A numerical study of planar arrays of correlated spin islands

I. Maccari¹, A. Maiorano¹,², E. Marinari³, and J. J. Ruiz-Lorenzo³,²

¹ Dipartimento di Fisica, Sapienza Università di Roma, P. A. Moro 2, 00185 Roma, Italy
² Instituto de Bio computación y Física de Sistemas Complejos (BIFI) 50018 Zaragoza, Spain
³ Dipartimento di Fisica, IPCF-CNR and INFN, Sapienza Università di Roma, P. A. Moro 2, 00185 Roma, Italy

Abstract. We analyze a system of interacting islands of XY spins on a triangular lattice. This model has been introduced a few years ago by Eley et al. to account for the phenomenology in experiments on tunable arrays of proximity coupled long superconductor-normal metal-superconductor junctions. The main features of the model are the separation of a local and a global interaction energy scale and the mesoscopic character of the spin islands. Upon lowering the temperature the model undergoes two crossovers corresponding to an increasing phase coherence on a single island and to the onset of global coherence across the array; the latter is a thermodynamical phase transition in the Ising universality class. The dependence of the second transition on the island edge-to-edge spacing is related to the proximity-effect of the coupling constant.

1 Introduction

Recently Eley et al. [1] have introduced a model of coupled islands of XY spins. Their goal was explaining the results of measurements of resistance in arrays of long superconducting-normal-superconducting junctions. The experimental devices are based on planar arrays of identical islands made of superconducting (Nb) grains, disposed in a triangular matrix over a metal (Au) film. The authors studied the dependence of the system resistance $R(T; h, \ell)$ on temperature $T$, on island (vertical) thickness $h$ and on inter-island spacing $\ell$. They found i) the resistance dropping to zero, by lowering $T$, in two steps, and they determined two transition temperatures $T_1$ and $T_2$ with $T_1 > T_2$; ii) an interesting dependence of both $T_1$ and $T_2$ on the island spacing, possibly (both) extrapolating to $T = 0$ at large $\ell$; iii) a strong dependence of the behavior of the system on the island thickness. In a following paper [2], they discussed a more detailed comparison between the experimental data and the predictions about the dependence of $T_2$ on $\ell$ given by the conventional theory of Lobb, Abraham, and Tinkham (LAT) [3]. They argued that for large inter-island spacing the superconducting transition is more likely to be driven by diffusive effects [4,5] in the normal metal substrate, and that it does not depend on the details of the superconducting islands, with the puzzling dependence on island height as a notable exception.

The superconducting transition in proximity-coupled macroscopic grains embedded in normal metal films has been the object of intensive work in the past years, [6,7,8]. Tunable realizations of 2D superconductivity were also object of previous experiments [9]. The classical model presented in Ref. [1] to account for a novel phenomenology is at difference with previous theoretical and experimental work, as it takes into account the intrinsic fluctuations of the superconducting state inside the single mesoscopic islands (see also refs. [10,11] for recent theoretical and experimental work on mesoscopic Sn islands laid on graphene). It is clear that, because of many reasons we will discuss in the following, this model does not try to reproduce faithfully the experimental situation (for example the use of an anisotropic coupling is not connected to the physical form of the Josephson interaction but is a tool needed to obtain a phase transition). The idea of [1], and our point of view here, is to analyze a very simple model that offers a behavior quite similar to the one detected in the experiments, and to try to learn from this behavior. Here we will present a detailed analysis of the model, that corroborates and supplements the hints coming from the first analysis of [1]. It is also worth mentioning that tunable two-dimensional superconductors are also of interest in a revived search for a non-conventional 2D, $T = 0$ metallic phase. [12,13,14,15,16,17,18,19]

