Using inhomogeneity to raise the superconducting critical temperature in a two-dimensional \(XY\) model

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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: \(T_c = A Y(0)\). 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.

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There is experimental evidence that many strongly correlated systems such as nickelates, cuprates, and manganese 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.\(^{25}\) 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, \(T_c \sim e^{-1/|U|}\); since \((e^{-1/|U|}) \gg e^{-1/|U(T)|}\), 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:

\[
H_{XY}[	heta] = -\sum_{(ij)} J_{ij} \cos(\theta_i - \theta_j),
\]

where \(i,j\) are site labels, \(J_{ij}\) are nearest-neighbor couplings (representing the local phase-coherence energy scale), and \(\theta_i\) 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 \(U(r)\), we choose to fix the average coupling, \(\bar{J}_{ij} = J_0\). 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 \(Y(T = 0)\) 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 \(Y(T)\). 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 \(Y = \gamma^2 \rho_s / (4m^*)\). We calculate this quantity via Monte Carlo simulations using

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

We use the Wolff cluster algorithm,\(^8\) which is the fastest serial algorithm for our purposes. The \(\theta\) variables are stored and manipulated as two-vectors to avoid trigonometric function calls.
In order to obtain reliable estimates of $T_c$, we have performed finite-size scaling (FSS) on $Y(L, T)$ in the following manner. The BKT transition can be described by a two-helicity modulus curve of how this comes about, we show how the shape of the inhomogeneity. In Fig. 3, we show our simulations of producing inhomogeneity. In Fig. 3, we show our simulations of forming finite-size scaling equations [Eq. 3] chosen to fit the data (crosses). The dashed line is $Y/T=\frac{2}{\pi}$. The black curve is $Y(L=\infty, T)$, obtained by FSS. The dashed line is $Y=\frac{2}{\pi}T$.

(i) with $J$ set equal to the spatial average of $J_u$ and $J_v$, $J=J_{\text{avg}}=[J_u+(\lambda-1)J_v]/\lambda$. Thus for all curves shown in Fig. 3, the zero-temperature helicity modulus $Y(T=0)$ 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 $Y''(0)=1/4$.[13,14] Curve (ii) in Fig. 3 shows the helicity modulus for $J_v=3.4$ and $J_u=0.2$. In this case, the transition temperature is enhanced by 8% above the homogeneous case. For the case of extreme inhomogeneity with

![FIG. 2. (Color online) Finite-size scaling. The crosses are Monte Carlo results for the helicity modulus $Y(L, T)$ of a 4 × 4-modulated XY model with $J_u=0$ and $J_v=4J_{\text{avg}}$, for $T=0.9, 1.0, \ldots, 1.5$ in units of $J_{\text{avg}}$ and $L=4, 8, \ldots, 1024$. (a) Dimensionless helicity modulus $u=Y/T$ 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 $Y/T=\frac{2}{\pi}$. (b) Helicity modulus as a function of temperature. The black line is $Y(L=\infty, T)$, obtained by FSS. The dashed line is $Y=\frac{2}{\pi}T$.](image)

![FIG. 3. (Color online) Y(T, L=\infty) for 2D XY models. (i) Homogeneous 2D XY model. (ii) 4 × 4 modulation with $J_v=3.4$ and $J_u=0.2$. (iii) 4 × 4 modulation with $J_v=4$ and $J_u=0$. The dashed line is $Y=\frac{2}{\pi}T$. The arrow indicates the theoretical upper bound $T_{\max}=\frac{2}{J_{\text{avg}}}$.](image)
$T_c=1.57$. 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

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

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 $J_{w}=\lambda J_{\text{avg}}$. Such patterns correspond to “decorated” lattices. By integrating out all doubly coordinated spins [that is, by applying the so-called decorated-iteration transformation, $J_{\text{eff}} = \tanh^{-1}(\tanh J_i \tanh J_j)$], one can reduce a decorated lattice to a primitive lattice and thus obtain an exact expression for its $T_c$ [Eq. (5)]. Unfortunately, the decoration-iteration transformation for $XY$ models involves an infinite set of Fourier components of the potential 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 $J_{w}=\lambda J_{\text{avg}}$ because for a given wavelength $\lambda$, this gives the largest enhancement of $T_c$ while conserving the average coupling $J_{\text{avg}}$. 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 $\lambda$ 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 $\lambda$.

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

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

$T_c$ is the transition temperature, $J_{\text{avg}}$ is the average coupling constant, and $\lambda$ is the wavelength of the modulation.
One of the occurrences of lambda in this equation is due to taking \( \lambda \) bonds in parallel, to form “bundles,” and the other occurrence is due to taking \( \lambda \) bundles in series. For \( XY \) models, the transition temperature also increases monotonically with modulation length \( \lambda \). 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.

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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 \( N_{clus}(L, T) \), based on the predictions of BKT theory that \( \chi(L, T_c) \sim L^{7/4}(\ln L)^{1/8} \) and that \( \chi(\infty, T-T_c) \sim r^{-11/6} e^{-r^{1/2}} \). The results agree with those obtained from finite-size scaling for \( Y \).
23. For more complicated patterns not amenable to decoration, \( T_c \) 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).