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The quasi-one-dimensional frustrated XY model

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Abstract. A quasi-one-dimensional version of the frustrated XY model used to describe Josephson junction arrays and granular superconductors is described. It is shown that there are two distinct types of ground state, depending on whether the frustration is greater than or less than a critical amount. The small fluctuations around the weak frustration ground state are analysed by diagonalising the Hessian matrix; this gives an expression for the low-temperature specific heat of the network. By an extension of this analysis to include the effect of twisted boundary conditions, the critical current of the system is calculated in the low-flux regime. Finally the effect of diamagnetic screening currents are included.

1. Introduction

The frustrated XY model [1–15] has been of recent interest because of its relevance to granular superconductors, artificially made networks of superconducting wires and Josephson junction arrays. It is now of even greater interest since the discovery of high-temperature superconductors. The existence of grains within these new materials is much more important than in conventional superconductors because of the short coherence lengths of the electron pairs, which are of the order of the grain boundary width. It is believed that some of the magnetic effects in these materials can be explained by their granularity [13].

In this paper the properties of the model are studied on a quasi-one-dimensional 'ladder' network which is simpler to treat both analytically and numerically but retains many of the features of the full model. This network has been studied previously by Kardar [15].

In §2 the model and the ladder network are described. In §3 the ground states of the system will be discussed and it will be shown that the ground states for weak frustration are qualitatively different from those with strong frustration and the existence of a critical value of the frustration will be inferred. In §4 the effects of small fluctuations about the ground state will be considered by diagonalising the Hessian matrix. This leads to an estimate of the low-temperature specific heat of the system. In §5 the small fluctuation analysis will be extended to the case of a weakly frustrated array with twisted boundary conditions which carries a bulk current along the ladder. The value of the net current at which the state becomes unstable, indicated by a soft mode in the fluctuation spectrum, will be determined and identified as the critical current of

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the array. Section 6 will include the self-consistent effects of the diamagnetic screening currents in the weak frustration ground state. Finally, §7 contains a brief summary.

2. The frustrated XY model and the ladder network

Consider an array of grains of superconducting material embedded in a normal matrix, as depicted in figure 1. Below the bulk transition temperature, T_{sc}, each grain has its own complex order parameter, $\psi = \rho \exp(i\theta)$. Well below T_{sc} the modulus, ρ, is approximately the same on each grain, but the phase angle, θ, is subject to strong thermal fluctuations (corresponding to Goldstone modes of the bulk transition). If the grains were widely separated then the phases would always be uncorrelated, but if the grains are very closely packed then the Josephson effect will couple the phases on adjacent grains (this is true if the matrix is an insulator; if it is a normal metal then the proximity effect leads to the same qualitative form for the coupling). In the absence of any external magnetic fields, the Josephson coupling has the normal XY model form, with the phase variables playing the role of XY spins. We can therefore write an effective Hamiltonian for the phase degrees of freedom of the form

$$H = -J(T) \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j). \tag{2.1}$$

Consequently, in two dimensions the model will have a Kosterlitz–Thouless transition [14], below which the phases will exhibit quasi-long-range order. The phases will of course not show true long-range order except at zero temperature.

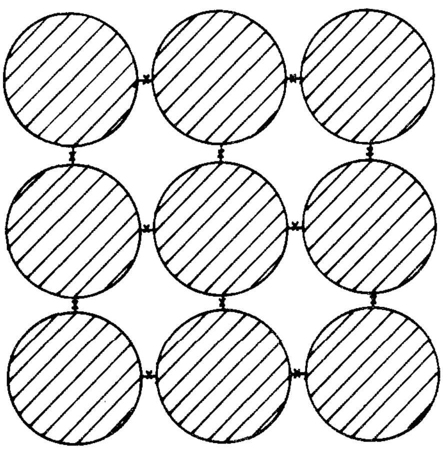

Figure 1. A schematic view of a regular granular superconductor. The shaded regions are superconducting while the unshaded regions are normal. The crosses mark the locations of the Josephson junctions.

