Theory of how to distinguish a scalar from a tensor order parameter in the high-T_c superconductors

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Using generalized Ginzburg-Landau equations, we discuss the possibility that the high-T_c superconductors do not have a scalar, but a tensor order parameter. We propose experiments to distinguish between these two possibilities both with lattice anisotropy included. A tensor order parameter implies a splitting of the upper critical field for a given setup as well as the appearance of a transverse magnetic field, when a field is applied parallel to the crystal cell axes. Only for a single scalar is the product of coherence and penetration lengths an invariant along the cell axes.

The pioneering work of Bednorz and Müller[1] and the subsequent discovery of superconductivity above liquid-nitrogen temperatures[2] has led to considerable interest in these materials, especially in their potential applications. Recently single crystals of sufficient size have been produced[3] and a first few experimental results have appeared.[4-7] From an analysis of these investigations the following picture emerges. The new high-T_c materials are highly anisotropic but do have *truly* three-dimensional superconductivity and show a large, temperature-dependent anisotropy of resistivity and critical fields. In addition, the new materials are strongly type-II superconductors with a lower critical field of about 10^2 G and an upper critical field of the order of 10^5 G. Therefore a Ginzburg-Landau (GL) approach can be expected to be extremely important because of existing spatial variations, vortices, and other spatial inhomogeneities.

The theoretical attempts to describe high-T_c superconductors have either been purely microscopic or focused on the application of the GL theory having a single scalar order parameter with lattice anisotropy,[8-10] that is if the mass matrix associated with the gradient part of the free energy has tensor character.

Here we suggest that the above theory is not sufficient to describe the strong anisotropy of the oxide superconductors. Hence we propose that such a strong anisotropy requires that the macroscopic wave function is of a tensorial nature.[11]

Since such anisotropies are expected to be more pronounced in the 90 K than in the 40 K superconductors, we list the experimental evidence for a multicomponent order parameter for this class of compounds. (a) Atomic replacement of Y by magnetic ions such as Gd (Ref.12) and Cu by metal such as Zn (Ref. 13) shows that the critical temperature is not and is severely affected, respectively. Thus superconductivity is directional in these compounds, predominantly happening in the Cu-O planes and chains. (b) Far-infrared spectroscopy indicates the possibility of more than one gap[14] and tunneling measurements give a broad range of gap values.[15,16] (c) Nuclear spin-lattice relaxation on the Cu sites indicates the existence of two gaps.[17] (d) Temperature behavior of the upper critical field[7] and a large anisotropy are measured for the lower critical field.[7,18] (e) A possible intermediate critical temperature is obtained from low-field magnetization measurements on small single crystals.[19] (f) Oxygen stoichiometry versus temperature shows a plateau at oxygen concentration around $\delta = 6.7$.[20]

Triggered by these observations we compare the results predicted from a phenomenological theory for a single scalar order parameter with lattice anisotropy with those obtained for tensor order parameters. The latter are basically unknown in the theory of superconductivity, but their application to other fluids is well established. These include the superfluid phases of ^{3}He (^{3}He-A, ^{3}He-B, ^{3}He-A_1, etc.)[21,22] and superfluid neutron star matter[23,24] as well as various classes of liquid crystals,[25,26] the mesophases mediating the solid-to-isotropic liquid transition in many organic compounds.

The method used in the present analysis is a generalized GL description[27] for the macroscopic wave function supplemented by general symmetry arguments above and below T_c. This approach allows us to make predictions, which can be tested experimentally and which will allow for a narrowing down of possible order parameters. Finally, we complement the generalized GL description by an evaluation of the possibility of new vortices and other defects using group theoretical methods. Measurements on single crystals are a *sine qua non* condition if one wants to distinguish among different options for the order parameter as we show in this Brief Report.

Our main predictions to experimentally distinguish between a single scalar and a tensor order parameter both with lattice anisotropy and for spin singlet pairing are the following.

(a) If an external magnetic field is applied in the direction of any of the axes defining the perovskite unit cell in a single crystal, we show that every tensor order parameter, except for a scalar, can lead to the occurrence of a transverse magnetic field along with a longitudinal component of the resulting current density. This is in addition to both the current density in the plane perpendicular to the vortex line direction and the magnetic field in the vortex line direction. Hence we predict that the Meissner effect changes qualitatively for a field along one of the crystalline axes.

(b) The measurement of the product of coherence and penetration length along each of the crystallographic axes of an orthorhombic or tetragonal lattice is expected to be invariant *only* for a single scalar order parameter with lattice anisotropy. Therefore the absence of this invariance at any temperature, for which the Ginzburg-Landau theory is valid, implies the existence of a multicomponent order parameter in the new materials.

