DILUTE METALS: SUPERCONDUCTIVITY, CRITICAL CURRENTS,
MAGNETIC PROPERTIES

V. N. Bogomolov
A. F. Ioffe Physical & Technical Institute,
Russian Academy of Science,
194021 St. Petersburg, Russia

(Dated: March 23, 2022)

Properties of oxides are interpreted as a result of existence of the virtual sublattices formed by the atomic quantum states. An infinite cluster with the superconductivity of the Bose-Einstein condensate kind can be formed in the ground state sublattice at certain oxygen atoms concentration in the effectively diluted system of metal atoms (above the percolation threshold). Then the electron pairs concentration $n/2$ can be much less than the metal atoms concentration $N$ in the oxide. The similar situation takes place in metals with superconductivity of the BCS type. Above the percolation threshold the superconductivity $T_c$ may be limited by the magnetic properties of the oxygen $2p^6$ quantum state sublattice. Data on the critical current density allows us to estimate the electronic density $n/2$ and to obtain an information on the superconductivity nature.

PACS numbers: 71.30.+h, 74.20.-z, 74.25.Jb

I. A structure of the metal oxides can be conceived as a superposition of four virtual sublattices formed by (i) - $yN$ metal atoms in the ground state, (ii) - $(1-y)N$ metal ions, (iii) - $(1-y)N$ O$^{2-}$ ions, and (iv) - $yN$ paramagnetic oxygen atoms $\tilde{\text{O}}$. These sublattices are related to the quantum states of the metal and oxygen atoms and to certain physical properties of the oxides. The value $N$ is an actual concentration of the metal atoms in the oxide, while the value $y$ is a portion of the ground state in the superposition of the ground and ionized states of the metal atoms. Such approach allows us to make several conclusions on superconducting, magnetic and ferroelectric properties of the oxides.

II. An actual density $n$ of superconducting electrons can be estimated from the data on the critical current density $j_c$, if we assume that $kT_c \sim mv_c^2/2$ and $j_c \sim euv_c$, where $v_c$ is the current carriers critical velocity. The current critical density $j_cL$ takes values (at $T$ and $H$ about zero) within the range $(10^5 - 10^6)$ A/cm$^2$ for low-temperature superconductors (LTS) (Nb-Ta with $T_{cL} \sim 10K$ $\tilde{\text{E}}$ $\tilde{\text{E}}$). At similar conditions, $j_{cH}$ reaches the magnitudes $(10^7 - 10^8)$ A/cm$^2$ for high-temperature superconductors (HTS) (for instance, YBa$_2$Cu$_{3-x}$O$_7$ with $T_{cH} \sim 90K$ or layers of CaCu$_2$O$_2$ intermitted with Ba$_{0.9}$Nd$_{0.1}$CuO$_{2+x}$ layers with $T_{cH} \sim 60K$ $\tilde{\text{E}}$ $\tilde{\text{E}}$).

At $m = 2.5m_e$, $n_L = 5.7 \times 10^{18}$cm$^{-3}$, $n_H = 1.8 \times 10^{20}$cm$^{-3}$.

It follows from the BCS model for metals with $N \sim 10^{22}$cm$^{-3}$ that $n_L/2 \sim N(kT_{cL}/E_F)$, where $(kT_{cL}/E_F) \sim 10^{-4}$. In the case of HTS oxides it is necessary to have a parameter $(kT_{cH}/E_F) \sim 10^{-2}$ in the BCS theory that formally is realistic for $E_F \sim 1$eV. Then the critical current density $j_{cH} \sim (kT_{cH})^{3/2}/E_F$.

However, one can try the model of Bose-Einstein condensing (BEC) hard electronic pairs in both of cases as well. Then $kT_{cB} = 3.3 \times (h/2\pi)^2(n/2)^{2/3}/2m^*$ and $kT_{cBL} \sim 12K$, while $kT_{cBH} \sim 120K$. Both of temperatures are near to experimental magnitudes (10K and 90K) in this version too. In other words, knowledge of only the transition temperature magnitude is not suffice to discriminate between the BCS and BEC mechanisms.

Data on critical currents can give an additional information on the nature of transition into the superconducting state. In the BEC case the current $j_c \sim (kT_c)^2$ and all electrons participate in it unlike the BCS metal case, where their participation ratio is $(kT_c/E_F)$. (The condition $j_c \sim (kT_c)^2$ corresponds to the relation $kT_{cB} \sim kT_{cF} \sim E_F$). This fact excludes BEC as a mechanism of the superconducting transition for metals, but can be an argument for applicability of this model at least in a restricted region taking into consideration that metals in oxides exist in an diluted state ("chemical" dilution $\tilde{\text{E}}$). Certainly, a real hundredfold dilution is not accessible, but an arbitrary effective dilution degree can be reached in the infinite cluster of metal atoms ground states. New collective properties appear, when an average effective density of ground states exceeds the percolation threshold $y$ for a density of quantum states per metal atom (Fig.1). The parameter $y$ is proportional to the similar parameter $x$ in the chemical formula YBa$_2$Cu$_3$O$_{6-x}$.

