



THE PHYSICS OF METALS AND METALLOGRAPHY

English Translation of Fizika Metallov i Metallovedenie

Editor-in-Chief Vladimir V. Ustinov

http://www.maik.ru

A Comprehensive Journal Containing Theoretical, Experimental, and Applied Studies on Various Metals, Alloys, and Metal Compounds Russian Academy of Sciences



MAUK "HAYKA/INTERPERIODICA" PUBLISHING

MAIK "Nauka/Interperiodica" Publishing

is pleased to present to the international scientific community simultaneous Russian- and English-language publication of the journals of the Russian Academy of Sciences

MAIK "Nauka/Interperiodica" 2002 volumes include the following titles:

- Computational Mathematics and Mathematical Physics
- · Doklady Earth Sciences
- · Doklady Mathematics
- · Entomological Review
- · Eurasian Soil Science
- · Geochemistry International
- · Geology of Ore Deposits
- · Geomagnetism and Aeronomy
- · Geotectonics
- · Herald of the Russian Academy of Sciences
- · Izvestiva, Atmospheric and Oceanic Physics
- · Izvestiya, Physics of the Solid Earth
- · Journal of Communications Technology and Electronics
- Journal of Computer and Systems Sciences International
- Journal of Ichthyology
- · Laser Physics
- · Oceanology

- · Paleontological Journal
- · Pattern Recognition and Image Analysis
- · Petroleum Chemistry
- Petrology
- · Polymer Science, Series A
- · Polymer Science, Series B
- · Polymer Science, Series C
- · Physics of Particles and Nuclei · Proceedings of the Steklov Institute of Mathematics
- · Russian Journal of Inorganic Chemistry
- · Russian Journal of Mathematical Physics
- · Russian Journal of Physical Chemistry
- Russian Metallurgy (Metally)
- · Stratigraphy and Geological Correlation
- · Studies on Russian Economic Development
- The Physics of Metals and Metallography
- Thermophysics and Aeromechanics*

- · Applied Biochemistry and Microbiology
- · Automation and Remote Control
- · Biochemistry (Moscow)
- Biology Bulletin
 Colloid Journal
- · Combustion, Explosion, and Shock Waves*
- Cosmic Research
- · Differential Equations
- Doklady Biochemistry and Biophysics
 Doklady Biological Sciences

- Doklady ChemistryDoklady Physical Chemistry
- · Fluid Dynamics*
- Functional Analysis and Its Applications*
- Glass Physics and Chemistry
 High Energy Chemistry
- · High Temperature
- · Human Physiology
- Inorganic Materials
- Instruments and Experimental Techniques
- · Journal of Analytical Chemistry
- Journal of Applied Mechanics and Technical Physics*
- Journal of Evolutionary Biochemistry and Physiology Journal of Mining Science*
- · Journal of Structural Chemistry*
- Kinetics and Catalysis

- Thermal Engineering

Please direct all inquiries about the above journals to: INTERPERIODICA, P.O. Box 1831, Birmingham, AL 35201-1831. For faster service call toll-free (800) 633-4931 or (205) 995-1567 (outside US and Canada). Fax: (205) 995-1588, E-mail: interperiodica@ebsco.com

- · Lithology and Mineral Resources
- Mathematical Notes*
- Microbiology Molecular Biology
- Motecular Biology
 Problems of Information Transmission
 Programming and Computer Software
 Protection of Metals
- Radiochemistry
- Russian Chemical Bulletin*

- Russian Chemical Butelin
 Russian Journal of Applied Chemistry
 Russian Journal of Bioorganic Chemistry
 Russian Journal of Coordination Chemistry
 Russian Journal of Developmental Biology
 Russian Journal of Ecology

- · Russian Journal of Electrochemistry
- · Russian Journal of General Chemistry
- Russian Journal of Genetics
- Russian Journal of Marine Biology
- Russian Journal of Nondestructive Testing
 Russian Journal of Organic Chemistry
- Russian Journal of Plant Physiology
- · Russian Microelectronics
- Siberian Mathematical Journal*
- Solar System Research
- Theoretical and Mathematical Physics*
- · Theoretical Foundations of Chemical Engineering
- Water Resources
- * The journal is produced under contracts between Plenum Publishing and the Russian Academy of Sciences and/or its divisions,the institutes, and the editorial boards, and under contract and subcontract between Kluwer Academic/Plenum Publishers and MAIK "Nauka/Interperiodica"

Please direct all inquiries about the above journals to: Kluwer Academic/Plenum Publishers, P.O. Box 322, 3300 AH Dordrecht, The Netherlands. Phone: (31 78) 657-6000. Fax: (31 78) 657-6474, E-mail: orderdept@wkap.nl

- · Acoustical Physics
- · Astronomy Letters
- · Astronomy Reports
- Crystallography Reports · Doklady Physics JETP Letters
- Journal of Experimental and Theoretical Physics

- Optics and Spectroscopy*
- · Physics of Atomic Nuclei
- · Physics of the Solid State Plasma Physics Reports
- Semiconductors
- Technical Physics
- Technical Physics Letters

Please direct all inquiries about the above journals to: **American Institute of Physics**, Circulation and Fulfillment Services, Suite 1NO1, 2 Huntington Quadrangle, Melville, NY 11747-4502 USA. Tel. (516) 576-2270, 1-800-344-6902. Fax: (516) 349-9704, E-mail: subs@aip.org

^{*} Thermophysics and Aeromechanics is only distributed by MAIK "Nauka/Interperiodica" Publishing

^{*}Optics and Spectroscopy: Optical Society of America, 2010 Massachusetts Ave., NW, Washington, DC 20036-1023, Atin.: Publications Department. Tel. (202) 223-8130, (800) 582-0416. Fax: (202) 416-6140.