(c) The single scalar theory with lattice anisotropy predicts for the upper critical field an anisotropy similar to that of the lattice. For the multicomponent theories we show the appearance of more than one intermediate upper critical field in a given direction.

The observation of any one of our three main predictions for nonscalar order parameters would immediately rule out the single scalar order parameter with lattice anisotropy, thus demonstrating the power and importance of a purely macroscopic approach.

Now we discuss our choice of the class of order parameters considered in this note. There is no experimental indication of any long-range magnetic order coexisting with superconductivity in the new materials close to the normal superconducting transition. Only at much lower temperatures (of order 2 K) a phase transition to a state, where antiferromagnetism and superconductivity coexist, has been observed. Therefore we conclude that the new materials have most likely spin singlet pairing. From this observation and the fact that the macroscopic wave function must be antisymmetric (electrons are fermions), it follows immediately that the orbit part of the macroscopic wave function must be symmetric under parity. This in turn rules out the possibility of a polar vector as the orbit part. Thus for tensors up to second rank we have three classes: a scalar (the usual quantity considered for low-temperature superconductors), an axial vector, and a symmetric traceless tensor (also called the deviator). The latter is familiar as an order parameter in the field of liquid crystals[25] and it is well known to contain uniaxial and biaxial nematics (long-range orientational order along one or two directions) as the two possible subclasses.[25,26] We interpret it as resulting from d-wave components in the electronic pairing.

In this note we give explicit formulas for the case of the axial-vector order parameter in a uniaxial environment (crystal lattice symmetry) and indicate in the text which results carry over to the case of the deviator and/or orthorhombic lattices. Explicit results for the latter classes will be given in a forthcoming publication. The generalized GL free energy for the axial-vector order parameter with uniaxial lattice anisotropy is

$$F=F_N+\int dV[1/2\mu_{ijkl}(D_i\psi_k)^*(D_j\psi_l)+\alpha_{ij}\psi_i^*\psi_j + \beta_{ijkl}\psi_i^*\psi_j\psi_k^*\psi_l+\mathbf{H}^2/8\pi]\ , \tag{1}$$

where $D_i=h/i2\pi\nabla_i-2e/cA_i$, $\mathbf{H}=\nabla\times\mathbf{A}$, and where we have for the structure of μ_{ijkl} and α_{ij}

$$\begin{aligned}\mu_{ijkl}=\mu_1\delta_{ij}^{\mathrm{tr}}\delta_{kl}^{\mathrm{tr}}+\mu_2/2(\delta_{ik}^{\mathrm{tr}}\delta_{jl}^{\mathrm{tr}}+\delta_{il}^{\mathrm{tr}}\delta_{jk}^{\mathrm{tr}})\\ +\mu_3n_in_jn_kn_l+\mu_4\delta_{ij}^{\mathrm{tr}}n_kn_l+\mu_5/4(\delta_{ik}^{\mathrm{tr}}n_jn_l+\delta_{jk}^{\mathrm{tr}}n_in_l+\delta_{il}^{\mathrm{tr}}n_jn_k+\delta_{jl}^{\mathrm{tr}}n_in_k)+\mu_6\delta_{kl}^{\mathrm{tr}}n_in_j\ ,\end{aligned} \tag{2a}$$

$$\alpha_{ij}=\alpha_\perp\delta_{ij}^{\mathrm{tr}}+\alpha_\parallel n_in_j\ . \tag{2b}$$

n_i characterizes the direction of uniaxial symmetry and $\delta_{ij}^{\mathrm{tr}}$ projects into the plane perpendicular to n_i: $\delta_{ij}^{\mathrm{tr}}=\delta_{ij}-n_in_j$.

Above T_c fluctuations on the order parameter must be isotropic and the only anisotropy left is due to the lattice structure. Hence for $T>T_c$, μ_{ijkl} and α_{ij} have the form

$$\begin{aligned}\mu_{ijkl}&=\mu\delta_{ij}^{\mathrm{tr}}\delta_{kl}+\mu' n_in_j\delta_{kl}+\mu''/2(\delta_{ki}\delta_{jl}+\delta_{kj}\delta_{il})\ ,\\ \alpha_{ij}&=\alpha\delta_{ij}\ .\end{aligned} \tag{3}$$

