Intrinsic frustration effects in anisotropic superconductors

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(I November 21, 2018)

Lattice distortions in which the axes are locally rotated provide an intrinsic source of frustration in anisotropic superconductors. A general framework to study this effect is presented. The influence of lattice defects and phonons in d and s + d layered superconductors is studied.

73.40.Gk,74.25.Bt,74.72.-h

I. INTRODUCTION.

In anisotropic superconductors, local rotations of the lattice modulate the order parameter. The most striking manifestation of this effect is the influence of grain boundaries in high-Tc superconductors. Less pronounced effects are also to be expected from lattice defects such as dislocations, as they twist the lattice axes in their vicinity. Transversely polarized phonons can, in principle, also couple to the superconducting order parameter through the local rotations that they induce.

If, along a given direction, there are strains which change the orientation of the lattice axes, the equilibrium order parameter must follow that distortion. For instance, in a two dimensional square lattice, a parameter with $d_{x^2-y^2}$ symmetry, $\Delta_{x^2-y^2}$, must change into $\cos(2\theta)\Delta_{x^2-y^2} - \sin(2\theta)\Delta_{xy}$ after a lattice rotation by an angle $\theta$. We express the local order parameter in terms of its components in a fixed frame of reference which is independent of the orientation of the lattice. We expand the local order parameter in terms of the functions $(\Delta_{x^2-y^2}, \Delta_{xy})$, defined in this external frame. In principle, the symmetry of the square lattice allows mixing of a pure $\Delta_{x^2-y^2}$ in one point and $\cos(2\theta)\Delta_{x^2-y^2} + \sin(2\theta)\Delta_{xy}$ in the other. The transformation which takes one expression into the other can be accomplished by modifying the two component vector $(\Delta_{x^2-y^2}, \Delta_{xy})$ by means of an operator of the type $e^{i\int \hat{A}_y d\vec{r}}$, such that:

$$i \int \hat{A}_y d\vec{r} = 2\theta\left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right)$$ (1)

and:

$$e^{i\int \hat{A}_y d\vec{r}} = \left( \begin{array}{cc} \cos(2\theta) & \sin(2\theta) \\ -\sin(2\theta) & \cos(2\theta) \end{array} \right)$$ (2)

The integral is to be taken along the path in real space along which the lattice is rotated. As $\theta$ is the total rotation along the path considered, we can write, for the example considered here:

$$\hat{A}_y = 2(\nabla R)\sigma_y = \hat{A}\sigma_y$$ (3)

where $\nabla$ is the gradient operator in real space, $R$ specifies the local rotation of the lattice axes, and $\sigma_y$ is a Pauli matrix. The rotation $R$ can be written as:

$$R = \frac{\partial_x u_y - \partial_y u_x}{2}$$ (4)
where $\mathbf{u}(\mathbf{r})$ are the local deviations of the lattice node at $\mathbf{r}$ from equilibrium. Eq. (3) is valid for small deviations (strains).

The expressions above allow us to relate the changes in the order parameter as seen in the two frames, and the rotations of the lattice, in terms of the local strains. The gradient term in the Ginzburg Landau description, which should be expressed with respect to the external frame, looks, in terms of the order parameter with respect to the local axes:

$$
\mathbf{F} = \frac{a_{x^2-y^2}T_c\xi_0^2}{2} \int \sum_{i=x,y} |(\partial_i - A_{gi})\Delta_{x^2-y^2}|^2 \\
+ \frac{a_{xy}T_c\xi_0^2}{2} \int \sum_{i=x,y} |(\partial_i - A_{gi})\Delta_{xy}|^2 \\
+ \frac{a_{0}(T - T_c^2)}{2} \int |\Delta_{x^2-y^2}|^2 \\
+ \frac{a_{0}(T - T_c^2)}{2} \int |\Delta_{xy}|^2 + \text{quartic terms} \quad (5)
$$

where $\mathbf{F}$ is the free energy, $T_c$ is a number with dimensions of temperature, and of order $T_c^2$. Finally, $a_{x^2-y^2} \sim a_{xy} \sim a_0$ are proportionality constants which play no role in the analysis presented below. We take the critical temperatures of the $\Delta_{x^2-y^2}$, $\Delta_{xy}$ order parameters as different, as appropriate for a square lattice. Equation (3) and the definitions (3) and (4) suffice to study the phenomenology of layered superconductors whose order parameter is well approximated by $|\cos(2\theta)|$, $|\sin(2\theta)|$.