The Physics of Metals and Metallography

(Fizika Metallov i Metallovica Come

ISSN: 0031-9.53

Editor-in-Chief **Vladimir V. Usti**nov

Corresponding Member of the Russian Academ. Director of the Institute of Metal Physics, Ural Division of the Research Education Services

> Address for correspondence. ul. S. Kovalevskoi 18, Ekaterinburg, 620219 R.... Phones: 7 (3432) 74-0230, 7 (3432) 49-9102 Fax: 7 (3432) 74-5244 E-mail: fmm@imp.uran.ru

Deputy Editors-in-Chief

Yurii A. Izyumov

Corresponding Member, RAS, Professor,

Vadim M. Schastlivtsev

Corresponding Member, RAS, Professor, Institute of Metal Physics, Ekaterinburg, Russia Institute of Metal Physics, Ekaterinburg, Russia

Executive Editor-in-Chief

Yurii N. Gornostyrev

Professor, Institute of Metal Physics, Ekaterinburg, Russia

EDITORIAL BOARD

Yurii I. Chumlyakov

Dr. Sci. (Phys.--Math.), Siberian Physico-Technical Institute. Torusk, Russia

Aleksandr V. Korolev

Cand Sci. (Phys.-Math.). Institute of Metal Physics, Ekaterinburg, Russia

Lev G. Korshunov

Dr. Sci. (Eng.), Institute of Metal Physics, Ekaterinburg, Russia

Vyacheslav V. Marchenkov

Cand. Sci. (Phys.-Math.). Institute of Metal. Physics, Ekaterinburg, Russia

Dzhalal A. Mirzaev

Professor, Dr. Sci. (Phys.-Math.), State Technical University, Chelyabinsk, Russia

Nikolai V. Mushnikov Cand. Sci. (Phys.–Math.). Institute of Metal Physics, Ekaterinburg, Russia

Valentin E. Naish

Dr. Sci. (Phys.-Math.), Institute of Metal Physics, Ekaterinburg, Russia

Vladimir V. Nikolayev

Cand. Sci. (Phys.-Math.), Institute of Metal Physics, Ekaterinburg, Russia

Sergei G. Ovchinnikov

Dr. Sci. (Phys.-Math.), Kirensky Institute of Physics, Krasnoyarsk, Russia

Vladimir G. Pushin

Dr. Sci. (Phys.-Math.), Corresponding Member, Russian Academy of Natural Sciences, Institute of Metal Physics, Ekaterinburg, Russia

Valerii V. Rybin

Professor, Dr. Sci. (Phys.-Math.), Prometei Central Research Institute of Structural Materials, St. Petersburg, Russia

Viktor V. Sagaradze

Professor, Dr. Sci. (Eng.), Institute of Metal Physics, Ekaterinburg, Russia

Vladimir G. Shavrov

Dr. Sci. (Phys.–Math.), Radio Engineering Institute, RAS, Moscow, Russia

Mstislav A. Shtremel'

Professor, Dr. Sci. (Phys.-Math.), Moscowa Institute of Steel and Alloys, Russia

Vladimir P. Silin

Corresponding Member, RAS, Lebedev Instof Physics, RAS, Moscow, Russia

Staff Editor Eduard P. Molchanov

Editor of the English Translation Vsevolod I. Okulov, Dr. Sci. (Phys.-Math.) and Nikolai V. Mushnikov, Cand. Sci. (Phys.-Math.)

SPONSORS OF THE RUSSIAN VERSION OF THE JOURNAL

Ekaterinburg Nonferrous Metal-Working Plant

SCOPE

The Physics of Metals and Metallography (Fizika Metallov i Metallovedenie) was founded in 1955 by the USSR Academy of Sciences. Its scienting involves the theory of metals and metal alloys, their electrical and magnetic properties, as well as their structure, phase transformations, and principal π : ical properties. The journal publishes scientific reviews and papers written by experts involved in fundamental, application, and technological studie annual volume of publications amounts to 250 papers submitted from 100 leading national scientific institutions. The Physics of Metals and Metallo. indexed in World Translations Index.

SUBSCRIPTION OFFICE

INTERPERIODICA P.O. BOX 1831, BIRMINGHAM, AL 35201-1831 USA PHONE: (800) 633-4931: (205) 995-1567 (outside US and Canada) EAX: (205) 995-1588

PUBLISHER

INTERNATIONAL ACADEMIC PUBLISHING COMPANY "NAUKA/INTERPERIODICA" PROFSOYUZNAYA UL. 90, MOSCOW, 11799 F PHONE: 7 (095) 336-1600; FAX: 7 (095) 336-066 E-mail: compmg@maik.ru Web Site: http://www.maik.ru

SUBSCRIPTION PRICES (2002, Volumes 93/94, 12 + 2 Supplementary issues)

US \$3290.00 (North America), \$3790.00 (elsewhere). A 5% discount is given on 2-year orders. Subscriptions may be entered at any time. Orders may at agencies or directly. There is a 5% discount to all subscription agencies. Cancellations not allowed except for duplicate payment. Prepayment Advance payment required in US\$/US bank. MasterCard/Visa accepted. Make checks payable to The Physics of Metals and Metallography or Inter-The Physics of Metals and Metallography (ISSN: 0031-918X) is published monthly for (US dollars) \$3290.00 (North America), outside North \$3790.00 per year by MAIK "Nauka/Interperiodica", 5724 Hwy. 280 East, Birmingham, Alabama 35242-5724 USA. Periodical postage paid at E Alabama, and additional mailing offices. POSTMASTER: Send address changes to The Physics of Metals and Metallography. P.O. Box 183 Birmingham, Alabama 35201 USA,

> The journal was founded in 1955. Original Russian Edition Copyright © 2002 by the Russian Academy of Sciences,
> Division of General Physics and Astronomy, and the Ural Division of the Russian Academy of Sciences,
> English Translation Copyright © 2002 by MAIK "Nauka/Interperiodica" (Russia). Printed in the USA by Pleiades Publishing, Inc.

PREFACE

The Euro-Asian Symposium "Trends in Magnetism" (EASTMAG 2001), organized by the Institute of Metal Physics, Russian Academy of Sciences, was held in the Ural Cultural Center, Ekaterinburg, Russia, from February 27 to March 2, 2001, under the motto "At the Border of Two Continents, at the Boundary of Centuries".

The purpose of the symposium was to provide an opportunity for scientists from all over the world to meet at the border of Europe and Asia to discuss recent advances in the study of the physics of magnetic materials. The EASTMAG symposia are aimed at continuing and developing the best traditions of the former All-Union Conferences on Magnetism that were organized previously in the former Soviet Union. EASTMAG 2001 was devoted to the memory of academician S.V. Vonsovsky, who made a great contribution to magnetism, and the development of science in Russia. Two hundred fifty participants from 15 countries took part.

Three supplementary issues of volumes 91, 92, and 93 of *The Physics of Metals and Metallography* contain the papers presented at the symposium and accepted for publication through a review process determined by *The Physics of Metals and Metallography*. Supplementary issues nos. 1 of vols. 91–93 consist of nine chapters devoted to the physics of new magnetic materials: multilayers and films, nanocrystalline and amorphous materials, manganites, hard magnetic materials, domain structures and domain walls, resonances, excitations, waves, model systems and computations, novel scientific instrumentation, and finally, magnetic alloys and compounds.

