in Fig. 1).

We are interested in optimizing the transition temperature. To study this, we focus on the behavior of the helicity modulus $\Upsilon(T)$. The helicity modulus measures the change in the free energy caused by a small change in the phase angle,[7] and it is related to the areal superfluid density by $\Upsilon = \hbar^2\rho_s/(4m^*)$. We calculate this quantity via Monte Carlo simulations using

$$\Upsilon = \frac{1}{2V}\left\langle \sum_{\langle ij\rangle} J_{ij}\cos(\theta_i - \theta_j) - \beta\left[\sum_{\langle ij\rangle} J_{ij}\sin(\theta_i - \theta_j)\right]^2 \right\rangle. \tag{2}$$

We use the Wolff cluster algorithm,[8] which is the fastest serial algorithm for our purposes. The θ variables are stored and manipulated as two-vectors to avoid trigonometric function calls.

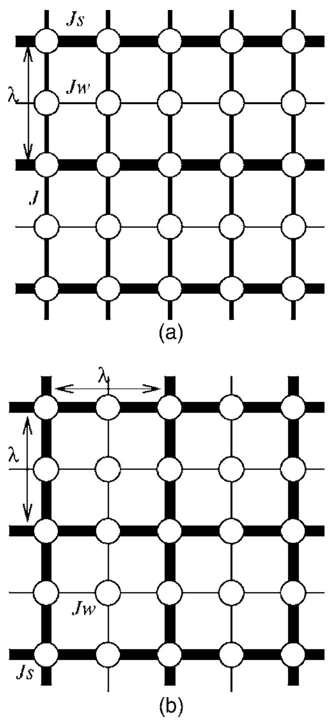

FIG. 1. In this Brief Report, we study the above inhomogeneity patterns, where certain bonds are made stronger (J_s) and others weaker (J_w) such that the total coupling is preserved. (a) ID modulation; (b) 2D modulation.

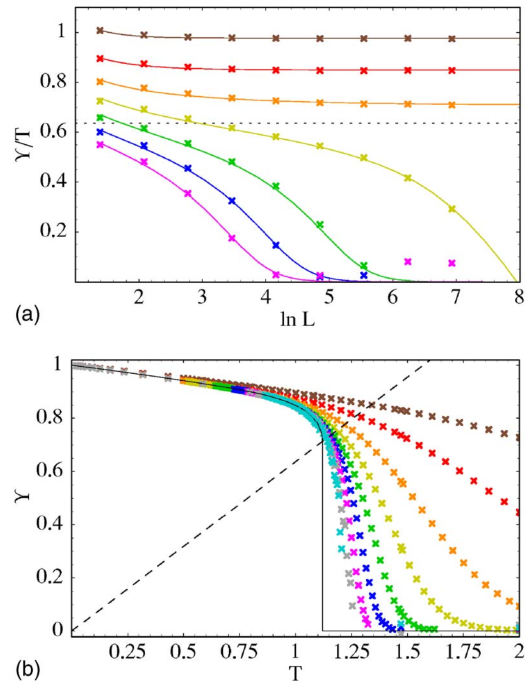

FIG. 2. (Color online) Finite-size scaling. The crosses are Monte Carlo results for the helicity modulus $\Upsilon(L,T)$ of a 4×4-modulated XY model with $J_w=0$ and $J_s=4J_{\text{avg}}$, for $T=0.9,1.0,\ldots,1.5$ in units of J_{avg} and $L=4,8,\ldots,1024$. (a) Dimensionless helicity modulus $u=\Upsilon/T$ as a function of system size. The curves are solutions of the scaling equations [Eq. 3] chosen to fit the data (crosses). The dashed line is $\Upsilon/T=\frac{2}{\pi}$. (b) Helicity modulus as a function of temperature. The black curve is $\Upsilon(L=\infty,T)$, obtained by FSS. The dashed line is $\Upsilon=\frac{2}{\pi}T$.

In order to obtain reliable estimates of T_c, we have performed finite-size scaling (FSS) on $\Upsilon(L,T)$ in the following manner. The BKT transition can be described by a two-parameter scaling flow[7,9–11] for the dimensionless helicity modulus $u=\Upsilon/T$ and the "vortex fugacity" y,

$$\frac{du}{dl}=-4\pi^3u^2y^2, \quad \frac{dy}{dl}=(2-\pi u)y, \tag{3}$$

where $l=\ln L$ is the length scale. This pair of differential equations can be solved numerically, given initial values $u(l_0)=u_0$ and $y(l_0)=y_0$ (where l_0 is some reference length scale). For each temperature T, we choose u_0 and y_0 so as to obtain a good fit of $u(l)$ to the Monte Carlo data for the available system sizes, $4\leqslant L\leqslant 1024$ [see Fig. 2(a)]. We then integrate the differential equations all the way to $l=\infty$. This gives $u(\infty)$ and hence the helicity modulus in the infinite-size limit $\Upsilon(T,L=\infty)$, shown in Fig. 2(b).[22]

