Possible Pressure Effect for Superconductors

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Abstract

We make an estimate of the possible range of $\Delta T_c$ induced by high-pressure effects in post-metallic superconductors by using the theory of extended irreversible/reversible thermodynamics and Pippard’s length scale. The relationship between the increment of the superconducting temperature and the increase of the pressure is parabolic.

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1 Introduction

The investigation of electron motions in polar crystal began 60 years ago [1]. Their influence in the phenomenon of pressure-enhanced superconductivity has attracted the attention of many researchers [2]. The work reported in [2] was limited to the study of low-temperature superconductivity in periodic systems. Recently, related studies of High-Temperature Superconductivity (HTS) in the cuprates [3] and MgB$_2$ [4-5] became the focus of attention.

It was the unusual high pressure effect on $T_c$ observed in (La, Ba)$_2$CuO$_4$ that first signaled the significance of cuprates in the search for high $T_c$ and led to the discovery of YBa$_2$Cu$_3$O$_7$ and related compounds. Meanwhile, as reported in Ref. [5] for MgB$_2$, the superconducting transition temperature $T_c \sim M^{\alpha_B}$, with $\alpha_B = 0.26$ ($M$ is the isotope mass) confirms the isotope relation for the important role that phonons play in traditional superconductors (which the BCS theory could be applied for). In addition, band structure calculations indicate a rather isotropic electrical transport instead of the very layered appearance of honeycombed boron and hexagonal magnesium networks in the material [6]. These facts support our present approach which will be described below. For simplicity, we will not consider the effect due to pressure-induced-charge-concentration in this study since it is beyond our present approach and interest.

Theoretically, from the theory of Quantum Mechanics [7], which in general treats very-small-scale particles/waves, however, we have the pressure defined by $p = F/A$ with $F = (\partial H/\partial \lambda)_{nn} = \partial E_n/\partial \lambda$, where $\lambda$ is a parameter on which the effective Hamiltonian $H$ (and therefore the energy eigenvalues $E_n$) depends. Here, $H$ comes from the pressure effect, $A$ is the area which is normally calculated with an artificial surface-cut across the characteristic domain., $F$ is the force acting upon $A$; $n = 0, 1, 2, \cdots$. The kinetic pressure from the (mostly spherical) particles

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acting upon $A$ is usually presumed equal to the hydrostatic pressure or the average of the trace from the stress tensor (on $A$) in thermodynamic equilibrium so that we can interpret the measurements easily and conveniently [8-9]. The trouble along this thinking is: how to find this $H$ directly so that we could interpret the pressure-effect easily?

Griessen [10] discussed a number of models which tried to explain the effect of pressure on the equilibrium phase transition of superconducting properties [10-13]. A theoretical approach to the pressure-effects for cuprates was recently discussed in [14] using a BCS-type mean field approach. Unfortunately most of the detailed structures of the high-pressure phases are not yet known.

To the best of our knowledge, the role of the pressure-gradient, which may drive electrons and/or phonons into a flow before the final equilibrium is reached, in the study of kinetic or non-stationary effects in superconductors is seldom mentioned [6,15]. In this Letter, we shall use the idea of Extended Reversible/Irreversible Thermodynamics (ER/IT)[8] to estimate the possible range of $\Delta T_c$ from the pressure-gradient resulting from the effect of uniaxial stress on $T_c$ in superconductors. In the frame of ER/IT, thermodynamic functions or potentials can be functions of the gradient of thermodynamic state variables as well as of thermodynamic state variables only [8-9].

Once the external pressure is imposed upon the sample, due to the highly anisotropic and heterogeneous feature of the material, there will be a net pressure- or density-gradient acting upon electrons (gases) inside a presumed very-small slender domain (considering the pressure from both longer sides of it) which may be bounded by near-by phonons. The unbalanced pressures imposed upon the inlet and outlet of a nano-channel (along which the electron gases pass through) in our consideration can thus give the pressure- or density-gradient and then drive the electron-gas flow. Our interests here are those stationary states or steady electron-gas flows so that we could consider the nearly equilibrium properties.

We assume the BCS [16] theory could be extended to the situations after the samples are imposed upon high pressures (they are already superconducting for whatever mechanism which we have no interests in investigating here) and in certain sense still valid here [10] for some periodic microdomains and the pressures or uniaxial stresses imposed on the samples can influence the passing through of the electron-pairs so that the superconductivity shifts with $T_c$. The overall effects of external stresses on phonons are presumed to be completely transmitted to those electron-pairs. Thus, we only need to consider the influences to electron-pairs from those imposed pressure or stress fields within their limits [17-18]. We must also assume, however, that there were no created micro- or nano-cracks inside during the imposing of the high pressures in the cuprates for previous measurements so that our approach described below could be well applied.
2 Formulation

In a strict analysis of transport problems it is seldom possible to deal solely with average properties such as the mean velocity and the mean energy, and it is necessary to determine the distribution of the particles both as regards position and their velocities. The fundamental equation determining the distribution function is an integro-differential equation known as the Boltzmann equation [17]

\[
\frac{\partial f}{\partial t} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} = G - L,
\]

where \( G, L \) means gain and loss of the number of electrons due to collisions; \( \mathbf{F} \) is the external field force, \( m \) is the mass. If the electron gas is dilute enough, then we can neglect the collisional integral (r.h.s. term of above equation). Furthermore, by considering only the stationary state or final equilibrium state, we can omit the first term in the left-hand-side of the above equation. We also assume that the contribution from \( \mathbf{F} \) is much weaker than the pressure-induced (into the velocity) term in the above equation. The complex boundary-interactions, e.g. electron-phonon scattering along the boundary, are also excluded.