If a magnetic field is applied perpendicular to the array then an extra phase shift is developed across each junction which is given by

$$A_{i,j} = \frac{2\pi}{\Phi_0} \int_i^j \boldsymbol{A}(\boldsymbol{r}) \cdot d\boldsymbol{l} \tag{2.2}$$

where Φ_0 is the flux quantum and $A(r)$ is the vector potential for the magnetic field. The Hamiltonian (2.1) is then replaced by

$$H = -J(T)\sum_{\langle i,j\rangle}\cos\phi_{i,j} \tag{2.3a}$$

$$\phi_{i,j} = \theta_i - \theta_j - A_{\langle i,j\rangle} \tag{2.3b}$$

which defines ϕ, the gauge-invariant phase difference across a junction. From the definition of the twist (2.2) it can be seen that the sum of the twists around a plaquette is proportional to the number of flux quanta threading that plaquette:

$$\sum_{\langle i,j\rangle\in\alpha} A_{\langle i,j\rangle} = 2\pi f_\alpha = 2\pi\Phi(\alpha)/\Phi_0. \tag{2.4}$$

It is also clear that f_α is a measure of the frustration on the plaquette: if f is an integer then the energy of each bond on the plaquette can be simultaneously minimised, if f is not an integer this cannot be done and the plaquette is frustrated.

The supercurrent flowing across a junction is given by

$$I_{i,j} = \bar{I}\sin\phi_{i,j} \tag{2.5}$$

where $\bar{I} = 2eJ(T)/\hbar$, while the sum of the currents around a plaquette is a local magnetisation

$$M_\alpha = \sum_{\langle i,j\rangle\in\alpha} I_{i,j}. \tag{2.6}$$

In this paper I propose to consider this model on the ladder network depicted in figure 2. Each site of the network is labelled by an integer coordinate and an 'up or down' label $s = \pm$. The magnetic field will be assumed to be uniform and to link a flux $f\Phi_0$ through each plaquette. In this case the gauge can be chosen so that there are no twists on the horizontal bonds and a twist of $A_i = 2\pi f i$ on the ith vertical bond. We now define the gauge invariant phase differences

$$\phi_i^\pm = \theta_i^\pm - \theta_{i-1}^\pm \qquad \phi_i^0 = \theta_i^+ - \theta_i^- - A_i \tag{2.7}$$

current variables

$$I_i^c = \bar{I}\sin\phi_i^c \qquad c = 0, \pm \tag{2.8}$$

and magnetisation variables

$$M_i = I_i^0 - I_i^+ - I_{i-1}^0 + I_i^-. \tag{2.9}$$

The Hamiltonian then has the form

$$H = -J(T)\sum_{i=1}^{N}\sum_{c=0,\pm}\cos\phi_i^c. \tag{2.10}$$

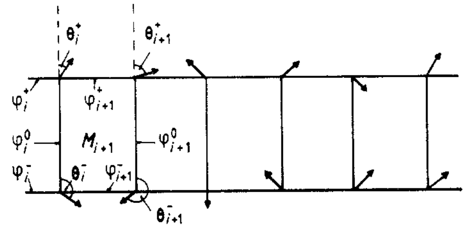

Figure 2. The ladder network of Josephson junction arrays showing the labelling of site, bond and plaquette variables.

Kardar [15] studied this network for a model including the effects of junction capacitance and showed that, in the limit of strongly anisotropic couplings: $J^{\pm} \gg J^0$, the network is equivalent to the 1+1-dimensional sine–Gordon model which has been exactly solved by Haldane [17].

3. Ground states of the model

The Hamiltonian (2.6) has an obvious global continuous symmetry: $\theta_i^s \mapsto \theta_i^s + \alpha$, consequently any state, including the ground state, is a member of a continuous, U(1), family of degenerate states. In addition to this, when f is not an integer, there are extra, discrete, degeneracies associated with the ordering of the magnetisation variables. In all of the following the trivial U(1) degeneracy will be assumed to have been removed by fixing the value of one phase angle.

Ground states were found numerically using a Langevin (gradient descent) algorithm. The system was initialised with a random configuration and then evolved according to the relaxational dynamics

$$\theta_i^s(t+\delta t) = \theta_i^s(t) - \delta t\, \partial H/\partial\theta_i^s + \eta_i^s(t) \tag{3.1}$$

where $\eta_i^s(t)$ was drawn from a Gaussian white noise distribution

$$\begin{aligned} &\overline{\eta_i^s(t)} = 0 \\ &\overline{\eta_i^s(t)\eta_j^t(t')} = 2T\delta_{s,t}\delta_{i,j}\delta(t-t') \end{aligned} \tag{3.2}$$

characterised by a temperature T. The temperature was slowly decreased to zero during each run until the changes in the spins fell below a threshold value. For a given value of f this was repeated using different sequeneces of noise terms and different start configurations (this last was not important as the start temperature was sufficiently high to wash out any initial condition effects).