2 The model

The Hamiltonian of the model is based on $O(2)$ vectors living on the individual grains (labeled with $i, j$). Groups
of grains form islands (labeled by $p$):
\[
H = -J \sum_{p} \sum_{(i,j) \in p} \mathbf{S}_i \cdot \mathbf{S}_j - \sum_{(p,p')} M_p \cdot J' M_{p'} ,
\]
where by a dot we denote the scalar product in the internal space and where $J'$ is a $2 \times 2$ matrix of couplings. Each island is a $D$-dimensional hyper-cubic array of grains of linear size $I$ (and volume $V_I = I^D$, with either $D = 1$ or $D = 2$ in our computations). Islands are arranged on a (two-dimensional) planar regular lattice of linear size $L$. Islands are mesoscopic: their linear size $I$ is not larger than a few grains. Because of that they may have large global phase fluctuations. The size of the underlying planar array is macroscopic, $L \gg I$. The case of one-dimensional island is an exercise useful to understand better the role of island dimensionality, and does not try to be a description of the experimental situation. On the contrary the case of two dimensional islands is probably closer to the experimental situation, where islands have many layers, but only one or few conure to build the inter-island interaction.

The first term of the Hamiltonian is a sum of nearest-neighbor interactions between grains contained in the same island. The second term couples neighboring islands in the array. Each spin in a given island interacts directly with its neighboring spins in the same island and with the average spin field of surrounding islands. In the model proposed in Ref. [1], the inter-island coupling matrix (in the internal $O(2)$ space) $J'$ is anisotropic:
\[
J' = \begin{pmatrix} J' & 0 \\ 0 & 0 \end{pmatrix} .
\]

This particular choice polarizes the islands in one specific direction in internal vector space, changing the nature of the inter-island phase transition. This is a technically useful choice (since it carries a phase transition in the game), but it does not aim at reproducing the details of the physical Josephson interaction. Finally, notice that in the isotropic case and if the energy scales $J$ and $J'$ are far apart, i.e. $J' \ll J$, so that at low temperatures all (mesoscopic) islands are magnetized, we recover a Kosterlitz-Thouless [20] phase transition.

The island-island couplings depend on the temperature and on the inter-island edge-to-edge spacing, according to the theory of diffusion of electron pairs in SC-Normal-SC junction. As in the work of [1] we take a “quasi-proximity-effect” [13] form for both couplings: in a proximity interaction $J'$ would depend on the inverse square of island spacing when the latter is small, but following [1] and for the same sake of simplicity we omit this part of the interaction, that is not expected to change the nature of the phase transitions here. We assume the proximity-effect form also for the grain-grain coupling $J$ and we take the grain-grain distance as the length (lattice) unit (and denote the inter-island spacing as $\ell$).
\[
J = J_0 \exp \left(-\sqrt{T} \right) , \tag{4}
\]
\[
J' = J'_0 \exp \left(-\ell \sqrt{T} \right) . \tag{5}
\]

The choice of an interaction of a proximity-like form implies that physically grains of the islands are also immersed into a metallic matrix. The authors of Ref. [1] introduced the model defined in [1] to explain the presence of two transitions (intra-island, $T_1$, and inter-island coherence, $T_2$) and the depression of $T_1$ for increasing island spacing $\ell$. Such a dependence of $T_1$ on $\ell$ has been observed and reported for the first time in [1] (for example in previous experiments on lead disks on a thin substrate [9] where islands were not mesoscopic, the effect was not observed).

The energy scales $J_0$ and $J'_0$ must be well-separated: we adjust them in order to clearly split the high-$T$ and the low-$T$ transition. We fix $J_0 = 1$ and vary $J'_0$, in order to easily compare data for different island sizes, we also take $J'_0 = J'_0/\sqrt{V_I}$ and adjust the parameter $J'_0$.

In Ref. [1] the authors also give some predictions by analyzing a $D = 1$ islands model, where it turns out that:
- $T_2 \leq T_1$ provided $J > J'$ and islands are small;
- $T_1 \to 0$ when $J' \to 0$.

The second statement is rather counter-intuitive, as it implies that islands are not superconducting when they are isolated. This implies that an array of superconducting islands can be superconducting even if the inter-island spacing is larger than the superconductor coherence length, but an isolated island of superconducting grains, where grains are packed closer than islands are in the array, loses phase coherence. In this respect, the one-dimensional and mesoscopic character of the islands plays a role, since for macroscopic chains we must expect $T_1 \sim 0$, and, as we will see in the following, for large $I$ the intra-island coherence is driven by inter-island ordering (also see the discussion in the Conclusions section).