On behalf of the organizing committee, I would like to express my sincere gratitude to all the participants of the symposium for their excellent contributions and to the authors who presented papers for the proceedings. I hope that the proceedings provide valuable information on the physics of magnetic phenomena and technology of magnetic materials.

March 2001 Vladimir Ustinov EASTMAG 2001 Chairman

Contents

IBUEL O	3. :	Supr	ol.	1.	20	O	2
---------	------	------	-----	----	----	---	---

The samplement is published only in English by MAIK "Nauka/Interperiodica" (Russia). The former of Metals and Metallography ISSN 0031-918X.

Chapter 9. Alloys and Compounds	Chapter	9.	Alloys	and	Compounds
---------------------------------	---------	----	--------	-----	------------------

Antiferromagnetic Intra-Sublattice Exchange Interaction	
Guanghua, N. P. Kolmakova, R. Z. Levitin, A. Yu. Sokolov, and D. A. Filippov	S1
Harman of Local Crystal Fields and Itinerant Magnetism in RNi _{5-r} Cu _r Alloys	
Ermolenko and A. G. Kuchin	S8
of Crystal Field in Metals and Magnetic Anisotropy of Rare-Earth Intermetallides	
= P. Irkhin and V. Yu. Irkhin	S14
Magnetothermal, and Magnetoelastic Properties of $Gd_5(Si_{1.95}Ge_{2.05})$ Magnetostructural Phase Transition	
S. Chernyshov, D. A. Filippov, M. I. Ilyn, R. Z. Levitin, A. O. Pecharskaya, S. Pecharsky, K. A. Gschneidner Jr, V. V. Snegirev, and A. M. Tishin	S19
infer of Interstitial Elements on the Magnetic Anisotropy and Magnetostriction and Elements of Elements on the Magnetic Anisotropy and Magnetostriction and Elements of Elements on the Elements of Eleme	
Tereshina, S. A. Nikitin, V. N. Verbetsky, and A. A. Salamova	S24
Temperature Paraprocess in DyCo ₅	
of A. Borovkova and R. S. Il'yasov	S31
Efect of External Pressure on Magnetism of UCoAl and U _{0.9} Co _{1.05} Al _{1.05}	
Mushnikov, A. V. Andreev, and T. Goto	S35
relationeous and Induced, by Field or Pressure, Magnetic Phase Transitions and Ce ₂ Fe _{17-x} Mn _x System	
G. Kuchin, V. I. Khrabrov, Z. Arnol'd, O. Prokhnenko, A. N. Pirogov, E. Teplykh, I. V. Medvedeva, E. V. Belozerov, G. M. Makarova, Kamarád, and A. S. Ermolenko	S40
Subsystem Magnetization Concentrational and Temperature Dependences In Mn, and Cosubstituted Y ₂ Fe ₁₄ B Intermetallic Compounds	
: V. Kudrevatykh, S. V. Andreev, M. I. Bartashevich, and A. N. Bogatkin	S45
estigation of Magnetic Properties of Compounds of Rare-Earth Metals are from Group in the Range of the Solid-Liquid Phase Transition	
K. Kuvandikov, H. O. Shakarov, D. A. Saifullaeva, and M. K. Salakhitdinova	S48
exactization and Magnetic Anisotropy of Tm and Fe Subsystems in Tm ₂ Fe ₁₇	
i Pirogov, J. Park, Y. Jo, J-G. Park, K. Prokes, S. Wel'yael', C. H. Lee, Kudrevatykh, E. Valiev, V. Kazantsev, and D. Sheptyakov	S54
eagmetism of Ca-3d Metal Laves-Phase Compounds Synthesized at High Pressure	
4. V. Tsvyashchenko, L. N. Fomicheva, M. V. Magnitskaya, V. A. Sidorov, E. N. Shirani, A. V. Kuznetsov, D. V. Eremenko, and V. N. Trofimov	S59
Extetic Properties of a Microinhomogeneous Mn _{0.55} Fe _{0.45} Pd Alloy	
E. Korolyov, N. V. Volkova, N. I. Kourov, and L. N. Tyulenev	S64
ctural and Magnetic Phase Transitions in Shape Memory Ni-Mn-Ga Alloys	
D. Buchel'nikov, A. T. Zayak, A. N. Vasil'ev, T. Takagi, P. Entel', and V. G. Shavrov	S69

