

PHYSICAL REVIEW B

For editorial and subscription correspondence,
please see inside front cover
(ISSN: 0163-1829)

PERIODICALS
Postmaster send address changes to:
American Institute of Physics
500 Sunnyside Boulevard
Woodbury, NY 11797-2999

THIRD SERIES, VOLUME 59, NUMBER 1

CONTENTS

1 JANUARY 1999-I

Subject Matter Categories for Physical Review B	iii
Physical Review B Editorial Policies and Practices	iv
Physical Review B Information for Contributors	vii
Guidelines for Estimating Length for Physical Review B	xi

BRIEF REPORTS

Structure, structural phase transitions, mechanical properties, defects, etc.

Vacancy ordering and medium-range structure in a simple monatomic liquid	1
B. Sadigh, M. Dzugutov, and S. R. Elliott	
Number of independent partial structure factors for a disordered n -component system	5
David L. Price and Alfredo Pasquarello	
Reliability of measuring the roughness exponent in a small-length-scale regime	8
Jie Deng, F. Ye, Q. Y. Long, and C. W. Lung	
Effect of A- and B-cation substitutions on the phase stability of PbTiO_3 ceramics	12
J. Frantti, V. Lantto, S. Nishio, and M. Kakihana	
Transient ordered phases with different structure types along a phase-decomposition path	16
Zhi-Rong Liu, Bing-Lin Gu, Hong Gui, and Xiao-Wen Zhang	
Inverse Kirkendall mixing in collision cascades	20
K. Nordlund and R. S. Averback	
Interconnection of defect parameters and stress-induced electric signals in ionic crystals	24
P. Varotsos, N. Sarlis, and M. Lazaridou	
Physical origin of the dynamical central peak in ferroelectric triglycine sulfate	28
Y. Tsujimi, T. Matsui, H. Furuta, and T. Yagi	

Inhomogeneous, disordered, and partially ordered systems

Singularities of the renormalization-group flow for random elastic manifolds	32
D. A. Gorokhov and G. Blatter	
Structure and dynamics of liquid sulphur	34
John S. Tse and Dennis D. Klug	
Spatial structure of boson peak vibrations in glasses	38
V. N. Novikov and N. V. Surovtsev	
Spectrum of waves in randomly modulated multilayers	42
V. A. Ignatchenko, Yu. I. Mankov, and A. A. Maradudin	



General localization lengths for two interacting particles in a disordered chain	46
Pil Hun Song and Felix von Oppen	
Dynamics, dynamical systems, lattice effects, quantum solids, etc.	
Excitation-power-dependent spectral shift in photoluminescence in dye molecules in strongly scattering optical media	50
K. Totsuka, M. A. I. Talukder, M. Matsumoto, and M. Tomita	
Hyper molecular dynamics with a local bias potential	54
X. G. Gong and J. W. Wilkins	
Higher-order effects on Shapiro steps in Josephson junctions	58
Kim Ø. Rasmussen, Vadim Zharnitsky, Igor Mitkov, and Niels Grønbech-Jensen	
Observation of the out-of-plane mode in the Raman scattering from the graphite edge plane	62
Yasushi Kawashima and Gen Katagiri	
Magnetism	
Edge critical behavior at the surface transition of Ising magnets	65
M. Pleimling and W. Selke	
Spin-glass properties of metallic nanoparticles conducted by quantum size effects	69
Wen-Chu Huang and Juh-Tzeng Lue	
Specific heat of α' -NaV ₂ O ₅ in magnetic fields up to 16 T	73
W. Schnelle, Yu. Grin, and R. K. Kremer	
Colossal resistive relaxation effects in a Pr _{0.67} Ca _{0.33} MnO ₃ single crystal	77
A. Anane, J.-P. Renard, L. Reversat, C. Dupas, P. Veillet, M. Viret, L. Pinsard, and A. Revcolevschi	
Very strong magnetic-field dependence of the oxygen isotope shift of the charge-ordering transition in La _{0.5} Ca _{0.5} MnO ₃	81
Guo-meng Zhao, K. Ghosh, H. Keller, and R. L. Greene	
Low-energy spectral density for the Alexander-Anderson model	85
C. A. Paula, M. F. Silva, and L. N. Oliveira	
Nonequilibrium spin distribution in a single-electron transistor	89
Alexander N. Korotkov and V. I. Safarov	
Spin accumulation in small ferromagnetic double-barrier junctions	93
Arne Brataas, Yu. V. Nazarov, J. Inoue, and Gerrit E. W. Bauer	
Microscopically homogeneous magnetic structure of La _{1-x} Sr _x MnO ₃ beyond the range of 0 < x < 0.1 observed by La NMR	97
K. Kumagai, A. Iwai, Y. Tomioka, H. Kuwahara, Y. Tokura, and A. Yakubovskii	
Thermodynamic properties of spin- $\frac{1}{2}$ transverse XY chains with Dzyaloshinskii-Moriya interaction: Exact solution for correlated Lorentzian disorder	100
Oleg Derzhko and Johannes Richter	
Crystal-field transition in PuO ₂	104
S. Kern, R. A. Robinson, H. Nakotte, G. H. Lander, B. Cort, P. Watson, and F. A. Vigil	
Ground state of the spin- $\frac{1}{2}$ Heisenberg antiferromagnet on a two-dimensional square-hexagonal-dodecagonal lattice	107
Piotr Tomczak and Johannes Richter	
Bond-operator approach to the bilayer Heisenberg antiferromagnet	111
Deng-Ke Yu, Qiang Gu, Han-Ting Wang, and Jue-Lian Shen	
Quantum magnetism in the stripe phase: Bond versus site order	115
Jakub Tworzydło, Osman Y. Osman, Coen N. A. van Duin, and Jan Zaanen	
Ground-state magnetization of polymerized spin chains	119
Daniel C. Cabra and Marcelo D. Grynberg	