Our most important result is that *by redistributing the bond strengths of an XY model in certain inhomogeneous patterns, it is possible to increase* T_c. As a concrete example of how this comes about, we show how the shape of the helicity modulus curve *vs* temperature is changed by introducing inhomogeneity. In Fig. 3, we show our simulations of $\Upsilon(T)$, extrapolated to infinite system size $L\to\infty$, for a 2D inhomogeneity of the type shown in Fig. 1(b) using $\lambda=4a$, where a is the underlying lattice constant. In curves (ii) and (iii) in Fig. 3, the coupling constant J_{ij} has been made stronger (J_s) on the thick lines in Fig. 1(b) and weaker (J_w) on the thin lines. We compare these to the homogeneous case [curve (i)] with J set equal to the spatial average of J_w and J_s, $J=J_{\text{avg}}\equiv[J_s+(\lambda-1)J_w]/\lambda$. Thus for all curves shown in Fig. 3, the zero-temperature helicity modulus $\Upsilon(T=0)$ and the zero-temperature free energy are the same.

In the homogeneous case, it is known that $T_c=0.8929J$ (Refs. 7 and 12) and that the low-temperature slope of the helicity modulus $\Upsilon'(0)=1/4$.[13,14] Curve (ii) in Fig. 3 shows the helicity modulus for $J_s=3.4$ and $J_w=0.2$. In this case, the transition temperature is enhanced by 8% above the homogeneous case. For the case of extreme inhomogeneity with

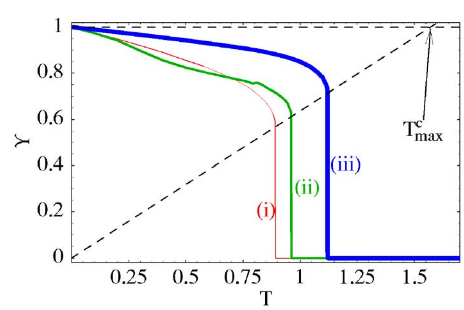

FIG. 3. (Color online) $\Upsilon(T,L=\infty)$ for 2D XY models. (i) Homogeneous 2D XY model. (ii) 4×4 modulation with $J_s=3.4$ and $J_w=0.2$. (iii) 4×4 modulation with $J_s=4$ and $J_w=0$. The dashed line is $\Upsilon=\frac{2}{\pi}T$. The arrow indicates the theoretical upper bound $T^c_{\text{max}}=\frac{\pi}{2}J_{\text{avg}}$.

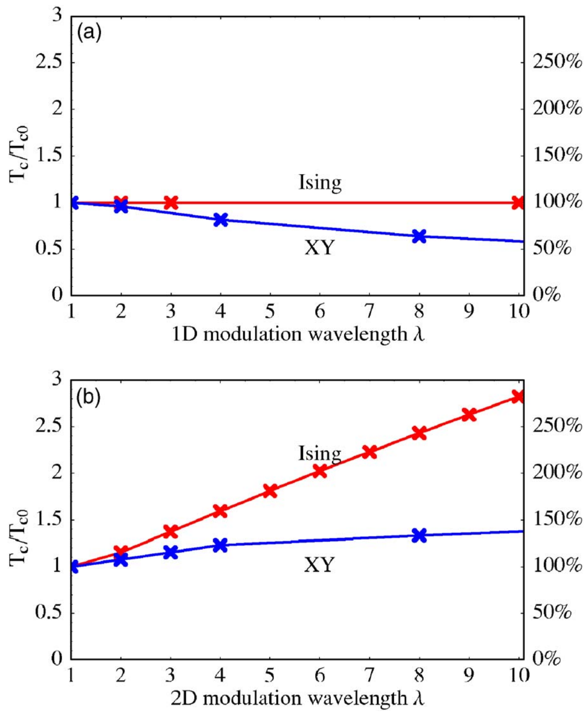

FIG. 4. (Color online) Critical temperatures T_c of the lattices depicted in Figs. 1(a) and 1(b) as a function of the wavelength of the inhomogeneity.

$J_s=4$ and $J_w=0$ [curve (iii)], the transition temperature is 25% higher than in the homogeneous case. The shape of curve (ii) demonstrates the separation of energy scales that happens with inhomogeneity. Notice that at the very lowest temperatures, curve (ii) is dominated by the long-wavelength average of the coupling constants, and the low-temperature linear slope of the helicity modulus is identical to that of the homogeneous case. As temperature is raised, the slope increases in magnitude as the weak plaquettes become disordered. Then, at a higher temperature, the slope approaches that of curve (iii), indicating that at higher temperatures the helicity modulus is dominated by J_s. It is this shallower high-temperature slope which causes the helicity modulus to overshoot the homogenous T_c and leads to an inhomogeneity-induced enhancement of the transition temperature.