Magnetic Properties of a Single Quasicrystal Al _{70.2} Pd _{21.3} Mn _{8.5}	
A. A. Rempel', S. Z. Nazarova, and A. I. Gusev	S74
Magnetism of Geometrically Frustrated Transition-Metal Sulfides: BaVS3 and Related Compounds	
H. Nakamura and M. Shiga	S78
Colossal Magnetoresistivity in Sulfides of $Me_xMn_{1-x}S$ ($Me=Cr$, Fe)	
G. A. Petrakovskii, L. I. Ryabinkina, G. M. Abramova, N. I. Kiselev, D. A. Balaes. O. B. Romanova, G. I. Makovetskii, K. I. Yanushkevich, A. I. Galyas, and O. F. Demidenko	S82
Optical Properties of α -MnS Single Crystal	
O. B. Romanova, G. M. Abramova, L. I. Ryabinkina, and V. V. Markov	S85
Itinerant Electron Metamagnetism and Magnetoelasticity of CoS ₂	
N. V. Mushnikov and T. Goto	S88
Semiconductor-Metal Transition in FeSi in Ultrahigh Magnetic Field	
Yu. B. Kudasov, A. G. Volkov, A. A. Povzner, P. V. Bajankin, A. I. Bykov, M. I. Dolotenko, V. G. Guk, N. P. Kolokol'chikov, V. V. Krjuk, M. P. Monakhov, I. M. Markevtsev, V. V. Platonov, V. D. Selemir, O. M. Tatsenko, and A. V. Filippov	S93
Magnetic Susceptibility and Disorder–Order Phase Transitions in Strongly Nonstoichiometric Compounds TiC _y and HfC _y	
S. Z. Nazarova, L. V. Zueva, and A. N. Zyryanova	S97
The Magnetic State and Spin Dynamics of Single Crystal CuB ₂ O ₄	
G. Petrakovskii, A. Pankrats, A. Balaev, A. Vorotinov, K. Sablina, M. Popov, B. Roessli, A. Amato, J. Schefer, and B. Ouladdiaf	S102
Peculiarities of Inhomogeneous Charge Density Distribution in Dielectric Oxides	
L. A. Boyarsky, S. P. Gabuda, S. G. Kozlova, I. V. Postnov, and S. V. Verkhovsky	S107
Investigation of the Cotton-Mouthon Effect in an α-Fe ₂ O ₃ Easy-Plane Antiferromagnet	
I. Sh. Akhmadullin, V. A. Golenishchev-Kutuzov, S. A. Migachev, and M. F. Sadykov	S111
Concentration Phase Transitions in Single-Crystal Solid Solutions V_x Fe $_{1-x}$ BO $_3$	
V. V. Markov, V. V. Rudenko, I. S. Edel'man, N. B. Ivanova, N. V. Kazak, A. D. Balaev, and S. G. Ovchinnikov	S114
Influence of Ga ³⁺ Ions on the Magnetic Properties of Ferrite NiFeCrO ₄	
L. G. Antoshina, A. N. Goryaga, and V. V. San'kov	S119
Electronic Structure and Magnetic Mechanism of Pairing in HTSC Transition Metal Oxides	
S. G. Ovchinnikov, I. O. Baklanov, A. A. Borisov, V. A. Gavrichkov, M. M. Korshunov, E. V. Kuz'min, I. S. Sandalov , and O. Erikson	S124
Low-Temperature Anisotropy of Magnetoresistance in Layered Single Crystals Nd _{2-x} Ce _x CuO _{4+δ}	
G. I. Harus, A. I. Ponomarev, A. N. Ignatenkov, T. B. Charikova, L. D. Sabirzjanova, N. G. Shelushinina, A. A. Ivanov, and I. A. Rudnev	S130
Magnetoresistance of TmBaCuO Single Crystals in the Antiferromagnetic State	
È. B. Amitin, A. G. Blinov, L. A. Boyarsky, V. Ya. Dikovsky, K. R. Zhdanov, M. Yu. Kameneva, and L. P. Kozeeva	S133
Spin Density Wave and Pseudogap in HTSC Cuprates	
L. S. Mazov	S137
Magnetic Properties of the Fe Impurity Spin System in Gapless Semiconductor HgSe	
G. A. Al'shanskii, V. L. Konstantinov, A. V. Korolyov, E. A. Neifel'd, V. I. Okulov, S. Yu. Paranchich, and L. D. Sabirzyanova	S142

CHAPTER 9. ALLOYS AND COMPOUNDS

Electronic Structure and Magnetic Mechanism of Pairing in HTSC Transition Metal Oxides

S. G. Ovchinnikov *, I. O. Baklanov *, A. A. Borisov *, V. A. Gavrichkov *, M. M. Korshunov ** E. V. Kuz'min **, I. S. Sandalov*, ***, and O. Erikson***

* Kirenskii Institute of Physics, Krasnoyarsk, 660036 Russia

** Krasnoyarsk State University, Krasnoyarsk, 660075 Russia

*** Condensed Matter Theory Group, Institute of Physics, University of Uppsala, Box 530, S-75121 Uppsala, Sweden

Abstract—Starting from the multiband p-d model of strongly correlated electrons, we derive the effective Hamiltonian in the form of the generalized singlet—triplet t-t'-J model which transforms to the usual t-t'-J model in the low-energy limit. Both n- and p-type copper oxides are considered in the mean field approximation for Gorkov type Green functions in the X-operator representation. Different signs of the t'/t ratio result in different normal state properties and T_c values conserving the $d_{x^2-v^2}$ gap symmetry both for n- and p-oxides.

Comparison with ruthenates and the coexistence of superconductivity and magnetism in RuSr₂GdCu₂O₈ are studied in the extended *t–J–I* model with ferromagnetic coupling between Ru ions.

INTRODUCTION

Currently, there is no widely accepted theory for the electronic structure of the undoped antiferromagnetic insulator, its concentration evolution with doping to the metal state, and for the pairing mechanism in cuprates of p- and n-type. A spin fluctuation mechanism of pairing is probably the best candidate for describing HTSC in copper oxides [1, 2]. One of the unsolved problems is the underlying electronic structure and how the specific electronic properties of a given material provide the rich variety of different properties in cuprates of the p- and n-type, ruthenates, and layered RuSr₂GdCu₂O₈. We discuss this problem in the framework of the multiband p-d model of transition metal oxides.

FORMULATION OF THE PROBLEM

The necessary ingredient for discussing possible mechanisms of HTSC is the band structure of the fermionlike quasiparticles. However, it is a difficult subject for *ab initio* calculations due to the strong electron correlations. For this reason, we use a model approach which is based on the possibility of rewriting the exact full Hamiltonian of the system in terms of larger-scale variables. Described briefly, the essence of the approach is as follows. Suppose we have a set of Wannier functions belonging to a chosen elementary cell which is generated by some single-electron problem for the crystal symmetry of interest. Then, the full electron field operator can be written in the form of an expansion:

$$\psi_{\sigma}(r) = \sum_{jL} \chi_{jL}(r) a_{jL}.$$

Here, the index $j = R_j$ gives the coordinate of the chose elementary cell of the lattice, L is the composite inde $L = \{\lambda, \sigma\}$, λ labels bands, and σ stands for the specific projection. Due to the orthogonality of the Wanner functions, we have $\{a_{jL}, a_{j'L'}^+\} = \delta_{jL,j'L'}$. The full nonreativistic Hamiltonian can be written in the form sum of intra- (H_c) and intercell (H_{cc}) terms:

$$H = H_c + H_{cc} = \sum_{i} H_i^c + \sum_{i \neq j} H_{ij}^{cc},$$

$$H_{i}^{c} = \sum_{LL'} h_{i}^{LL'} a_{iL}^{+} a_{iL'} + \frac{1}{2} \sum_{LL'} v_{iL,iL',iL'',iL'''} a_{iL}^{+} a_{iL'}^{+} a_{iL'} a_{iL'} a_{iL'}$$

$$H_{ij}^{cc} = \sum_{LL'} h_{ij}^{LL'} a_{iL}^{\dagger} a_{jL'}$$

$$-\frac{1}{2} \sum_{II'} \mathsf{v}_{iL,\,jL',\,iL'',\,jL'''} a_{iL}^{+} a_{jL'}^{+} a_{iL''} a_{jL'''}.$$