Another striking aspect of the phenomenology of the system [12] is the dependence of its behavior from the height of columnar grains. Realistic islands extend in more than one dimension. We have analyzed by numerical simulations the behavior of one and two-dimensional islands. The dependence on thickness may suggest that it would be interesting to go to $D = 3$, too (in case of a very large value of $I$ this should turn the $T_1$ transition to a true second-order one). If energy scales are adequately separated (i.e. $J \gg J'$), this should not change the properties of the $T_2$ (KT) transition, when phases of grains in the same island are mutually locked. Mesoscopic islands can then have a crossover at $T_1$ from a disordered to an ordered phase; for $D \geq 2$ and large $I$ this crossover is related to a true thermodynamic transition.

3 Numerical simulations
We have studied the model defined in [1]. By following a very slow annealing protocol, with constant ratios between
adjacent temperature (a logarithmic annealing scale), we have cooled down the system in order to get a signal for the two transitions. At each temperature we collected measurements during the evolution of the Monte Carlo dynamics. Our Monte Carlo step consists of \( n_m \) sweeps of the whole lattice by single-spin moves Metropolis dynamics, followed by \( n_o \) sweeps by over-relaxation \( [22] \). The choice of \( n_m = 10 \) and \( n_o = 12 \) have shown to be appropriate for most island and array sizes considered (and an overkill for the smaller sizes), and allowed an estimate of integrated auto-correlation times not larger than ten Monte Carlo steps at most temperatures. Although averages always stabilize quickly after any temperature change, we drop the first half of the collected measurements at all \( T \) values. The simulated annealing protocol, together with over-relaxation, is appropriate to the needs of this problem. All observables of interest converge very fast to a plateau at all temperatures. Although averages always stabilize quickly after any temperature change, we drop the first half of the collected measurements at all \( T \) values.

Since the devices in the experimental setup \([1,2]\) are triangular arrays, we consider a triangular lattice. A simple implementation choice in simulation is to consider a triangular array with regular hexagonal shape with helical boundary condition (in this way we preserve the symmetries of the triangular array and avoid involved bulk properties extrapolations); each side of the hexagon has a width of \( L \) islands, and the number of islands is \( V_S = 3L(L - 1) + 1 \). We simulated systems with \( L = 8, 16 \) and \( 32 \): for \( D = 1 \) systems we have islands of sizes \( I = 16, 36, 64, 100 \) and 144, while for \( D = 2 \) we have \( I = 6, 8, 10 \) and 12. The inter-island edge-to-edge spacing \( \ell \) has been varied in the set \( \{2, 4, 8, 12\} \) for \( D = 1 \) and \( \{2, 4, 8, 12, 16, 24\} \) for \( D = 2 \) (the SNS arrays in Ref. \([1]\) had edge-to-edge spacings up to approximately 10 times the grain size in their experiments, and \( \ell \) up to 20 in Ref. \([2]\) ). We have considered both free (FBC) and periodic (PBC) boundary conditions on the single islands. Although we found no qualitative differences, FBC is a more realistic choice when dealing with mesoscopic objects, for which we expect finite-size effects to play a role. We measured the following quantities.

- The single island magnetization magnitude (averaged over islands):

\[
M_I = \frac{1}{V_S} \sum_p \left| \frac{1}{V_I} \sum_{i \in p} S_i \right|. \tag{6}
\]

This should be, in the limit of infinitely extended islands, a good order parameter for island internal ordering (in any direction in internal spin space, and globally over the array: it has a non-zero value whenever any island starts to order internally and it is maximum when all islands are locally ordered, independently of the relative orientation between different islands).

- The total magnetization:

\[
M = \frac{1}{V_S V_I} \sum_p \sum_{i \in p} S_i. \tag{7}
\]

- A renormalized magnetization:

\[
\mu_p = \frac{\sum_{i \in p} S_i}{\sum_{i \in p} |S_i|}, \tag{8}
\]

which is a unit vector on the single island, and its average over the array.