For 2D patterns like those in Fig. 1(b), the enhancement of the transition temperature increases with λ, as shown by curve (ii) in Fig. 4(b). However, the enhancement is constrained by the zero-temperature helicity modulus. Even in the presence of inhomogeneity, in two-dimensions, the system remains in the BKT universality class and the helicity modulus has a universal jump at the transition such that $\Upsilon(T_c)=0.6365T_c$. Since thermal fluctuations introduce disorder, $\Upsilon(T_c)<\Upsilon(T=0)$, so that $T_c/\Upsilon(0)\leqslant 1.57$ or, equivalently, $T_c/T_{c0}\leqslant 1.76$. This theoretical upper bound on T_c is illustrated in Fig. 3. That is, although the zero-temperature properties of the system may be used as a predictor of the transition temperature, $T_c=A\Upsilon(T=0)$, the constant A is non-universal. In fact, $A=T_c/\Upsilon(0)$ may be useful for *characterizing* the degree of inhomogeneity: it increases from 0.89 for the homogeneous *XY* model up to a theoretical maximum of 1.57. For a 2D system, a large measured value of this ratio may indicate substantial inhomogeneity. (An increase in this ratio may also indicate higher dimensionality.[13])

We have also considered one-dimensional (1D) modulations, like those in Fig. 1(a). Since this type of inhomogeneity drives the system towards more 1D physics where a phase transition is forbidden by the Mermin-Wagner theorem, the transition temperature decreases, as shown in Fig. 4(a). Therefore, the enhancement of T_c is not additive—the effect of a 2D modulation is *not* double that of a 1D modulation. Reference 1 found that for an attractive Hubbard model, 1D modulation of the potential U produces simultaneous 1D modulation of the pairing energy scale and phase stiffness, which have opposing tendencies to raise and to lower T_c. According to our results, 2D modulations of the pairing and phase stiffness should *cooperate* to raise T_c.

Figure 4 also shows the effect of inhomogeneity in the Ising model for comparison. Inhomogeneous Ising models may be described by the Hamiltonian

$$\mathcal{H}_{\text{Ising}}[\sigma]=-\sum_{\langle ij\rangle}J_{ij}\sigma_i\sigma_j, \quad \sigma_i=\pm 1. \tag{4}$$

As with the *XY* model, we restrict ourselves to two dimensions. For the purpose of studying different length scales of inhomogeneity, we focus on an extreme type of inhomogeneity with $J_w=0$ and $J_s=\lambda J_{\text{avg}}$. Such patterns correspond to "decorated" lattices. By integrating out all doubly coordinated spins [that is, by applying the so-called decorated-iteration transformation, $J_{\text{eff}}=\tanh^{-1}(\tanh J_1 \tanh J_2)$], one can reduce a decorated lattice to a primitive lattice and thus obtain an exact expression for its T_c [Eq. (5)].[23] (Unfortunately, the decoration-iteration transformation for *XY* models involves an infinite set of Fourier components of the potential[11] and it does not lead to exact results for T_c.)

In Fig. 4, we show the effect of extreme inhomogeneity (i.e., with $J_w=0$) on the transition temperatures in Ising and *XY* models. We use the maximum value of $J_s=\lambda J_{\text{avg}}$, because for a given wavelength λ, this gives the largest enhancement of T_c while conserving the average coupling J_{avg}. While we are interested primarily in superconductors with small superfluid density, which can be captured with an *XY* model, we also show results for the Ising model for which results can be obtained analytically as described above. Figure 4(a) shows the effect of a purely 1D modulation, as a function of distance λ between strong bonds J_s, chosen so as to preserve the zero-temperature, long-wavelength properties of the system. The pattern of coupling constants is shown in Fig. 1(a). In the Ising case, the transition temperature is unchanged by this procedure. In the *XY* case, the transition temperature decreases monotonically with λ.

The effect of a 2D modulation is shown in Fig. 4(b). Again, parameters are chosen so as to preserve the zero-temperature properties of the system. Figure 1(b) shows the pattern of coupling constants. Here, the transition temperature in the Ising case increases as

$$T_c=\frac{2\lambda J_{\text{avg}}}{\sinh^{-1}\left[\operatorname{csch}\left(\frac{1}{\lambda}\sinh^{-1}1\right)\right]}. \tag{5}$$

One of the occurrences of lambda in this equation is due to taking λ bonds in parallel, to form "bundles," and the other occurrence is due to taking λ bundles in series. For *XY* models, the transition temperature also increases monotonically with modulation length λ. In this case, there is an upper bound, set by the zero-temperature properties of the system, as shown in Fig. 3. That is, the maximum enhancement of T_c possible with this type of inhomogeneity in an *XY* model is 76%.