Now suppose that we are able to find the many-early tron states for the intracell Hamiltonian in an appropriation better than Hartree-Fock, so that it takes account (at least, partly) strong intra-atomic and intra-luster interactions. Then,

$$H_i^c|i,\Gamma_n\rangle = E_{n\Gamma}^{(0)}|i,\Gamma_n\rangle$$

and the full Hamiltonian can be rewritten in terms of the Hubbard's operators

$$X_{i}^{m} \equiv X_{i}^{\Gamma_{n-1}, \Gamma_{n}} \equiv |i, \Gamma_{n-1}\rangle\langle i, \Gamma_{n}|,$$

$$Z_{i}^{\xi} \equiv Z_{i}^{\Gamma_{n}, \Gamma_{n}'} \equiv |i, \Gamma_{n}\rangle\langle i, \Gamma_{n}'|.$$

The Hubbard model is often used to study the electronic structure of strongly correlated electron systems (SCES). To take into account the chemistry of metal oxides, it is generalized to the p-d model; the simplest version of such a model has been proposed by Emery [3] and Varma et al. [4]. In this 3-band p-d model, only the $d_{x^2-y^2}$ Cu and p_{σ} O orbitals are considered. There are many indications of the importance of the d_z : Cu orbital (see review [5]). A multiband p-d model with both $d_{x^2-y^2}$ and d_{z^2} states has been proposed by Loktev et al. [6]. To calculate the electronic structure in SCES, the generalized tight-binding (GTB) method combining the exact diagonalization of the Hamiltonian for small clusters (intracell part of the Hamiltonian) with the cluster perturbation theory for the intercell part of the Hamiltonian was proposed by Ovchinnikov and Sandalov [7]. Recently, the electronic structure of the undoped antiferromagnetic (AF) insulator like Sr₂CuO₂Cl₂ and its evolution with doping have been studied by Gavrichkov et al. [8]. The dispersion equation in the GTB method for two sublattice AF states is given by

$$\left\| \frac{(E - \Omega_m^G)}{F_\sigma^G(m)} \delta_{mn} - 2 \sum_{\lambda \lambda'} \gamma_{\lambda \sigma}^*(m) T_{\lambda \lambda}^{PG}(\mathbf{k}) \gamma_{\lambda' \sigma}(n) \right\| = 0, (1)$$

where the zero frequency of the transition $\Omega_{i,m}^{(0)} = E_{n+1,\Gamma}^{(0)} - E_{n,\Gamma}^{(0)}$ is renormalized by the Coulomb interaction within the analogue of the Hubbard-I approximation as follows:

$$\begin{split} &\delta_{n:m_1}\Omega_{i,m} = \delta_{mm_1}\Omega_{i,m}^{(0)} \\ &+ \sum_{j(\neq i)} (B_{ij}^{\Gamma_1\Gamma_2, \Gamma_3\Gamma_4} \varepsilon_{m_1}^{m, [\Gamma_1, \Gamma_2]} \langle Z_j^{\Gamma_3, \Gamma_4} \rangle \\ &- B_{ji}^{\Gamma_1\Gamma_2, \Gamma_3\Gamma_4} \varepsilon_{m_1}^{m, [\Gamma_3, \Gamma_4]} \langle Z_j^{\Gamma_1, \Gamma_2} \rangle), \end{split}$$

where the matrix elements $B_{ij}^{\Gamma_1\Gamma_2, \Gamma_3\Gamma_4}$ are

$$B_{ij}^{\Gamma_1\Gamma_2,\,\Gamma_3\Gamma_4} = \nu_{iL,\,jL',\,jL'',\,iL''} [a_{iL}^+ a_{iL'''}]^{\Gamma_1\Gamma_2} [a_{jL'}^+ a_{jL''}]^{\Gamma_3\Gamma_4}.$$

Here, excitations $[\Gamma_1, \Gamma_2]$ and $[\Gamma_3, \Gamma_4]$ are Bose-like ones, and the splitting in fermionlike excitations originates, obviously, from the crystal-field splitting of the states Γ by Coulomb interaction with the neighboring clusters. Against a background of $\Omega_{i,m}^{(0)}$, which is of the

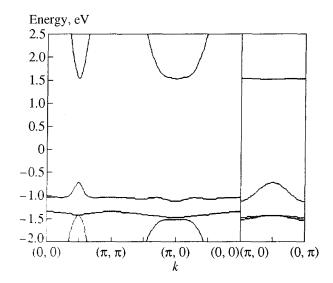


Fig. 1. Band structure of the undoped CuO₂ layer.

order of Hubbard's U of the cluster, these effects are small. Below, we consider the antiferromagnetic state and the lattice index i runs over the sublattices P, G.

Here, $m \leftrightarrow (p, q)$ numerate a quasiparticle described by the Hubbard's operator X^{pq} , and $\gamma_{\lambda\sigma}(m)$ is a parameter of X-operator representation for the single-electron annihilation operator with orbital λ and spin σ ,

$$a_{f\lambda\sigma} = \sum_{m} \gamma_{\lambda\sigma}(m) X_f^m.$$

Equation (1) has the same structure as the usual tight-binding equation of the single-electron approach but differs in the following: (i) the local energy Ω_m is given by the multielectron resonance $\Omega_m = E_{n+1}(p) - E_n(q)$, between the n- and (n+1)-electron terms of the cell; (ii) filling factors $F(m) = \langle X^{pp} \rangle + \langle X^{qq} \rangle$ result in a concentration and temperature dependences of the band structure.

The electronic structure for the undoped case with hole concentration $n_h = 1$ is shown in Fig. 1. It was calculated for the following set of model parameters (in eV):

$$t_{pq} = 1$$
, $\varepsilon(d_{x^2 - y^2}) = 0$, $\varepsilon(d_{z^2}) = 0$,
 $\varepsilon(p_x) = 1.6$, $\varepsilon(p_z) = 0.5$,
 $t_{pp} = 0.46$, $t'_{pp} = 0.4$, $U_d = 9$,
 $U_p = 4$, $V_{pd} = 1.5$, $J_d = 1$.

The wide charge transfer gap $E_{ct} \approx 2$ eV separates the empty conductivity band mainly of $d_{x^2-y^2}$ character and the filled valence band formed by a complex mixture of different copper and oxygen orbitals.