Critical exponents of the ferromagnetic-paramagnetic phase transition of $\text{La}_{1-x}\text{Sr}_x\text{CoO}_3$ ($0.20 \leq x \leq 0.30$)	123
J. Mira, J. Rivas, M. Vázquez, J. M. García-Beneytez, J. Arcas, R. D. Sánchez, and M. A. Señas-Rodríguez	
Specific heat of $\text{Nd}_{0.67}\text{Sr}_{0.33}\text{MnO}_3$	127
J. E. Gordon, R. A. Fisher, Y. X. Jia, N. E. Phillips, S. F. Reklis, D. A. Wright, and A. Zettl	
Sublinear temperature dependence of resistivity in metallic heterogeneous ferromagnets at high magnetic fields	131
I. Ya. Korenblit, A. Gerber, A. Milner, and M. Karpovsky	
Effect of disorder on the magnetization of a spin glass	135
D. Walton, A. McCleary, C. V. Stager, and N. P. Raju	
Ballistic electron transport through magnetic domain walls	138
Jeroen B. A. N. van Hoof, Kees M. Schep, Arne Brataas, Gerrit E. W. Bauer, and Paul J. Kelly	
Stability of stripe magnetic domain in magnetic multilayers: Prediction and observation	142
Sug-Bong Choe and Sung-Chul Shin	
Isotropic strain and magnetic properties in Ni films	146
Luca Callegaro and Ezio Puppini	
Oscillating exchange and spin wave stiffness in magnetic monolayers	149
V. Kamberský, B. A. Ivanov, and E. V. Tartakovskaya	
Temperature and magnetic field dependent optical spectral weight in the cation-deficient colossal-magnetoresistance material $\text{La}_{0.936}\text{Mn}_{0.982}\text{O}_3$	153
V. Golovanov, L. Mihaly, C. O. Homes, W. H. McCarroll, K. V. Ramanujachary, and M. Greenblatt	
Competition of interbilayer magnetic couplings in $R_{1.4}\text{Sr}_{1.6}\text{Mn}_2\text{O}_7$ ($R = \text{La}_{1-z}\text{Nd}_z$)	157
Y. Moritomo, K. Ohoyama, and M. Ohashi	