It is easy to see that, when $\Delta_{x^2-y^2}$ and $\Delta_{xy}$ have the same critical temperature, and $\nabla \times \mathbf{A} = 0$, the effects of the field can be made to vanish by performing a local rotation of the order parameter. In this case, the system has isotropic superconducting properties. Hence, rotations of the underlying crystal lattice leave the (degenerate) order parameter unaffected.

The formalism described here can be expressed in terms of a connexion, which depends on the lattice orientation. The definition of parallel transport of a vector, in our case $(\Delta_{x^2-y^2}, \Delta_{xy})$, needs to be modified by the rotation of the lattice. The usual derivative is changed into a covariant derivative. This technique lies at the basis of the extensive work done in topological phases, and has found use in many fields in condensed matter physics.

In addition to the effects described by (3), there may be an explicit coupling of the order parameter to the lattice strains. The simplest coupling is proportional to $\frac{\partial\mathbf{F}}{\partial\mathbf{r}} \int \sum_i \epsilon_{ii} |\Delta_{x^2-y^2}|^2$, where $\sum \epsilon_{ii}$ defines the local compression, or expansion, in terms of the symmetric part of the strain tensor. This term can also exist in a s wave superconductor. A coupling of this type is not negligible in the high-$T_c$ compounds, due to the strong dependence of $T_c$ on pressure 4.

The previous analysis can be generalized to three dimensional superconductors with arbitrary order parameters. Local rotations of the lattice can be expressed in terms of the parameter:

$$R_i = \frac{\epsilon_{ijk} \partial_j u_k}{2} \quad (6)$$

where $\epsilon_{ijk}$ is the fully antisymmetric tensor. In order to determine the transformations induced by these rotations in the order parameter, we must first decompose it into spherical harmonics with well defined transformation properties. Then, a gauge field which performs rotations in order parameter space is added to each component. Finally, as in (3), all terms allowed by the lattice symmetry are included in the free energy. The procedure is cumbersome, but straightforward. For instance, we can add to (6) higher harmonics which transform like $|\cos(4n+2)\theta|$, $|\sin(4n+2)\theta|$. The gauge field associated to these components is of the type $\mathbf{A}_g = 4(2n+1)\sigma_y^G \mathbf{y} \nabla(\partial_x u_y - \partial_y u_x)$, where $\sigma_y^G$ transforms one of these parameters into the other. The gauge field induced by the higher harmonics of the order parameter are also proportional to the gradient of the lattice rotations, but with a larger constant of proportionality. The term with $|\mathbf{A}_g|^2$ in the free energy induces a reduction of these components of the order parameter. This reduction will be stronger for higher harmonics than for lower ones.

### III. Static Distortions.

We now consider specific lattice distortions within the layers. The simplest static defect is a dislocation. The strains in the vicinity of a dislocation can be calculated from the theory of elasticity. If the Burgers vector is $\mathbf{b}$, then

$$\frac{\partial_x u_y - \partial_y u_x}{2} = \frac{\mathbf{b} \cdot \mathbf{r}}{\pi|\mathbf{r}|^2} \quad (7)$$

where we are neglecting a possible anisotropy in the elastic constants of the lattice. We now assume that the $\Delta_{xy}$ component is negligible, which is justified if, for instance, the parameter $T_c^2$ in (3) is less than one. Then, the coupling of the lattice rotations to $\Delta_{x^2-y^2}$ is due to terms quadratic in the gauge potential, and we obtain:

$$\frac{a_{xy}T_c\xi_0^2}{2} \int |\Delta_{x^2-y^2}|^2 |\mathbf{A}|^2 \quad (8)$$

and $|\mathbf{A}|^2 = \frac{|\mathbf{b}|^2}{2\pi|\mathbf{r}|^2}$. The effect of this term is to reduce the effective critical temperature near the dislocation. It suppresses a possible local enhancement of $T_c$ due to the explicit dependence of the critical temperature on pressure 4. In the presence of a magnetic field, the normal cores of vortices will be attracted towards the dislocations, to take advantage of the suppression of $T_c$, leading
to pinning. Near the core of the dislocation, \( r \sim \xi_0 \), we can estimate the reduction of \( T_c \) (see below) as \( \frac{\Delta T_c}{T_c} \sim \frac{\xi_0^2}{\xi_0} \). This effect can be significant in a material with a short coherence length, such as the copper oxides.