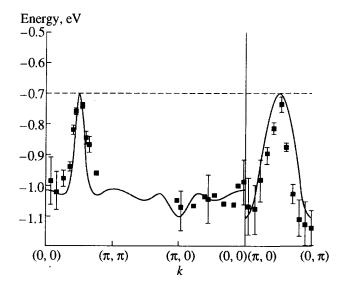


Fig. 2. The dispersion of the top part of the valence band in comparison with ARPES data on Sr₂CuO₂Cl₂ [9].

The dispersion of the top of the valence band is shown in Fig. 2 together with the ARPES data [9]. It should be noted that the valence band is formed by hole excitations from the initial single-hole state $|1, \sigma\rangle$ to different final two-hole states, both singlet $|S\rangle$ and triplet $|T, M\rangle$, M = -1, 0, +1 being essential. One more unusual result of GTB calculations [8] is the dispersionless virtual level shown by the dashed line in Fig. 2. It has zero weight in the undoped case but acquires the spectral weight $\sim x$ in the hole doped system with $n_h = 1 + x$, providing formation of the in-gap state at the top of the valence band. The dispersion of the in-gap state and its concentration evolution is shown in Fig. 3.

The calculation [8] was not self-consistent, magnetic order is given ad hoc. Thus, the curve for x = 0.1 in Fig. 3 is the interpolation, its justification being the large correlation length of the short-range antiferromagnetic order.

THE EFFECTIVE HAMILTONIAN OF THE SINGLET-TRIPLET T-T-J MODEL

The t-t'-J model is derived by exclusion of the intersubband hopping between the low (LHB) and upper (UHB) Hubbard's subbands for the Hubbard model [10] and for the 3-band p-d model [11]. We write the Hamiltonian in the form

$$H = H_0 + H_1,$$

where the excitations via the charge transfer gap are included in H_1 . Then, we define an operator $H(\varepsilon) = H_0 + \varepsilon H_1$ and make the unitary transformation

$$\tilde{H}(\varepsilon) = e^{-is\hat{S}}H(\varepsilon)e^{i\varepsilon\hat{S}}.$$

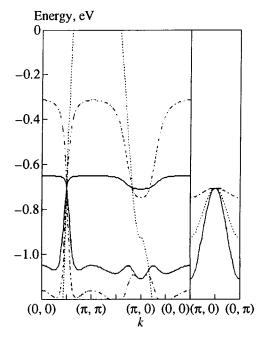


Fig. 3. Concentration dependence of the band structure in the antiferromagnetic (x = 0.01, solid line; x = 0.1, dot-dashed line) and paramagnetic (x = 0.2, dashed line) phases.

The vanishing of linear terms in ε of $\tilde{H}(\varepsilon)$ gives the equation for matrix \hat{S} :

$$H_1 + i[H_0, \hat{S}] = 0. (3)$$

The effective Hamiltonian is obtained in the second order in ε and at $\varepsilon = 1$ is given by

$$\tilde{H} = H_0 + \frac{1}{2}i[H_1, \hat{S}].$$
 (4)

It is convenient to express the matrix \hat{S} in terms of X-operators. Thus, for the multiband p-d model with a hole doping, the effective Hamiltonian has the form of a singlet-triplet t-t'-J model [12]:

$$\tilde{H} = H_0 + H_t + H_J, \tag{5}$$

where H_0 (unperturbed part of the Hamiltonian), H_t (kinetic part of \tilde{H}), and H_J (exchange part of \tilde{H}) are given by the following expressions:

$$H_{0} = \sum_{i} \left(\varepsilon_{1} \sum_{\sigma} X_{i}^{\sigma\sigma} + \varepsilon_{2S} X_{i}^{SS} + \varepsilon_{2t} \sum_{M} X_{i}^{TMTM} \right)$$

$$H_{i} = \sum_{\langle i,j\rangle,\sigma} t_{ij}^{bb} X_{i}^{S\bar{\sigma}} X_{j}^{\bar{\sigma}S}$$

$$+ \sum_{\langle i,j\rangle,\sigma} t_{fg}^{aa} (\sigma \sqrt{2} X_{i}^{T0\bar{\sigma}} - X_{i}^{T2\sigma\sigma}) (\sigma \sqrt{2} X_{j}^{\bar{\sigma}T0} - X_{j}^{\sigma T2\sigma})$$

$$+ \sum_{\langle i,j\rangle,\sigma} t_{ij}^{ab} 2\sigma \gamma_{b} [X_{i}^{S\bar{\sigma}} (\sigma \sqrt{2} X_{j}^{\bar{\sigma}T0} - X_{j}^{\sigma T2\sigma}) + H.c.]$$

$$H_{J} = \frac{1}{2} \sum_{\langle i,j \rangle} (J_{ij} + \sigma J_{ij}) \left(\mathbf{S}_{i} \mathbf{S}_{j} - \frac{1}{4} n_{i} n_{j} \right)$$
$$- \frac{1}{2} \sum_{\langle i,j \rangle,\sigma} \delta J_{ij} X_{i}^{\sigma\sigma} X_{j}^{\sigma\sigma}.$$

The J_{ij} is the exchange integral $J_{ij} = 4\frac{\left(t_{ij}^{0b}\right)^2}{E_{ci}}$, and δJ_{ij} is the correction to it (dependent on the triplet's contribution) $\delta J_{ij} = 2v^2\frac{\left(t_{ij}^{ab}\right)^2}{E_{ci}}$. For the nearest neighbors (i=0,j=1), the estimation gives $\frac{\delta J_{iJ}}{J_{ij}} \sim 10^{-2}$.

Previously, the motion of triplet holes and the simplest version of the singlet—triplet model were studied in [13].