Superfluidity and superconductivity

Emission of the second sound with an expanding ^3He -concentrated droplet and phase-separation kinetics in a superfluid ^3He - ^4He mixture	161
Serguei N. Burmistrov and Takeo Satoh	
Superflow-stabilized nonlinear NMR in rotating ^3He -B	165
V. V. Dmitriev, V. B. Eltsov, M. Krusius, J. J. Ruohio, and G. E. Volovik	
Low-temperature transport through a quantum dot coupled to two superconducting leads	169
T. I. Ivanov	
Superconducting phases in the presence of Coulomb interaction: From weak to strong correlations	173
Tadeusz Domański and Karol I. Wysokiński	
Effects of energy-level quantization on the supercurrent decay of Josephson junctions	177
B. Ruggiero, M. G. Castellano, G. Torrioli, C. Cosmelli, F. Chiarello, V. G. Palmieri, C. Granata, and P. Silvestrini	
Static properties of stacked Josephson junctions: Comparison of experiments with the inductively coupled sine-Gordon model	181
N. Thyssen, R. Monaco, A. Petraglia, G. Costabile, H. Kohlstedt, and A. V. Ustinov	
Vortex lattice effects on low-energy excitations in d -wave and s -wave superconductors	184
Masanori Ichioka, Akiko Hasegawa, and Kazushige Machida	
Finite-temperature depinning of a flux line from a nonuniform columnar defect	188
Deniz Ertas	
Thermopower of high- T_c cuprates	192
Mu-Yong Choi and J. S. Kim	
Extended Van Hove singularity in electronic Raman scattering in $\text{YBa}_2\text{Cu}_4\text{O}_8$	195
E. Ya. Sherman and O. V. Misochko	
Experimental evidence for vortex lines in the vortex-liquid phase of $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$ in a geometry of tilted vortices	199
Alain Pautrat, Charles Simon, Alexandre I. Rykov, and Setsuko Tajima	

Giant T_c shift in $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$ and $\text{TlBa}_2\text{CaCu}_2\text{O}_{7-\delta}$ superconductors due to Hg-Tl exchange	203
A. A. Gapud, J. Z. Wu, B. W. Kang, S. L. Yan, Y. Y. Xie, and M. P. Siegal	
Magnetoresistance of $\text{YBa}_2\text{Cu}_3\text{O}_7$ in the cold spots model	207
Anatoley T. Zheleznyak, Victor M. Yakovenko, and H. D. Drew	

ARTICLES

Structure, structural phase transitions, mechanical properties, defects, etc.

Soft-x-ray-emission study of the influence of Li^+ -doping, irradiation, and plastic deformation on CuO	211
D. A. Zatsepin, V. R. Galakhov, B. A. Gizhevskii, E. Z. Kurmaev, V. V. Fedorenko, A. A. Samokhvalov, S. V. Naumov, and R. Berger	
Pressure-induced cubic-to-orthorhombic phase transition in ZrW_2O_8	215
J. D. Jorgensen, Z. Hu, S. Teslic, D. N. Argyriou, S. Short, J. S. O. Evans, and A. W. Sleight	
Random and channeling stopping powers and charge-state distributions in silicon for 0.2–1.2 MeV/u positive heavy ions	226
W. Jiang, R. Grötzschel, W. Pilz, B. Schmidt, and W. Möller	
Mixed finite element and atomistic formulation for complex crystals	235
E. B. Tadmor, G. S. Smith, N. Bernstein, and E. Kaxiras	
Anharmonicity of Cu-based shape-memory alloys in the vicinity of their martensitic transition	246
Alfons González-Comas, Lluís Mañosa, Antoni Planes, and Michel Morin	
Hypersonic anomalies and optical properties of RbTiOAsO_4 and KTiOPO_4 single crystals	251
Chi-Shun Tu, Ram S. Katiyar, V. Hugo Schmidt, Ruyan Guo, and A. S. Bhalla	
Phase transitions in defect chalcopyrite compounds under hydrostatic pressure	257
V. V. Ursaki, I. I. Burlakov, I. M. Tiginyanu, Y. S. Raptis, E. Anastassakis, and A. Anedda	
Elastic soft mode and charge ordering of Yb_4As_3	269
Terutaka Goto, Yuichi Nemoto, Akira Ochiai, and Takashi Suzuki	