A grain boundary can be modelled as an array of dislocations. The gauge fields induced by each of them can be added, to obtain the effect of the whole boundary. After some algebra, we find that, if the rotation of the axes across the boundary is not large:

\[
|\vec{A}|^2 = \frac{\pi^2}{2a^2} \left[ 1 - \cos \left( \frac{\pi x}{a} \right) \cosh \left( \frac{\pi x}{a} \right) \right]^2 + \sin^2 \left( \frac{\pi x}{a} \right) \left[ \cos \left( \frac{\pi y}{a} \right) - \cos \left( \frac{\pi y}{a} \right) \right]^4 \nonumber \\
\sim \frac{\pi^2}{4a^2 \xi^2} \theta \left( x - \frac{\pi a}{2} \right), \quad \xi \to \infty \quad (9)
\]

where \( a \) is the lattice constant, \( \theta \) is the angle between the axes at both sides of the boundary, and \( \bar{a} = \frac{at_0}{\xi_0} \). From (8) and (9), we can estimate the reduction of the critical temperature at the boundary. We assume that \( \alpha_{x^2} \approx \alpha_{y^2} \approx \alpha_0 \), and \( T_c \sim T_c^{x^2-y^2} \). Then, \( \frac{\Delta T_c}{T_c} \sim \frac{\pi \xi^2}{2a^2} \sin^2 \left( \frac{\pi x}{a} \right) \), where \( T_c = T_c^{x^2-y^2} \). This calculation is rigorously valid when \( \sin(\theta) \ll 1 \), that is, when strains change slowly. A significant reduction of \( T_c \) can be expected near a twin boundary, which will act in a way similar to a weak link. It would be interesting to check this experimentally [12].

**IV. DYNAMIC ROTATIONS.**

The orientation of the lattice can also be modified dynamically, by transversely polarized phonons. A longitudinal phonon induces local compressions and dilatations of the lattice. A transverse phonon does not change the volume of the unit cell, but induces a shear deformation which changes from position to position. This deformation can be viewed as a local rotation of the axes. In a material with a complex unit cell, there are also optical phonons which rotate locally the axes. The rotations can be analyzed by means of the formalism discussed before. The only difference with a static distortion is that the gauge field which accounts for the lattice rotations depends on dynamic displacements. The time scales associated to the superconducting response are of the order of the inverse plasma frequency. This frequency is much higher than typical phonon frequencies, so that the changes in \( T_c \) induced by phonons can be studied as if the lattice distortions were static.

Transversely polarized acoustic phonons give rise to strains proportional to the gradient of their amplitudes. Hence, we expect that the Fourier components of \( \mathbf{R} \) are given by:

\[
\mathbf{R}_k \sim \vec{k}_\perp \times \vec{u}_k \quad (10)
\]

where \( \vec{u}_k \) is the amplitude of a phonon of momentum \( \vec{k} \), and \( k_\perp \) is the component of \( \vec{k} \) perpendicular to \( \vec{u}_k \). For transversely polarized phonons, \( \vec{k} \) is always perpendicular to \( \vec{u}_k \), and we do not need to take this restriction into account.

The gauge potential in (3) has a finite average, related to the thermal (or quantum) average value of the phonon amplitudes. It is given by:

\[
|\vec{A}_g|^2 \sim \sum_k |\vec{k}^2| (\vec{k} \times \vec{u}_k)|^2 \quad (11)
\]

We are analyzing materials which show strong differences in the superconducting properties along the in plane and out of plane directions. Phonons, however, need not be so anisotropic. We assume that they are described by an isotropic sound velocity, \( c \), and a Debye frequency \( \omega_D \approx \frac{\hbar c}{\xi_0} \), where \( a \) is the lattice constant, which we take to be of the same order of magnitude in all directions. The three dimensional integral implicit in (11) is extended to those modes such that \( \hbar c k \leq \hbar k_B T \) and \( a \leq k^{-1} \) and \( \xi_0 \leq k^{-1} \). Note that the Ginzburg-Landau description used here is valid at length scales greater than \( \xi_0 \) [11]. For simplicity, we take the Bose occupancy of a phonon to pinning. Near the core of the dislocation, \( r \sim \xi_0 \), we can estimate the reduction of \( T_c \) (see below) as \( \frac{\Delta T_c}{T_c} \sim \frac{\xi_0^2}{\xi_0} \). This effect can be significant in a material with a short coherence length, such as the copper oxides.