The problem may be treated within a regular diagram technique (DT) developed earlier for strongly correlated electron systems [14, 15]. Recently, a version of DT that allows the introduction of the exact expressions for self-energies and vertices via functional derivatives of the Green's functions and derives the perturbation expansion in terms of dressed Green's functions was derived [16]. Here, we can give only the idea of the DT, omitting the details. The effective Hamiltonian in terms of cluster variables can be written in the form

$$H = \sum_{j} E_{jm}^{(0)} + \sum_{jj',mm'} B_{jj'}^{\bar{a}a'} X_{j}^{\bar{a}} X_{j}^{a'}.$$

The commutation relations for these operators are $[X_j^a, X_{j'}^{\bar{a}^i}] = \delta_{jj'} \epsilon_b^{a\bar{a}^i} Z_j^b$, where X_j^a are Fermi-like and Z_j^b are Bose-like operators; $[X_j^a, Z_{j'}^{\bar{z}}] = \delta_{jj'} \epsilon_b^{a\bar{z}} X_j^b$. As shown in [16], the structure constants $\epsilon_b^{a\bar{a}^i}$, $\epsilon_b^{a\bar{z}}$ contain information on the overlapping of the many-electron states even in the case when they are constructed within the nonorthogonal basis set. The overlap matrices, however, will be replaced by the Kronecker symbols in the present model calculation. Introducing the Kadanoff-Baym S matrix [17], $S = \exp(-i \int d1 \ U(1)Z(1))$ with exter-

nal time-dependent field $U_{i_1}^{i_1}(t_1) \equiv U(1)$ (which causes the transitions a_1 between different states $|i_1, m\rangle$ of the same ion i_1) and, using equations of motion for X(1), we obtain the closed system of equations for correlators $N(1) \equiv \langle TZ(1)\rangle_U = \langle TSZ(1)\rangle/\langle TS\rangle$ and Green's functions of quasi-fermion $G(1, 1') = -i\langle TX(1)X(1')\rangle_U$ and quasi-boson hoppings $K(1, 1') = -i\langle\langle TZ(1)Z(1')\rangle_U - \langle\langle TZ(1)\rangle\langle\langle TZ(1')\rangle_U\rangle$ in terms of functional derivatives with respect to the following fields:

$$\begin{split} D_0^{-1}(1,2)G(2,1') \\ &= P(1,1') + B(2,3)\epsilon_4^{12} \bigg(N(4) + i\frac{\delta}{\delta U(4)} \bigg) G(3,1'), \\ \text{where } D_0^{-1}(12) &\equiv (\delta_{12}i\partial_{t_1} - A_{12}(t_1) - \Omega_{12}^0)\delta(t_1 - t_2), \\ A_{12}(t_1) &\equiv \epsilon_{3_b}^{1\bar{2}} U^{3_b}(t_1) \quad \text{and} \quad P(1,-1') &= \delta(t_1 - t_1')\epsilon_{3_b}^{1\bar{2}} \langle Z^{3_b}(t_1') \rangle_U. \end{split}$$

We look for a solution in the form G(3, 1') = D(3, 5)P(5, 1'). Defining D by the equation $D^{-1}(1, 2) = D_0^{-1}(1, 2) - \Sigma(1, 2)$, the vertex as $\Gamma(1, 2; 3) = \delta D^{-1}(1, 2)/\delta U(3)$ and using the relation $\delta G(1, 2)/\delta U(3) = -D(1, 4)\Gamma(4, 5; 3)G(5, 2) + D(1, 4)\delta P(42)/\delta U(3)$ with $\delta P(42)/\delta U(3) = \varepsilon_6^{42} K(6, 3)$, we obtain a closed equation for the GF in terms of the vertices:

$$D_{+}^{1}(1,2)G(2,1') = P(1,1') + \delta P(1,1') + B(2,3)\varepsilon_{4}^{12}N(4)G(3,1') - B(2,3)\varepsilon_{4}^{12}D(36)\Gamma(6,7;4)G(7,1)$$

with $\delta P(1, 1') = B(2, 3) \varepsilon_4^{12} D(3, 5) \delta P(51) / \delta U(4)$. Iterating this exact equation via vertex and self-energy, we obtain an expansion in terms of dressed Green's functions

For the electron-doped systems, the exclusion of all two-hole states results in the usual t-t'-J model. Thus, the asymmetry of the electronic structure of p- and n-type doped copper oxides results from the different structure of the Hilbert subspaces for $n_h = 0$ (one vacuum state $|0\rangle$) and $n_h = 2$ (a set of two-hole singlet $|S\rangle$ and triplet $|TM\rangle$, a Zhang-Rice singlet being one of them). In the low excitation energy region $E \ll \Delta$, where $\Delta = E_T - E_S$ is the energy of the lowest spin exciton, one can omit all excited two-hole states and obtain the effective t-t'-J model both for p- and n-type systems. The typical value of Δ is 0.5 eV. That is much less than the Mott-Hubbard or charge transfer gaps.

In the t-t'-J model, the difference between p- and n-type systems is provided by the different sign of the t'/t ratio. It was shown that to fit the ARPES data the following ratios are required [18]: for $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ t'/t = -0.2, for $\text{YBa}_2\text{Cu}_3\text{O}_7$ t'/t = -0.45, and for $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$ t'/t = +0.2. A direct calculation [8] gives $t'_{\text{eff}}/t_{\text{eff}} = -0.24$ for the p-type doping.

MAGNETIC MECHANISM OF PAIRING FOR HOLE- AND ELECTRON-DOPED CUPRATES

An early suggestion that AF spin fluctuations could give rise to singlet $d_{x^2-y^2}$ —wave pairing in hole-doped cuprate superconductors was made by Bickers, Scalapino, and Scalettar [19]. This suggestion has been sup-

ported by the FLEX approximation to the Hubbard model [20] that is, however, not valid in the case of $U \gg t$. In this limit of SCES, the proper model is the *t*–*J* model. Exact diagonalization and the quantum Monte Carlo method results for small clusters have been discussed by Dagotto [21]. For the infinite lattice, the most adequate perturbation approach to the t-J model has been formulated in the X-operator representation because of the exact treatment of local constraint due to X-operators algebra. The mean-field solution [22-24] of the t-J model and an analysis of the self-energy correlations beyond the mean-field approximation by the diagram technique [25] and by the high-order decoupling scheme [26] has confirmed the $d_{x^2-y^2}$ -pairing in the hole-doped system with typical $T_c(x)$ dependence. Nevertheless, the optimal concentration of holes is $x_{opt} \approx$ 0.33, which is twice more than the experimental value.

As concerns n-type cuprates, the gap symmetry was unclear for a long time. Recently, phase-sensitive tunnel experiments by Tsuei and Kirtley [27] found evidence for dominant $d_{x^2-y^2}$ symmetry in electron-doped cuprates. We obtain that the mean-field solution of the t-t'-J model results in $d_{x^2-y^2}$ -gap symmetry for both p- and n-type systems. The difference in sign of t'/t provides a quantitative difference in the superconducting phase as well as in the normal phase.