Inhomogeneous, disordered, and partially ordered systems

Two-dimensional discrete Coulomb alloy	277
Yuqing Xiao, M. F. Thorpe, and J. B. Parkinson	
Monte Carlo simulations of icosahedral quasicrystal growth and melting	286
V. E. Dmitrienko, S. B. Astaf'ev, and M. Kléman	
Slow dynamics and ergodicity breaking in a lanthanum-modified lead zirconate titanate relaxor system	294
Zdravko Kutnjak, Cene Filipič, Raša Pirc, Adrijan Levstik, Robert Farhi, and Mimoun El Marssi	
Existence and localization of surface states on Fibonacci quasicrystals: A tight-binding study	302
E. S. Zijlstra, A. Fasolino, and T. Janssen	
Magnetic and transport properties of single-grain R -Mg-Zn icosahedral quasicrystals [$R = \text{Y}, (\text{Y}_{1-x}\text{Gd}_x), (\text{Y}_{1-x}\text{Tb}_x), \text{Tb}, \text{Dy}, \text{Ho}, \text{and Er}$]	308
I. R. Fisher, K. O. Cheon, A. F. Panchula, P. C. Canfield, M. Chernikov, H. R. Ott, and K. Dennis	
Bethe ansatz for the Harper equation: Solution for a small commensurability parameter	322
I. V. Krasovsky	
Molecular-dynamics study of melting on the shock Hugoniot of Al	329
Ji-Wook Jeong, In-Ho Lee, and K. J. Chang	
Parameter-free test of alloy dendrite-growth theory	334
Craig B. Arnold, Michael J. Aziz, Matthias Schwarz, and Dieter M. Herlach	
Electron-electron scattering times in low-diffusivity thick RuO_2 and IrO_2 films	344
J. J. Lin, W. Xu, Y. L. Zhong, J. H. Huang, and Y. S. Huang	

Dynamics, dynamical systems, lattice effects, quantum solids, etc.

Experimental verification of Herring's theory of anharmonic phonon relaxation: TeO_2	349
E. P. N. Damen, A. F. M. Arts, and H. W. de Wijn	
Quasiharmonic free energy and derivatives for three-body interactions	353
M. B. Taylor, N. L. Allan, J. A. O. Bruno, and G. D. Barrera	
Raman spectroscopy of SrRuO_3 near the paramagnetic-to-ferromagnetic phase transition	364
M. N. Iliev, A. P. Litvinchuk, H.-G. Lee, C. L. Chen, M. L. Dezaneti, C. W. Chu, V. G. Ivanov, M. V. Abrashev, and V. N. Popov	
Interpretation of the nonlinear optical susceptibility of borate crystals from first principles	369
Chung-gang Duan, Jun Li, Zong-quan Gu, and Ding-sheng Wang	
Anharmonicity in thermal motion and electrostatic forces on nuclei: Pulsed neutron diffraction from MnF_2	373
W. Jauch, A. J. Schultz, and R. F. Stewart	

Magnetism

Quantum-classical crossover in the spin-1/2 XXZ chain	381
Klaus Fabricius and Barry M. McCoy	
Multilayer $S = \frac{1}{2}$ Heisenberg antiferromagnet	387
Zheng Weihong	
Magnetization properties of some quantum spin ladders	396
Kunj Tandon, Siddhartha Lal, Swapan K. Pati, S. Ramasesha, and Diptiman Sen	
Transport, optical, and electronic properties of the half-metal CrO_2	411
I. I. Mazin, D. J. Singh, and Claudia Ambrosch-Draxl	
Calculated magnetic properties of binary alloys between Fe, Co, Ni, and Cu	419
P. James, O. Eriksson, B. Johansson, and I. A. Abrikosov	
Magnetic properties of Dy-Zr nanocomposites	431
A. Giguere, M. Foldeaki, R. A. Dunlap, and R. Chahine	
Metallic ferromagnetism from kinetic-energy gain: The case of EuB_6	436
J. E. Hirsch	
Classical spin liquid: Exact solution for the infinite-component antiferromagnetic model on the <i>kagomé</i> lattice ...	443
D. A. Garanin and Benjamin Canals	
Effect of disorder on the magnetic properties of SmCo_5	457
Diandra L. Leslie-Pelecky and R. L. Schalek	
Bilinear and biquadratic interlayer exchange coupling in sputtered Co/Cu multilayers damaged with residual gas impurities	463
C. H. Marrows and B. J. Hickey	
Influence of Au and Cu overlayers on the magnetic structure of Co films on W(110)	468
Thomas Duden and Ernst Bauer	
Biquadratic exchange in ferromagnetic/nonferromagnetic sandwiches: A spin-polarized low-energy electron microscopy study	474
T. Duden and E. Bauer	
Nonlinear transport in tunnel magnetoresistance systems	480
L. Sheng, Y. Chen, H. Y. Teng, and C. S. Ting	
Spontaneous two-ion magnetostriction of the Hubbard itinerant ferromagnet $\text{Y}_2\text{Fe}_{14}\text{B}$	486
C. Abadía, A. del Moral, K. Kulakowski, and P. A. Algarabel	
Zero-field ^{139}La nuclear magnetic resonance in $\text{La}_{1-x}\text{Ca}_x\text{MnO}_3$ for $0.125 \leq x \leq 0.5$	492
Joonghoe Dho, Ilryong Kim, Soonchil Lee, K. H. Kim, H. J. Lee, J. H. Jung, and T. W. Noh	
Evidence for breakdown of ferromagnetic order below T_C in the manganite $\text{La}_{0.8}\text{Ca}_{0.2}\text{MnO}_3$	497
Vladimir Chechersky, Amar Nath, I. Isaac, Jurgen P. Franck, Kartik Ghosh, Honglyoul Ju, and Richard L. Greene	