The gauge fields induced by each of them can be added, to obtain the effect of the whole boundary. After some algebra, we find that, if the rotation of the axes across the boundary is not large:

\[
|\vec{A}|^2 = \frac{\pi^2}{2a^2} \left[ 1 - \cos \left( \frac{\pi x}{a} \right) \cosh \left( \frac{\pi x}{a} \right) \right]^2 + \sin^2 \left( \frac{\pi x}{a} \right) \left[ \cos \left( \frac{\pi y}{a} \right) - \cos \left( \frac{\pi y}{a} \right) \right]^4 \\
\sim \frac{\pi^2}{4a^2 \xi^2} \theta \left( x - \frac{\pi a}{2} \right), \quad \xi \to \infty \quad (9)
\]

where \( a \) is the lattice constant, \( \theta \) is the angle between the axes at both sides of the boundary, and \( \bar{a} = \frac{at_0}{\xi_0} \). From (8) and (9), we can estimate the reduction of the critical temperature at the boundary. We assume that \( \alpha_{x^2} \approx \alpha_{y^2} \approx \alpha_0 \), and \( T_c \sim T_c^{x^2-y^2} \). Then, \( \frac{\Delta T_c}{T_c} \sim \frac{\pi \xi^2}{2a^2} \sin^2 \left( \frac{\pi x}{a} \right) \), where \( T_c = T_c^{x^2-y^2} \). This calculation is rigorously valid when \( \sin(\theta) \ll 1 \), that is, when strains change slowly. A significant reduction of \( T_c \) can be expected near a twin boundary, which will act in a way similar to a weak link. It would be interesting to check this experimentally [12].
\[ \langle \Delta T_c^2 \rangle \sim \left\{ \begin{array}{ll} T_c^9 & k_B T_c \ll \hbar \omega_D^{\text{opt}} \frac{\xi_0}{\xi_0} \\ T_c^7 & k_B T_c \ll \hbar \omega_D^{\text{opt}} \\ T_c & k_B T_c \gg \hbar \omega_D^{\text{opt}} \end{array} \right. \]  

by comparing (13) and this expression, one can see that fluctuations cannot be neglected. Finally, the typical length scale for fluctuations inside the planes is

\[ \xi \sim \max \left( \frac{\hbar c}{k_B T_c}, \xi_0 \right) \sim \max \left( \frac{\hbar \theta_D}{k_B T_c}, \frac{W}{k_B T_c} \right) \sim \xi_0 \quad (16) \]

where \( W \) is the electronic bandwidth. Hence, we expect large fluctuations in small scale domains. Transport measurements will be unable to resolve this structure, and the average \( T_c \) will be observed.

Transverse optical phonons of frequency \( \omega_{\text{opt}} \), give an additional reduction of \( T_c \),

\[ \frac{\Delta T_c}{T_c} = \left\{ \begin{array}{ll} \frac{\omega_c^2}{\omega_{\text{opt}}^2} & k_B T_c \ll \hbar \omega_{\text{opt}}^{\text{opt}} \\ \frac{\omega_c^2}{\omega_{\text{opt}}^2} & k_B T_c \gg \hbar \omega_{\text{opt}}^{\text{opt}} \end{array} \right. \quad (17) \]

where \( \langle a^2 \rangle \) denotes the mean square displacement of the phonon. It is, typically, a fraction, \( 10^{-3} - 10^{-1} \) of \( a^2 \). As in the previous case, we assume that the superconducting order parameter has a short coherence length in the out of plane direction. There is a contribution like (17) for each optical phonon transversely polarized in the plane.

The frustration of the order parameter in anisotropic superconductors by dynamical vibrations implies that \( T_c \) cannot be much larger than the frequency of the phonons responsible of the effect.

V. COUPLING BETWEEN DISTORTIONS AND CURRENTS.

The Ginzburg Landau expression (5) contains terms which are linear in \( \tilde{A}_y \), which couple one component of the order parameter and the spatial derivatives of the other (note that \( \tilde{A}_y \) is an operator which rotates one component into the other). These derivatives are different from zero in the presence of a supercurrent, because of the variation in the phase. In the case described by (5), however, these terms do not contribute, as \( \Delta_{xy} \sim 0 \).