Matching at $T=T_c$ yields

$$\mu_1=\mu_4=\mu,\ \mu_6=\mu',\ \mu_2=\mu_5=\mu'',\ \mu_3=\mu'+\mu''\ , \tag{4}$$

$$\alpha_\perp=\alpha_\parallel=\alpha\ . \tag{5}$$

An attractive feature of a tensor order parameter, not possible in the framework of a single scalar order parameter, is that it allows for structural changes in the order parameter within the superconducting phase. As the order parameter becomes more isotropic near the critical temperature, an intermediate transition can take place ($T_c^*<T_c$) where one of the components begins to fluctuate first. In the context of our working example, an uniaxial pseudovector order parameter, this means, say $\alpha_\perp=c_\perp(T-T_c)$ and $\alpha_\parallel=c_\parallel(T-T_c^*)$. For the second rank symmetric tensor this could mean a d-to-s wave and/or biaxial to uniaxial transitions.

Using the abbreviations $\psi_i=\rho_i\exp(i\phi)$, $\rho=(\rho_i^2)^{1/2}$, $\Phi_0=hc/2e$, and $r_i=\rho_i/\rho$ we have for the equations for the Meissner effect

$$A_k+c^2/[16\pi(e\rho)^2](\Omega^{-1})_{kl}(\nabla\times\mathbf{A})_l=\Phi_0/2\pi\nabla_k\phi\ , \tag{6}$$

where $\Omega_{kl}=\mu_{klij}r_ir_j$ and choosing $n_i \parallel z$, the existence of the off-diagonal terms, $\Omega_{xy}=\mu_2r_xr_y$, $\Omega_{xz}=\mu_5r_xr_z/2$, and $\Omega_{yz}=\mu_5r_yr_z/2$ results.

We see clearly that both the current density and the magnetic field acquire off-diagonal components due to the presence of μ_2 and μ_5. The main result for the case of a magnetic field applied perpendicular to the Cu-O planes is summarized in Fig. 1. The measurement of any field in

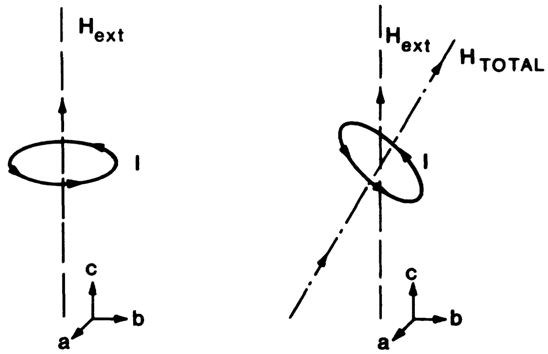

FIG. 1. An external magnetic field is applied parallel to the crystallographic axis c. The left and right figures show the resulting current density (solid line) and the total magnetic field (dash-dotted line) for a scalar and a nonscalar order parameter, respectively. For the scalar the total magnetic field is in the same direction as the external field (dashed line), whereas for the tensor order parameter this is not the case.

the Cu-O planes or any current density perpendicular to them would conclusively rule out a scalar order parameter. The converse is not true, since the off-diagonal contributions might be small. The same conclusion applies for tetragonal and orthorhombic symmetry of the lattice and also for the case of the traceless, symmetric second-rank tensor.

Experimentally one could test these predictions, e.g., via neutron scattering[8] and torque measurements (whose feasibility has been demonstrated recently for a granular sample of the new materials[28]) on well-aligned single crystals.

For a single scalar order parameter with anisotropic lattice we have a simple relation for the product of coherence length and penetration depth in each direction of symmetry; we find for example for an orthorhombic lattice in the clean limit

$$\lambda_1\xi_1=\lambda_2\xi_2=\lambda_3\xi_3=hc/[4\pi e\,|\psi|\,(2\pi|\alpha|)^{1/2}]\ , \tag{7}$$

where $|\psi|$ is the modulus of the order parameter and α measures the relative distance from T_c. Such invariance should hold in the dirty limit too because $\lambda^d\xi^d$ is independent of the mean free path and proportional to the clean limit product $\lambda\xi$.[27] Equation (7) is violated as soon as an order parameter other than a single scalar is considered, although the deviation might be small close to T_c. It is intuitively plausible that (7) does not hold for tensor order parameters since the London penetration depth depends, in contrast to the coherence length, on the condensate density, which varies for an anisotropic tensorial gap as a function of direction. As it is well known from the anisotropic single scalar theory,[8] the upper critical fields in the directions parallel and perpendicular to the Cu-O planes are related to the coherence lengths via $H_{c2\parallel}=\Phi_0/2\pi\xi_\perp^2$ and $H_{c2\perp}=\Phi_0/2\pi\xi_\perp\xi_\parallel$.