Using an extension of BCS theory, a general expression has been derived [19] \( T_c = 0.25\tilde{\Omega}(e^{2/\eta} - 1)^{-1/2} \), where \( \tilde{\Omega} = \langle \Omega^2 \rangle^{1/2} \) stands for the characteristic phonon frequencies and sets the energy scale (\( \sim \) the Debye temperature for certain cases), \( \eta \) is the strength of the electron-phonon coupling. The weak-coupling BCS formula [16] gives \( T_c = \omega_D \exp\{1/[N(E_F)\lambda]\} \), where \( \lambda \) is the attractive interaction due to the exchange of phonons, \( N(E_F) \) is the Density of States (DOS) at the Fermi energy \( E_F \), \( \omega_D \) is the energy scale. The direct relations between \( \Delta T_c \) and \( \Delta p \) [20], however, cannot be easily obtained up to now [6,14].

One of the crucial parameters for our approach is related to the density-gradient driven speed (say, \( \bar{v} \))[9,21] or flux of electrons in the microdomain when the phonons are stiffened by the imposing pressure in the prescribed direction. This flux will then be linked to the resistivity, and thus finally \( T_c \) as the equilibrium is reached. There is, however, one fundamental length : the extended Pippard’s coherence distance \( \xi_0 \), which is associated by means of the uncertainty principle with the energy \( kT_c \) [22],

\[
\frac{\hbar v_F}{\xi_0} \sim kT_c.
\]

\( \hbar = 1.0546 \times 10^{-34} \) J s, \( k = 1.38 \times 10^{-23} \) J K\(^{-1}\). This length scale can give us clues about the pressure-induced correlation length which is the distance beyond which the momenta are essentially uncorrelated.

We now let \( T_c \) be a function of \( dp/dx \) as well as \( p \), which is valid by the assumptions of Extended Reversible/Irreversible Thermodynamics [8-9,21] that the final state is not far from the statistical equilibrium. \( x \) is linked to the effective distance for the pressure imposed and within this range the electron-gas flow is weakly compressible [23] and fully-developed.

Furthermore, as mentioned above, the BCS theory is presumed also valid over the region we considered (already post-metallic) after the imposing high-pressure. Then, by considering the
equilibrium limit of the evolutional electron(pair)-gas motion (characterized by $\bar{v}$), and taking the limit of $\bar{v} \sim v_F$, besides, as $\bar{v} = K_a c$ ($c$ : the sound speed $\equiv \sqrt{(dp/d\rho)}|_s = \sqrt{dp/dx \cdot dx/d\rho}$; the latter relation is under the ER/IT formulations) or $\bar{v} \sim K_0 |(dp/dx)|^{0.5}$ (to certain limit of the flux [9,21]), so with (1), $T_c$ may be linked to $|dp/dx|$ for some situations [24]. This consideration can be understood that there is certain resonance existing between the propagating phase-speed of the interface of electron pairs and the phonons. This resonance is induced by the possible localization due to the dynamical environment near-by. From equation (1) with the effective length scale being $O(\xi_0)$ and by considering the data re-arrangement, i.e. $\Delta T_c$ (K) vs. $\Delta p$ (GPa), we could obtain the net increase of $T_c$ (K) due to the imposed pressure $p$ (GPa) by

$$\Delta T_c = \kappa (\Delta p)^{0.5},$$

where $\kappa$ is strongly dependent on $dx/d\rho$ for unit width ($\rho$ is the density; we take the average of long-range correlations). This expression might be extended and thought of an possible limit for those anisotropic cases which are common in HTS cuprates or other type of superconductors [24-27]. Note that once the moving particles or pairs are composed of holes, the sign convention for the density $\rho$ and the (local) coordinate $x$ (as the coordinate system for quasi-one-dimensional electron motion has been prescribed and fixed) should be thus changed as the hole motion is opposite to that of the electron. Meanwhile, considering the definition of the concentration and the pressure of particles (pairs), the sign convention will be reversed once the electron is replaced by the hole. It means if $dp/dx$ is positive for the motion of electrons then $dp/dx$ is negative for that of holes. The subsequent result is that $\Delta T_c$ could be either positive or negative!

3 Results and Discussions

We obtain an $ad$ $hoc$ estimate of the limit of $\Delta T_c$ (K) vs. $\Delta p$ (GPa) from equation (2) for some superconductors which could be possibly extended to HST if they are already post-metallic (thus the BCS theory then applies for [6]) under very-high pressures. This approach might be universal for similar superconductors and independent of the experimental procedures (except the selection or tuning of $\kappa$ [9,27]). This is because, at least in part, $T_c$ is related to the equilibrium phase transition which in general has no close link to the flow-history, and partly, $|dp/dx|$ may change the mean free path ($\lambda$) of the electrons but the latter is independent of $T_c$ [28] in most cases. The presence of inequivalent layers may lead to more complicated $\Delta T_c$ v.s. $\Delta p$ curves.

The interesting thing is : our result has the similar trend with that of [6] and [29] obtained from the series of measurements at increasing and decreasing pressure, for different types of superconductors, respectively. In fact, the granular limit of superconductivity under very high pressure could be reached once the perovskite structure of HTS suffers considerable changes [24]. If the resonance induced by the possible localization is relaxed due to a delocalization then the power (of $\Delta p$) shown in the equation of (2) will not be 0.5! Our approach will not be valid, however, once the dissipation produced by the pressure-driven flow of electron gas is too large so that the basic assumptions of the $Extended$ $Reversible/Irreversible$ $Thermodynamics$ [8-9] being
violated. In that case, we cannot predict in which way $T_c$ starts to decrease (or increase) even the pressure still increases. Perhaps, the approach of pressure-induced charge transfer (effect) [14,30] might help us understand the HTS behavior for this kind of large-dissipation flow [31] of electron gases. We shall investigate more complicated problems [32] in the future.

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