Terms of this type play a role in materials where the superconducting properties differ significantly along the lattice axes. Let us consider an orthorhombic superconductor, where the order parameter is \( s + d \). In addition to the terms in (5) we also have:

\[ \Delta \mathcal{F}_{\text{ortho}} = \frac{\bar{a} T_c \xi_0^2}{2} \int \partial_x \Delta_s \partial_y \Delta_s^{\ast} \Delta_{x^2-y^2} - \partial_y \Delta_s \partial_x \Delta_s^{\ast} \Delta_{x^2-y^2} + \partial_x \Delta_x \partial_y \Delta_x^{\ast} \partial y \Delta_s^{\ast} + \text{c.c.} \]

\[ + \frac{a_s (T - T_c^s)}{2} \int |\partial_i \Delta_s|^2 + \frac{a_s (T - T_c^s)}{2} \int |\Delta_s|^2 \]  

where \( \Delta_x \) is the \( s \) component of the order parameter. For the sake of simplicity, we ignore terms induced by the orthorhombic symmetry which are quadratic in the order parameter. These terms, needed for a complete description of the anisotropy in the penetration depth, do not modify qualitatively the picture discussed in the previous sections.

In the absence of internal lattice rotations, \( \Delta_{xy} = 0 \). The first term in (18) leads to a difference in the penetration depth along the two lattice axes. Local rotations of the lattice can be incorporated by adding the gauge field \( \vec{B} \) to the derivatives of the \( d \) components of the order parameter in (18). Then, assuming that the equilibrium order parameter has both \( \Delta_{x^2-y^2} \) and \( \Delta_x \) components, we obtain terms of the type:

\[ \frac{\bar{a} T_c \xi_0^2}{2} \int \partial_x \Delta_s \partial_y \Delta_s^{\ast} \Delta_{x^2-y^2} + \partial_y \Delta_s \partial_x \Delta_s^{\ast} \Delta_{x^2-y^2} + \text{c.c.} \quad (19) \]

This expression gives a contribution if \( \nabla \Delta_s \neq 0 \), and, in particular, in the presence of a current. The changes in a current carrying state induced by lattice rotations are best studied within London’s framework, which is valid if the magnitude of the order parameter does not change. We define the London tensor, with the same symmetry properties of the perfect lattice, such that \( \vec{j} = m^{-1} \tilde{A}_{\text{elec}} \), where \( \tilde{A}_{\text{elec}} \) is the electromagnetic vector potential. For the study of currents within the layers, we have:

\[ m^{-1} \equiv c \begin{pmatrix} \lambda_x^{-2} & 0 \\ 0 & \lambda_y^{-2} \end{pmatrix} \quad (20) \]

where \( \lambda_x, \lambda_y \) are the penetration depths along the two axes, and \( c \) is the velocity of light. London’s expression for the free energy is (3):

\[ \mathcal{F}_L = \frac{1}{8 \pi} \int |\nabla \times \tilde{A}_{\text{elec}}|^2 + \frac{\pi}{\epsilon^2} \int \lambda_x^2 \frac{j_x^2}{2} + \lambda_y^2 \frac{j_y^2}{2} \quad (21) \]

The deviation of tetragonal symmetry is given by \( \lambda_x^{-2} - \lambda_y^{-2} \propto \bar{a} T_c \xi_0^2 |\Delta_s \Delta_s^{\ast} \Delta_{x^2-y^2}|. \)

Taking into account that the gauge field related to the lattice distortions, \( \tilde{A}_s \), is itself a derivative, we can integrate by parts in eq. (14), to obtain:

\[ \Delta \mathcal{F}_L = \frac{\bar{a} T_c \xi_0^2}{2} \int \partial_x \Delta_s \partial_y \Delta_s^{\ast} \Delta_{x^2-y^2} \]

\[ \propto (\lambda_x^2 - \lambda_y^2) \lambda_x^2 \lambda_y^2 \int j_x (\partial_x u_y - \partial_y u_x) j_y \quad (22) \]

This equation can be interpreted as a rotation of the London tensor, (20), induced by the distortion of the lattice. The currents adjust to the directions of the local
principal axes. At a grain boundary, for instance, $\mathbf{A}_{elec}$ must be continuous. The component of the current parallel to the boundary must be discontinuous, leading to a kink in the direction of the total current, as the London tensor which gives the current at both sides is discontinuous [14–16]. If, on the other hand, the boundary conditions prevent the current from acquiring a transverse component, the vector potential shows a kink, and a perpendicular magnetic field is generated at the boundary, as sketched in fig(1 [18]. This picture, derived from London’s theory, is valid at distances comparable to the penetration depth. The discontinuity at the boundary is rounded off at shorter scales.