For the case of an axial-vector order parameter where the external magnetic field is applied perpendicular to the Cu-O planes we get $H_{c2\parallel}^{(1)}=\Phi_0/2\pi\xi_4^2$, $H_{c2\parallel}^{(2)}=\Phi_0/2\pi\xi_1^2$ with $\xi_4^2=-h^2\mu_4/8\pi^2\alpha_\parallel$ and $\xi_1^2=-h^2\mu_1/8\pi^2\alpha_\perp$. The upper critical field that totally destroys the superconducting state is the largest one of the two mentioned above. However, there is a second upper critical field for a magnetic field applied in one direction, in contrast to the case of a single scalar order parameter. For experimental results this can lead to the interpretation of a value for H_{c2} which is not sharply defined[6] close to T_c, $H_{c2\parallel}^{(1)}\approx H_{c2\parallel}^{(2)}$, if Eq. (5) holds. At lower temperatures one expects an increasing difference between the two.

If one applies a magnetic field inside the plane, one finds that one of the upper critical fields is $H_{c2\perp}^{(1)}=\Phi_0/2\pi\xi_1\xi_6$ where $\xi_6^2=-h^2\mu_6/8\pi^2\alpha_\perp$. For the case $\mu_2=\mu_5=0$ we can evaluate a second critical field analytically and obtain $H_{c2\perp}^{(2)}=\Phi_0/2\pi\xi_3\xi_4$ with $\xi_3^2=-h^2\mu_3/8\pi^2\alpha_\parallel$. For nonvanishing μ_2 and μ_5 the analogue of $H_{c2\perp}^{(2)}$ cannot be obtained analytically. This can be traced back to the fact that (a) the external field makes the system biaxial, and (b) that the terms μ_2 and μ_5 couple spatial variations in the plane and perpendicular to the plane.

The upper critical fields have been derived from the linearized GL equations assuming that for a given direction the critical fields are nearly equal and so the nonlinearities are simultaneously neglected. If this is not so, one must take into account that the component associated to a smaller upper critical field disappears in the presence of the component related to the maximum upper critical field which destroys superconductivity. The corresponding equation contains a nonlinear cross coupling to the other fields and this leads to an effective renormalization of the critical temperature. Consequently the smaller upper critical field involves this effective renormalized temperature $T_c'<T_c$. Such an effect might have been experimentally observed in Fig. 2 of Ref. 7. It seems to us that this phenomenon is very similar to the field-induced phase transitions observed in the superfluid phases of ^{3}He. An alternative scenario for Fig. 2 of Ref. 7 follows once nonlinearities are neglected simultaneously and there are two intrinsic critical temperatures in the GL equations as previously explained. These two scenarios lead to different consequences whose study will be given elsewhere.

Finally, we briefly indicate that the changes in the vortex and defect structure are drastic as one goes from a scalar to an axial-vector order parameter. In a classical type-II superconductor the only possible defects are vortex lines of strength quantized in units of the flux quantum $\Phi_0=hc/2e$. Assuming as above constant modulus for the order parameter, we predict two additional classes of defects. The first one is disclinations in r of half-integer strength. The second class corresponds to point defects in the director field r similar to those observed in uniaxial nematic liquid crystals.[29] A cross coupling between spatial variations of the director and the modulus, which has been found before for liquid crystalline phases, superfluid ^{3}He and neutron star matter,[30] leads to changes in the core structure. For the deviator two cases emerge; for the one equivalent to uniaxial nematics the defect structure is identical to the one for the axial vector, where for the "biaxial nematic" case it is different. The derivation of these results is based on homotopy groups and will be given elsewhere.

In conclusion, we have demonstrated that by careful evaluation of observable quantities such as the structure of the upper critical fields, the anisotropy of the Meissner effect along with the possibility of additional types of defects, a scalar order parameter can be distinguished from a tensor order parameter. The unequivocal experimental observation of any one of the predictions made here for a more structured order parameter would rule out a single scalar order parameter in the high-T_c materials.

Using the Ginzburg criterion[31,32] we can easily show that mean-field theory (i.e., no fluctuations) is applicable. We find, however, that Ginzburg's criterion is not as well satisfied for the high-T_c materials as it is for the classical low-temperature superconductors. Universality arguments indicate that measurements of critical exponents can distinguish between a scalar and a nonscalar order parameter. It will also be easier to observe the critical exponents in the new materials, since the critical regime is larger. Corresponding experimental results will then in turn stimulate further theoretical work to distinguish between the various options for nonscalar Ginzburg-Landau theories. Although we have studied here a tensor order parameter having a single phase, we mention the possibility of more than one phase leading to an internal Josephson behavior.

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