As would be expected for a frustrated spin system there are many low-lying metastable states, but the absence of disorder and the consequent expectation of periodic ground states means that the task of finding good ground states is not that hard for simple rational values of f. Ground states were found for values of f of the form $f = p/q$ for systems of length $N = lq$, for $l = 1, 2, \ldots$, and periodic boundary conditions, for $q = 1, \ldots, 13$ and all values of p which gave $0 \le f \le 1/2$ and p/q an irreducible fraction.

It was found that for a given q there existed a critical $P(q)$ such that $p \leq P(q)$ gave a unique, non-chiral (i.e. all magnetisations equal) ground state with period $2q$, whereas each $p \geq P(q)$ gave a set of degenerate chiral ground states with period q. The values of $P(q)$ found are at least consistent with the existance of a critical f (i.e. $P(q) \sim f_c q$): $f_c \simeq 0.295$.

For $p < P(q)$ the ground states have the form

$$\overline{\theta_i^{\pm}} = \pm i\pi f. \tag{3.3}$$

The case $f = 1/4$ is shown in figure 3. The frozen-in supercurrents in the ground state are therefore

$$I_i^{\pm} = \pm\bar{I}\sin\pi f \tag{3.4}$$

and the magnetisations

$$M_i = -2\bar{I}\sin\pi f. \tag{3.5}$$

The ground-state energy is $-NJ(0)(1 + 2\cos\pi f)$. It is noticeable that all of these quantities are simple functions of f.

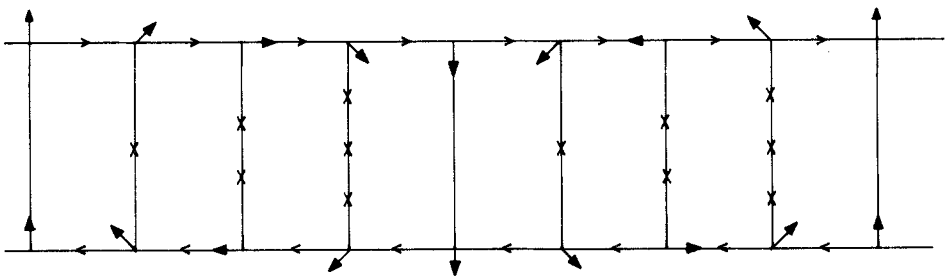

Figure 3. The forms of the ground state for $f = 1/4$. The upper left-hand phase in each case has been fixed to be zero to remove the U(1) degeneracy. The crosses on bonds each represent a twist of $2\pi f$. Arrows on the bonds indicate the direction of current flow.

The ground states for $p \geq P(q)$ are more complex and are no longer unique. As an example the ground states for $f = 1/2$, where all the plaquettes are maximally frustrated, are shown in figure 4. This case has two degenerate ground states given by

$$\theta_{2i}^{+} = 0 \qquad \theta_{2i+1}^{+} = \mp\phi \qquad \theta_{2i}^{-} = \pm\pi/2 \mp \phi \qquad \theta_{2i+1}^{-} = \pm\pi/2 \tag{3.6}$$

where $\tan\phi = 1/2$, $\phi \simeq 0.148\pi$. The magnitudes of the currents are $\bar{I}\sin\phi = \bar{I}/\sqrt{5}$ on horizontal bonds and $\bar{I}\cos\phi = 2\bar{I}/\sqrt{5}$ on vertical bonds, while the magnetisations are of magnitude $6\bar{I}/\sqrt{5}$. The ground state energy is $-NJ(0)\sqrt{5}$. The introduction of the staggered magnetisation

$$\Xi_i = (-1)^i M_i\left(\sqrt{5}/\bar{I}\right) \tag{3.7}$$

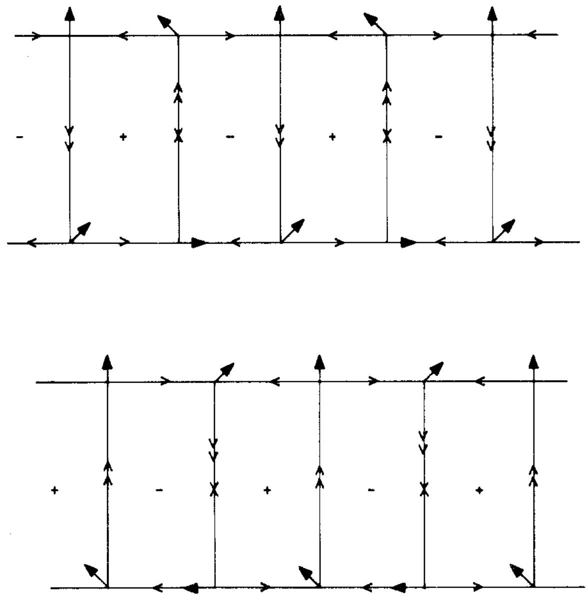

Figure 4. The two distinct chiral ground states for $f = 1/2$.