- \( M_R \), which characterizes the globally-ordered phase, even if islands are not yet internally fully ordered:

\[
M_R = \frac{1}{V_S} \sum_p \mu_p. \tag{9}
\]

We also consider the fluctuations of the magnetizations

\[
\chi \equiv V_I V_S \left[ \langle M^2 \rangle - \langle |M| \rangle^2 \right], \tag{10}
\]

\[
\chi_I \equiv V_I \left[ \langle M_I^2 \rangle - \langle M_I \rangle^2 \right], \tag{11}
\]

\[
\chi_R \equiv V_S \left[ \langle M_R^2 \rangle - \langle M_R \rangle^2 \right], \tag{12}
\]
where $\langle M_j^2 \rangle$ and $\langle M_j \rangle$ are averaged over all islands. $\chi$ is the total susceptibility of the system. At very low temperatures, when $M_j \sim 1$, we have $\chi_j \sim \chi/V_1$. At $T_2$, that we define as the location of the peak of the inter-island susceptibility $\chi_R$, $\chi_R$ and $\chi$ have very similar sharp peaks (both in shape and location). We take the location of the (very smooth) maximum of $\chi_I$ as a rough estimate of the temperature $T_1$ at which islands order internally (in this way we give an operative definition of $T_1$ in our model: since islands are of finite extent the $T_1$ defined in this way is indeed a crossover temperature).

4 Results and discussion

In Fig. 1 we report the results for arrays of one-dimensional chains. The $T_1$ temperature value goes to zero very fast as the island size grows, as expected for linear spin chains. Upon lowering $T$, coherence between island builds up and also drives the internal ordering; the two transitions can be resolved only for very small island sizes and by lowering considerably the value of coupling constant $J_0$. The effect is also strongly dependent on island size.

The situation is far clearer for two-dimensional islands (see Fig. 2), where we still have a finite temperature thermodynamic transition for isolated islands in the limit of large sizes. For mesoscopic islands, the crossover between unordered and ordered island depends more weakly on island size than in the linear chains case. Our numerical simulations show that the temperature $T_1$ does not depend on the island spacing, or the dependence is very weak. This effect has been also reported in experimental results on non-mesoscopic island samples [9]. Also the dependence of $T_1$ on island size is very weak.

We try a more quantitative approach studying the depression of $T_2$ by increasing the inter-island spacing. We take as an estimate for $T_2$ the midpoint of the temperature interval bracketing the peak at its half-height. The dependence of $T_2$ on $\ell$ and $I$ for the largest simulated array size $L = 32$ is shown in Fig. 3.

Following Ref. [1], we notice that $T_2(\ell)$ compares well to a proximity-effect prediction

$$T_2 = \Delta \exp(-C \ell \sqrt{T_2}) ,$$

(13)

corresponding to the solid straight line in Fig. 3 suggesting a diverging $\ell(T_2 = 0)$; we report in Table 1 our best fit estimates of the parameters $\Delta$ and $C$.

We have run more accurate numerical simulations in the temperature region close to the $T_2$ transitions, with a four times smaller cooling rate and ten times more measurements. We measured the Binder cumulant

$$G_4 = \frac{1}{2} \left( 3 - \frac{\langle M^2 \rangle^2}{\langle M^2 \rangle} \right) ,$$

(14)

The value of $G_4$ at the $T_2$ transition point is universal [22]; we report data for $I = 6$, $\ell = 4$ and various array sizes $L$ in Fig. 4. Note that the largest system sizes in Fig. 4 are due to the breakdown of the $O(2)$ internal symmetry introduced by the anisotropic form of $J$ in Eq. 5. This is the behavior one would expect, since at high temperature the $G_4$ value depends on the symmetry of the system. The fluctuations of the magnetization in the infinite volume limit are Gaussian dis-
tributed and the Binder parameter for the two-component magnetization of a XY system should approach the value $G_1(T \to \infty) = 0.5$, whereas for Ising spins the corresponding high-temperature value is $G_1(T \to \infty) = 0$. When long range order in the system builds up at low temperatures, the value of the Binder parameter must approach unity: $G_1(T \to 0) = 1$. The data in Fig. 3 show that $G_4$ is not monotonically increasing when the temperature decreases: it starts at a value around 0.5 but, as soon as the inter-island term becomes more important with respect to the intra-island interaction in the Hamiltonian, the effects of the Ising symmetry sets in and in proximity of the critical region, just above $T_2$, the value of $G_4$ drops to low values, as expected for an Ising system. The minimum of the dip decreases as the system size $L$ increases.