Numerous other physical systems, besides superconductors with low superfluid density, can be described by *XY* models. Thus, our work may have applications to Josephson junction arrays, superfluidity in nanostructured porous media, and magnetism in inhomogeneous systems. The question of the effects of inhomogeneity is even related to materials engineering and operations research. For example, composite materials often have superior mechanical properties compared to pure ones; efficient design of traffic and communications networks often uses links of differing capacities or reliabilities.

In conclusion, we have shown that certain types of inhomogeneity can increase the transition temperature of Ising and *XY* models. Specifically, two-dimensional modulations of the coupling constants that preserve the spatial average coupling increase the transition temperature over that of the homogeneous case. One-dimensional modulations depress the transition in *XY* models and leave the transition temperature unchanged in Ising models. Our results for 2D *XY* models may indicate that certain types of inhomogeneity can result in an enhancement of superconductivity in systems with low superfluid density.

It is a pleasure to thank S. A. Kivelson, E. Manousakis, and D. Stroud for helpful discussions. This work was supported by Purdue University (Y.L.L.), Research Corporation (Y.L.L.), and by the Purdue Research Foundation (E.W.C.). E.W.C. is a Cottrell Scholar of Research Corporation. This research was supported in part through computing resources provided by Information Technology at Purdue-The Rosen Center for Advanced Computing, West Lafayette, Indiana.

[1] I. Martin, D. Podolsky, and S. A. Kivelson, Phys. Rev. B **72**, 060502(R) (2005).

[2] K. Aryanpour, E. R. Dagotto, M. Mayr, T. Paiva, W. E. Pickett, and R. T. Scalettar, Phys. Rev. B **73**, 104518 (2006).

[3] E. Arrigoni and S. A. Kivelson, Phys. Rev. B **68**, 180503(R) (2003).

[4] V. L. Berezinskii, Zh. Eksp. Teor. Fiz. **59**, 907 (1970).

[5] V. L. Berezinskii, Sov. Phys. JETP **34**, 610616 (1972).

[6] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).

[7] N. Schultka and E. Manousakis, Phys. Rev. B **49**, 12071 (1994).

[8] U. Wolff, Phys. Rev. Lett. **62**, 361 (1989).

[9] J. M. Kosterlitz, J. Phys. C **7**, 1046 (1974).

[10] D. R. Nelson and J. M. Kosterlitz, Phys. Rev. Lett. **39**, 1201 (1977).

[11] J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977).

[12] U. Wolff, J. Phys. A **38**, 5869 (2005).

[13] E. W. Carlson, S. A. Kivelson, V. J. Emery, and E. Manousakis, Phys. Rev. Lett. **83**, 612 (1999).

[14] E. Roddick and D. Stroud, Phys. Rev. Lett. **74**, 1430 (1995).

[15] E. Dagotto, Science **309**, 257 (2005).

[16] E. W. Carlson, V. J. Emery, S. A. Kivelson, and D. Orgad, in *Concepts in High Temperature Superconductivity*, edited by J. Ketterson and K. Benneman, The physics of Superconductors Vol. II (Springer-Verlag, Berlin, 2004).

[17] S. Bose, P. Raychaudhuri, R. Banerjee, P. Vasa, and P. Ayyub, Phys. Rev. Lett. **95**, 147003 (2005).

[18] M. E. Fisher, J. Math. Phys. **7**, 10 (1966).

[19] Y. L. Loh and E. W. Carlson, Phys. Rev. Lett. **97**, 227205 (2006).

[20] For recent reviews, see Refs. 15 and 16.

[21] For a review, see Ref. 17.

[22] This treatment neglects the tiny corrections due to nonzero winding numbers, (Ref. 12) but it is adequate for the level of accuracy of the present work. As a check, we have estimated T_c using other methods, such as finite-size scaling for the susceptibility $\chi(L,T)$ and for the Wolff cluster size $N_{\rm clust}(L,T)$, based on the predictions of BKT theory that $\chi(L,T_c)\sim L^{7/4}(\ln L)^{1/8}$ and that $\chi(\infty,T-T_c)\sim t^{-1/16}e^{ct^{-1/2}}$. The results agree with those obtained from finite-size scaling for Υ.

[23] For more complicated patterns not amenable to decorationiteration, T_c can be calculated using either the Pfaffian method (Ref. 18) (e.g., for periodic inhomogeneity) or the recently developed bond-propagation algorithm (Ref. 19) (which is the most efficient in the case of bond dilution).