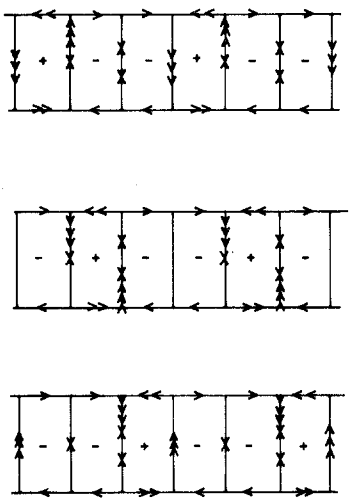

Figure 5. A schematic depiction of the ground states for $f = 1/3$. The signs in the plaquette centres denote the direction of current circulation (magnetisation). The arrows denote the magnitude of the current on each bond: >= $0.34\bar{I}$, >>= $0.64\bar{I}$, >>>= $0.98\bar{I}$.

which is invariant under global (and small local) phase rotations provides an order parameter for distinguishing between the two distict chiral ground states.

The ground states for the case $f = 1/3$ are shown schematically in figure 5, the crosses denoting a positive magnetisation of magnitude $3.25\bar{I}$ and the minuses a negative magnetisation of magnitude $1.67\bar{I}$; the arrows denote the direction of current flow along the bonds.

Figure 6 is a graph of ground state energy against flux per plaquette; it is clear that for $f > f_c$ the variation is complex with a strong dip at $f = 1/2$ and marked features at $f = 1/3$ and $f = 2/5$. This curve is strongly reminiscent of the graph of ground-state energy against flux for the 2D system found by Teitel and Jayaprakash [2]; the strong features at simple rational flux values correspond to similar effects seen by Halsey [8] in his analytically constructed 2D ground states.

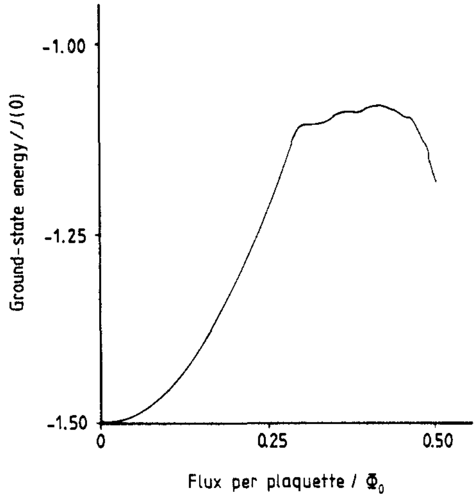

Figure 6. A plot of ground-state energy versus applied flux for the ladder model.

It is perhaps useful to relate the structure of these ground states to the properties of continuum superconductors [15]. The weak frustration states are analagous to the Meissner phase with diamagnetic screening currents flowing on the 'surface', while the strong frustration states correspond to the Abrikosov phase with the positive magnetisation plaquettes playing the role of fluxoids. We can, for example, consider the $f = 1/3$ states to be composed of a weak frustration-type state with vortices or flux kinks [15] introduced on every third plaquette, similarly the $f = 1/2$ state contains kinks on every second plaquette. Hence we draw an analogy between f_c and H_{c1} for type-II superconductivity.

There is no analogue of the Meissner phase in the two-dimensional model, presumably because charging effects are neglected and the local flux density is not calculated self-consistently, althought there is evidence of a change in the nature of the ground states around $f = 1/3$ [8]. It is tempting to believe that for $f < 1/3$ the two dimensional system is trying to form a flux lattice whereas for $f > 1/3$ there are too many vortices and the staircase states (flux density waves) of Halsey [8] are favoured.

The existence of a critical frustration f_c agrees with Kardar's work on the strongly anisotropic case. The sine–Gordon formulation idicates a transition at $f_c = 2/\pi^2 \simeq 0.2$. Kardar's calculation also implies that near this critical value of f the ordering is destroyed by any non-zero value of $1/C$ the inverse capacitance of the junctions; whereas for $f < f_c$ and $f > f_c$ there is a critical value of $1/C$ below which the ordering exists. The results found using the Hamiltonian given in §2 are, therefore, probably not stable to the addition of charging effects for $f \simeq f_c$.