![FIG. 1. Currents and electromagnetic vector potentials near a twin boundary, in a slab much narrower than the penetration depth. When the current is constant, and flows parallel to the boundaries, the vector potential must have a discontinuity at the twin. This discontinuity induces a magnetic field in the direction perpendicular to the slab.](image)

The present analysis implies that currents can also be deflected by other types of static defects, and by phonons. The currents flowing near a dislocation, and the instantaneous current in the presence of phonons, are sketched in fig.(2). Magnetic fields will be induced. It is interesting to note that phonons can modulate the currents and give rise to electromagnetic fields.

![FIG. 2. Sketch of the a currents flowing near a dislocation (a), and instantaneous current in the presence of a transverse acoustic phonon (b).](image)

So far, we have only considered the role of in plane distortions in layered superconductors. If we include rotations around in plane axes, we must allow for components like $\Delta_{x^2-r^2}, \Delta_{xz}, \Delta_{yz}$ in the order parameter. Because of the strong anisotropy of these compounds, components which transform like higher powers of $z^2$ are also to be expected. In analogy with (21), these components lead to contributions of the type $\int j_i (\partial_i u_z - \partial_z u_i) j_z$, where the direction $i$ lies in the planes. Note that this effect should also be present in layered superconductors with $s$ symmetry within the layers. The magnitude of the $\int j_\perp j_\parallel$ coupling is proportional to $\frac{\lambda_1^2 - \lambda_2^2}{\lambda_1^2 + \lambda_2^2}$. 

![FIG. 3. (a) Sketch of the currents around a vortex pinned by a screw dislocation. Dashed line is the dislocation axis. (b) Currents flowing along a twisted monocrystalline whisker.](image)

A particular defect which generates rotations in the out of the plane direction is a screw dislocation, which seems to be common in sputtered films [19]. In cylindrical coordinates, we have that only $\partial \theta u_z = \frac{1}{2\pi}$ is different from zero [8]. Hence, the free energy of the superconductor has a term like $\int j_\theta j_z$. A current flowing around the dislocation induces a current parallel to the axis of the dislocation. This situation may arise if a vortex is pinned by a screw dislocation. A similar effect can be realized in a monocrystalline whisker subject to shear strains. Then, $\partial_z u_\theta \neq 0$, leading again to a $\int j_\theta j_z$ coupling. A current flowing along the axis of the whisker induces a tangential component, giving rise to a magnetic field in its interior. A schematic picture of both situations is sketched in fig.(3).

VI. CONCLUSIONS.

We have presented a formalism to study the influence of lattice rotations on anisotropic superconductors. The analysis has been particularized to d-wave layered systems, but it is general enough to be applicable to more complex lattices and order parameters. We expect the scheme outlined here to be also useful for the study of heavy fermions and other materials which show an anisotropic order parameter.

For the systems considered here, we find that
i) Lattice distortions couple directly to an anisotropic order parameter, irrespective of other mechanisms, like the dependence of $T_c$ on pressure.

ii) Higher harmonics of the order parameter are more strongly frustrated by local rotations [20].

iii) Lattice defects, such as dislocations, reduce locally $T_c$. In the presence of a magnetic field, the vortex cores will be attracted to these regions, giving rise to pinning.

iv) Transversely polarized phonons also reduce $T_c$. The value of the critical temperature cannot be much larger than the typical frequency of these phonons.

v) Local rotations deflect supercurrents in superconductors with inequivalent lattice axes. In particular, the current through a grain boundary is deflected.

VII. ACKNOWLEDGEMENTS.

This work was done with support from CICyT (Spain) through grant PB96-0875. Valuable discussions with K. Maki, and hospitality at the Istituto Eduardo Caianello (Vietri, Italy), are acknowledged.

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