Moreover, the critical value of the Binder cumulant (which is universal) for the two-dimensional Ising model is known to great accuracy [23]. The values $G_4 = 0.9160386(24)$ compares extremely well with our value of the Binder parameter at crossing, close to $T_2 \sim 0.335$ (for comparison, from the position and width at half-height of the peak of the susceptibility for the same simulated system we obtain $T_2 \simeq 0.340 \pm 0.004$). We report in Fig. 4 the details of the crossing of the Binder curves. This provides a clear numerical evidence for a second order phase transition in the two-dimensional Ising universality class. The asymptotic value of the crossing points of the Binder cumulants curves (see inset of Fig. 4, $T_{2c}(L, 2L)$ which asymptotically tends to $T_2$, is clearly different from zero. We finally remark that the value of the Binder cumulant below the critical temperature is almost unity as expected asymptotically (as the size of the system goes to infinity).

![Fig. 3. A scaling plot of the $T_2$ transition temperature for arrays of $D=2$ island based on the behavior $\Delta \exp(-C(T_2/2))$ as suggested by Eq. (L = 32 data).](image)

![Fig. 4. Binder cumulant $G_4$ versus $T$ for $D=2$ islands with $I = 6$ and $\ell = 4$ and for the five simulated sizes ($L$).](image)

### Table 1

| $I$ | $\Delta$ | $C$     |
|-----|----------|---------|
| 6   | 3.74(10) | 0.935(6) |
| 8   | 5.21(15) | 0.890(6) |
| 10  | 7.56(28) | 0.889(7) |
| 12  | 8.15(26) | 0.840(6) |

Best fit estimates of $\Delta, C$ parameters in Eq. (3) from $T_2$ data for various island size $I$ ($D = 2$, $L = 32$, $\ell = 8, 12, 16, 24$). Data points for the shortest distances $\ell = 2, 4$ have been excluded from the fits. The chi-square per degree-of-freedom values vary between 2.4 and 3.7 and the quality-of-fit parameters between 0.11 and 0.32. Uncertainties are gnuplot estimates corrected as in [21].

### 5 Conclusions

It has been very difficult to resolve the crossover at $T_1$ (internal island ordering) and the $T_2$ transition (inter-island ordering) in the case of one-dimensional islands. In $D = 1$ and in the limit of large islands sizes we expect $T_1 \to 0$ and no thermodynamic transition at finite temperatures. In the range of simulated island sizes the measured crossover temperature at which the mesoscopic island order internally is as small as $T_2$. The island internal magnetization remains small and no clear maximum of the susceptibilities signals a crossover down to $T_2$. At $T_2$ the inter-island interaction couples the fluctuations of the magnetizations of neighboring islands, making them coherent: at this point spins inside each islands starts to align to the average field of neighboring islands. The mesoscopic character of the islands is crucial: in the limit of large islands we expect the fluctuations of local magnetization to be too small (we did not try an experiment in that direction). Then, although $J' < J$, it is the $T_2$ transition that drives both inter-island and internal ordering. As the inter-island spacing grows the depression of $T_2$ implies the depression of $T_1$, too. This is compatible with the counterintuitive requisite that $T_1 \to 0$ as $J' \to 0$ discussed above.

Since islands in experimental setups are not laid down on the substrate as unidimensional chains of columnar...
Appropriate variations of the basic model we have discussed here could lead to interesting developments in the study of the superconducting transition in arrays of SNS junctions. We think it is an interesting starting point to understand many striking experimental evidences, as for instance the dependence of the transition temperatures on island thickness, or the strong depression of the $T_1$ and $T_2$ transitions.

We thank Kay Kirkpatrick for introducing us to the model studied in this work and her and Jack Weinstein for interesting discussions. This work was partially supported by European Union through Grant No. PIRSES-GA-2011-295302, and ERC Grant No. 247328, by the Ministerio de Ciencia y Tecnología (Spain) through Grant No. FIS2013-42840-P, and by the Junta de Extremadura (Spain) through Grant No. GRU10158 (partially founded by FEDER).

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