4. Small fluctuations around the ground state

For the weak frustration ground states, (3.1), it is straightforward to write down the Hessian matrix

$$(\partial^2 H/\partial\theta_i^s\partial\theta_j^t)_{\bar{\theta}} = J[\delta_{s,t}\gamma(2\delta_{i,j} - \delta_{i+1,j} - \delta_{i-1,j}) + st\delta_{i,j}] \tag{4.1}$$

where $\gamma = \cos\pi f$. The eigenvalues of this matrix can be found analytically and have the form

$$\begin{aligned} \lambda_-(k) &= 2J(0)\gamma(1-\cos k) \\ \lambda_+(k) &= 2J(0)[1+\gamma(1-\cos k)] \end{aligned} \tag{4.2}$$

where $k = 2\pi m/N$, $m = 0,\ldots,N-1$. This leads to the following form for the density of states for fluctuations:

$$\rho(\omega) = \frac{\theta(\omega)\theta(4J\gamma-\omega)}{\sqrt{\omega(4J\gamma-\omega)}} + \frac{\theta(\omega-2J)\theta(2J(2\gamma+1)-\omega)}{\sqrt{(\omega-2J)[2J(2\gamma+1)-\omega]}}. \tag{4.3}$$

Making the usual assumption that each of these modes is occupied with a probability given by the Gibbs factor corresponding to the energy of the mode, gives the following expression for the low-temperature specific heat of the network

$$C \sim \int_0^\infty \omega^2\rho(\omega)\exp(-\omega/T)\,\mathrm{d}\omega \sim (J\gamma)^{-1/2}T^{5/2}. \tag{4.4}$$

This is of course only valid within the model as stated in equation (2.3), the neglected charging effects will have a contribution to the specific heat. In addition, this form is only valid for temperatures sufficiently low that the flux kinks or vortices cannot be created by thermal processes.

5. Critical currents

Consider a ladder array with fixed boundary conditions at the ends (i.e. the phases at the ends of the ladder are set to zero). If the the flux threads $p/q < f_{cr}$ of a flux quantum through each plaquette and the length of the ladder is $N = 2lq$ for some integer l, then the ground state of the system is the same as for the system with periodic boundary conditions, $\bar{\theta}_i^s$. If we now slightly increase the phases at the right-hand end of the ladder to a value, δ, then the phases will relax to distribute the twist right along the system to give a state of the form

$$\bar{\theta}_i^{\pm}(\delta) = i\delta/N \pm i\pi f \tag{5.1}$$

such that $\phi_i^{\pm}(\delta) = \pm\pi f + \delta/N$; $\phi_i^0 = 0$. Consequently there is now a net flow of supercurrent through the system of magnitude

$$I_{tot} = 2\bar{I}\cos\pi f\sin\delta/N. \tag{5.2}$$

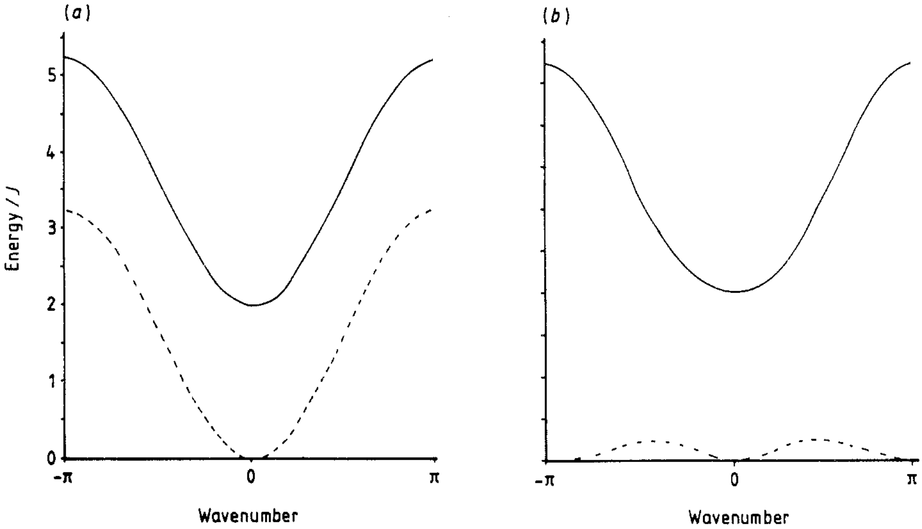

Figure 7. The dipersion curves for the fluctuation modes around the weak frustration ground states, for $f = 1/5$. (*a*) $\delta = 0$, i.e. periodic boundary conditions; (*b*) $\delta = \delta_c$, at the metastable state carrying the critical current.