COMPARISON OF MAGNETIC MECHANISMS OF PAIRING FOR CUPRATES AND RUTHENATES

The different electronic structure formed by $(t_{2g}-p)-\pi$ bonding in ruthenates in comparison with $(d_{x^2-y^2}-p)-\sigma$ bonding can result in a ferromagnetic coupling I between nearest Ru⁴⁺ ions. To compare superconductivity in cuprates and ruthenates, the t-J-I model has been proposed. Its mean-field solution [28, 29] has shown that, for $J \gg I$ (cuprates), there is the $d_{x^2-y^2}$ gap, while for $J \leq I$ (ruthenates) the triplet p symmetry gap occurs. The equation for T_c is similar in both cases, nevertheless the different gap symmetry results in a two orders of magnitude difference of T_c values. The reason is cancellation of the Van-Hove singularity for p-pairing, while for d-pairing high- T_c is a result of the spinfluctuation mechanism in SCES enhanced by the Van-Hove singularity. A similar conclusion was obtained previously in [24, 30].

The coexistence of ferromagnetism and superconductivity in RuSr₂GdCu₂O₈ [31] can also be studied in the framework of the t-J-I model. Superconductivity in the CuO₂ layer ($J \ge I$) has $d_{x^2-y^2}$ symmetry, while for the RuO₂ layer ($J \le I$) there is a competition of the ferromagnetic and triplet superconducting order. According to the mean-field phase diagram [32], a small

decrease of hole concentration in the RuO₂ layer in comparison to Sr₂RuO₂ results in the magnetic phase.

CONCLUSION

A generalized tight-binding analysis of the realistic multiband p-d model gives rather good agreement with ARPES and other spectroscopic data for the whole range of doping and provides the effective low-energy. Hamiltonian of the t-t'-J model. The mean-field solution of this model implies $d_{x^2-y^2}$ gap symmetry both for n- and p-type doped cuprates that is induced by AF spin fluctuations. In addition, the ferromagnetic fluctuation in the t-J-I model allows the comparison of magnetic pairing in cuprates and ruthenates on an equalifooting.

ACKNOWLEDGMENTS

The authors thank the Russian Federal State Program. "Integration," grant A0019, RFFI, grant 00-02-16110, and Krasnoyarsk Regional Scientific Foundation, grant 9F0039, for financial support. The support from the Swedish National Science Foundation (NFR and TFR), the Goran Gustafsson Foundation, and the Swedish Foundation for Strategic Research (SSF) is acknowledged.

REFERENCES

- 1. Yu. A. Izyumov. Uspekhi. Fiz. Nauk. 169 (1999) 225.
- 2. T. Moria and K. Ueda. Adv. Phys. 49 (2000) 555.
- 3. V. J. Emery. Phys. Rev. Lett. 58 (1987) 2794.
- 4. C. M. Varma, S. Schmitt-Rink, and E. Abrahams. Solid St. Commun. 62 (1987) 681.
- 5. S. G. Ovchinnikov. Physics-Uspekhi. 40 (1997) 993.
- Yu. B. Gaididei and V.M. Loktev. Phys. Stat. Sol. B. 147 (1988) 307.
- S. G. Ovchinnikov and I. S. Sandalov. Physica C. 198 (1989) 607.
- 8. V. A. Gavrichkov, S. G. Ovchinnikov, A. A. Borisov, and E. G. Goryachev. JETP. 91 (2000) 369.
- 9. B. O. Wells et al. Phys. Rev. Lett. 741 (1995) 964.
- K. A. Chao, J. Spalek, and A. M. Oles, J. Phys. C: Sol Stat. Phys. 10 (1977) 271.
- V. I. Belinicher, A. I. Chernyshev, and V.A. Shubin. Phys. Rev. B. 53 (1996) 335.
- M. M. Korshunov and S. G. Ovchinnikov. Fizika Tverdogo Tela. 43 (2001) 399.
- J. Zaanen, A. M. Oles, and P. Horsch. Phys. Rev. B. 46 (1992) 5798; R. Hayn, V. Yushannkhai, and S. Lotsov. Phys. Rev. B. 47 (1993) 5253.
- 14. R. O. Zaitsev, Sov. Phys. JETP, 43, (1976) 574.
- Yu. A. Izyumov, B. M. Letfulov, E.V. Shipitsyn, M. Bartkowiak, and K.A. Chao, Phys. Rev. B46 (1992) 15 697.
- I. S. Sandalov, B. Johansson, O. Eriksson, and U. Lundin: preprints cond-mat/0011259, 0011260, 0011261: submitted.

- L. Kadanoff and G. Baym, Quantum Statistical Mechanics, W. A. Benjamin, Inc., NY 1962.
- A. Nazarenko, K. J. E. Vos, S. Haas, and E. Dagotto, R. J. Gooding. Phys. Rev. B. 51 (1995) 8676.
- N. E. Bickers, D. J. Scalapino, and R. T. Scalettar. Int. J. Mod. Phys. B. 1(1987) 687.
- N. E. Bickers, D. J. Scalapino, and S. R. White. Phys. Rev. Lett. 62 (1989) 961.
- 21. E. Dagotto. Rev. Mod. Phys. 66 (1994) 763.
- 22. N. M. Plakida, V. Yushannkhai, and I. V. Stasyuk. Physica C. 160 (1989) 80.
- V. Yu. Yushannkhai, N. M. Plakida, and P. Kalinay. Physica C. 174 (1991) 401.
- J. Beenen and D. M. Edwards. Phys. Rev. B. 52 (1995) 13636.

- Yu. A. Izyumov and B. M. Letfulov. J. Phys.: Condens. Matter. 3 (1991) 5373.
- N. M. Plakida and V. S. Oudonenko. Phys. Rev. B. 59 (1999) 11949.
- C. C. Tsuei and J. R. Kirtley. Phys. Rev. Lett. 85 (2000) 182.
- 28. E. V. Kuz'min, S. G. Ovchinnikov, and I. O. Baklanov. JETP. 89 (1999) 349.
- E. V. Kuz'min, S. G. Ovchinnikov, and I. O. Baklanov. Phys. Rev. B. 61 (2000) 15392.
- E. Dagotto, A. Nazarenko, and A. Moreo. Phys. Rev. Lett. 74 (1995) 310.
- C. Bernard, J. L. Tallon, Ch. Niedermayer, et al. Phys. Rev. B. 59 (1999) 14099.
- 32. E. V. Kuz'min, S. G. Ovchinnikov, I. O. Baklanov, and E. G. Goryachev. JETP. 91 (2000) 353.