Above the percolation threshold for forming of the superconducting state, the ground states associate into the infinite cluster with the electronic pair density $n_e/2$, where $0 < n_e < N$ that leads to forming of the superconducting state. The metal atoms ground states concentration in the cluster (the order parameter) grows with $y$, while the effective interatomic distances and effective electron masses decrease (Fig.1). Tunneling of the atomic electron pairs can lead to their BEC. However,
further increase of $n_c$ leads to a drop of the electronic pair binding energy and, at some magnitude of $n_{cc}$, it would be favorable for the cluster electrons to transit into the Fermi state, i.e. into the metal or insulator state. The BEC - BCS crossover condition $\Delta \sim 5.5kT_{cB}$ can be estimated setting the electron energy density in metal and in the Bose-condensate equal one to another: $E_F^c \sim 2.87(h/2\pi)^2n_{cc}^{5/3}/m \sim \Delta n_{cc}/2$. An increase of $x$ up to 8 (or $y$ up to 1) transforms the oxide YBa$_2$Cu$_3$O$_{8-x}$ into the metal YBaCu. Only Cooper’s pairs remain, while the most of electrons are in the Fermi degeneracy state in result.

Perhaps, such evolution of a system can take place in the noble gas (NG) condensation process [8]. The concentration of virtually excited two-atom molecules with two paired electrons increases with compression, and the infinite cluster of chains of divalent particles is formed in the NG insulator (atoms in the ground state) above the percolation threshold: an irregular 3D conducting (superconducting) “cobweb” is created [6]. Such a “cobweb” structure of the superconducting cluster “gossamer” [9] can exist in HTS as well as it has been told above. Metallization of molecular condensates can be a useful model for study of the HTS materials. S and O$_2$ are metallized by now [10, 11]; their transition temperatures $T_c$ are respectively $\sim 17K$ and $0.6K$. Low temperatures can be due to strong local magnetic fields of these paramagnetic atoms ($r_O = 0.45\text{Å}; r_S = 0.81\text{Å}; r_{Sc} = 0.92\text{Å}$ [12]). Similar effect of the oxygen atoms can limit $T_c$ of the HTS oxides as well (Fig.1).

III. Some physical property can be traced back to any of 4 sublattices of quantum states. Sublattice (iv) is based on quantum ground state of O (2p$^5$) atoms, which have two parallel spins. A presence of parallel spins determines paramagnetism of the O$_2$ (2p$^2 - 2p^6$) or (O$^{2+}$$-$$O^{2-}$) molecule. Similar molecule-like state exists in the form of dynamically equilibrium bonds ($Me^0 - O^0$) -- ($Me^{2+} - O^{2-}$) in oxides. Below the percolation threshold for superconductivity, there are almost 10$^{22}$cm$^{-3}$ oxygen atoms in the oxide; their paramagnetism is only partly compensated by metal atoms ($Me^{2+} - O^{2-}$). Above the percolation threshold $y_p$, magnetic properties of the virtual sublattice of the oxygen paramagnetic states turn to be compensated by increasing collective properties of electrons of the cluster with increase of $y$ (Fig.1). Coexistence of superconductivity and magnetism manifests a relation between physical properties and quantum states of atoms in oxides. Synthesis of materials free of atoms, which have real or at least virtual magnetic states, can be a perspective way of the transition temperature rise. (For instance, ($M^1$)$_x$(M$^2$)$_{1-x}$B$_6$ with quantum states 2p$^0 - 2p^6$ of B atoms in B$_6$ molecule or B$^{1+} - B^{3-}$ bonds). Sulphides and selenides instead of oxides may be preferable for HTSC too.

[1] V.N.Bogomolov, e-print http://xxx.lanl.gov/abs/cond-mat/0411574 Percolation Threshold. Techn. Phys. Lett., 21, No. 11, 928 (1995).
[2] G.Otto, E.Saur, H.Witzgall, Journ. Low.Temp. Phys. 1, 19 (1969).
[3] G.Bogner, Electrotechn. Zs. 89, 321, (1968).
[4] B.Dam at al., Nature 399, 439 (1999).
[5] G.Balestrino at al., Phys. Rev. Lett. 89, paper 156402 (2002).
[6] V.N.Bogomolov, "Metallic xenon. Conductivity or superconductivity?" Preprint 1734, A.F.Ioffe PTI St-Peterburg (1999); e-print http://xxx.lanl.gov/abs/cond-mat/9902353 /9912034.
[7] V.N.Bogomolov, Metallization of Molecular Condensates under Pressure as a Result of a Transition through the
 FIG. 1: Schematic picture of some oxides properties

$y$ is the effective number of ground states per atom in the oxide;

$P(y)$ is the effective number of ground states per atom of the metal in the superconducting cluster;

$M$ is the total magnetic moment of oxygen atoms $2p^4$ states in the oxide;

$y_p$ is the percolation threshold for forming of the infinite superconducting cluster;

$\Delta$ is the electron pair binding energy. $\Delta_c \sim 5.5kT_c$;

$x$ is the parameter in the chemical formula $YBa_2Cu_3O_{8-x}$. 