If we now adiabatically (i.e. sufficiently slowly that the phase configuration is always a local minimum of the Hamiltonian) increase δ to 2π the system will once again be equivalent to the system with periodic boundary conditions (as far as ground state properties) but the phase configuration will be in a metastable minimum carrying a bulk supercurrent. If δ is increased further the state will eventually become unstable and there will be a drastic rearrangement of the phase angles resulting in a state carrying a lower net current. The current at the critical value of δ

$$I_c = 2\bar{I} \cos \pi f \sin \delta_c \qquad (5.3)$$

is then interpreted as the critical current of the network [2,8].

The Hessian for the state (5.1) is

$$(\partial^2 H/\partial\theta_i^s \partial\theta_j^t)_{\bar{\theta}_i(\delta)} = J[\delta_{s,t} \cos(s\pi f + \delta/N)(2\delta_{i,j} - \delta_{i+1,j} - \delta_{i-1,j}) + st\delta_{i,j}] \qquad (5.4)$$

which has eigenvalues

$$\lambda_\pm(k) = J\{1 + 2(1 - \cos k)\cos(\delta/N)\cos \pi f \pm [1 + 4(1 - \cos k)^2 \sin^2(\delta/N)\sin^2(\pi f)]^{1/2}\} \qquad (5.5)$$

The critical value of δ is reached when one of these modes (other than the $k = 0$ Goldstone mode) goes soft. Figure 7 shows $\lambda_\pm(k)$ for $\delta = 0$ and for $\delta = \delta_c$. It can be seen that the first mode to go soft is at the zone boundary giving

$$\cos(\delta_c/N) = -\tfrac{1}{4}[\cos(\pi f) + (1 + 15\sin^2(\pi f))^{1/2}]. \qquad (5.6)$$

The resultant critical current is plotted against f in figure 8.

6. Self-consistent field effects

One of the shortcomings of the model as described in §2 is the lack of self-consistent treatment of the field in the system, i.e. the neglect of the diamagnetic contribution of

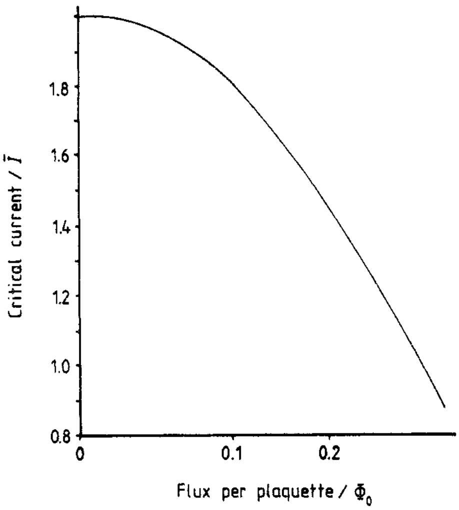

Figure 8. The variation of critical current versus external flux for $f < f_c$.

the supercurrents to the local field. In the chiral type of ground states this is hard to include because a uniform external field produces a non-uniform magnetisation, but in the weak frustration regime we can include these effects. Let F be the 'applied flux per plaquette', ie the flux that would thread each plaquette were it not bounded by junctions carrying current. The true flux per plaquette is then

$$f_\alpha = F_\alpha + gM_\alpha\{f_\beta\} \tag{6.1}$$

where $g = \mu_0/\Phi_0$ is an effective coupling constant. If $f < f_{cr}$ then

$$M_\alpha = -2\bar{I}\sin\pi f \tag{6.2}$$

which leads to the relation

$$F = f_\alpha + 2g\sin\pi f_\alpha. \tag{6.3}$$

Hence the local field is uniformly reduced by the diamagnetic current as one would expect.

7. Summary

The ground-state properties of a quasi-one-dimensional version of the frustrated XY model have been studied. It has been shown that if the applied flux/frustration is weak enough then the system has an unique, non-chiral ground state. In this regime exact calculations have been performed for the fluctuation spectrum, the low-temperature specific heat and zero temperature critical current. The diamagnetic effect of the frozen supercurrents on the local field has also been evaluated in this regime.

Acknowledgments

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