Magnetocaloric effect and heat capacity in the phase-transition region	503
A. M. Tishin, K. A. Gschneidner, Jr., and V. K. Pecharsky	
Magnetic structure of GdCu through the martensitic structural transformation: A neutron-diffraction study	512
J. A. Blanco, J. I. Espeso, J. García Soldevilla, J. C. Gómez Sal, M. R. Ibarra, C. Marquina, and H. E. Fischer	
Magnetic-field-dependent thermodynamics of Mn ₁₂ -acetate single crystals at low temperatures	519
F. Fominaya, J. Villain, T. Fournier, P. Gandit, J. Chaussy, A. Fort, and A. Caneschi	
Transport properties of the one-dimensional ferromagnetic Kondo lattice model: A qualitative approach to oxide manganites	529
J. J. Betouras and S. Fujimoto	
Transition-element doping effects in La _{0.7} Ca _{0.3} MnO ₃	533
K. Ghosh, S. B. Ogale, R. Ramesh, R. L. Greene, T. Venkatesan, K. M. Gapchup, Ravi Bathe, and S. I. Patil	
Dynamic and nonlinear magnetoconductance: Numerical analysis in two dimensions	538
Weidong Sheng, Qingrong Zheng, Jian Wang, and Hong Guo	
Influence of structural disorder on the temperature dependence of the transport and magnetic properties of β -phase Co _x Al _{1-x} alloy films	546
Y. P. Lee, K. W. Kim, J. Y. Rhee, and Y. V. Kudryavtsev	
Superfluidity and superconductivity	
Critical properties of the topological Ginzburg-Landau model	554
C. de Calan, A. P. C. Malbouisson, F. S. Nogueira, and N. F. Svaiter	
Dynamics of an SO(5)-symmetric ladder model	561
R. Eder, A. Dorneich, M. G. Zacher, W. Hanke, and Shou-Cheng Zhang	
Doping dependence of the pseudogap in the <i>ab</i> plane infrared spectra of Bi ₂ Sr ₂ Ca _{1-x} Y _x Cu ₂ O _{8+δ}	576
N. L. Wang, A. W. McConnell, B. P. Clayman, and G. D. Gu	
Double-vertically-stacked Josephson junctions: Numerical and analytical analyses of a current-biased system in a magnetic field	581
S. R. Maglic, P. R. Auvil, Jr., and J. B. Ketterson	
Theory of the π junctions formed in atomic-scale superconductor/ferromagnet superlattices	587
V. Prokić, A. I. Buzdin, and L. Dobrosavljević-Grujić	
Experimental study of the geometrical barrier in type-I superconducting strips	596
H. Castro, B. Dutoit, A. Jacquier, M. Baharami, and L. Rinderer	
Nonlinear flux-line dynamics in vanadium films with square lattices of submicron holes	603
V. Metlushko, U. Welp, G. W. Crabtree, Zhao Zhang, S. R. J. Brueck, B. Watkins, L. E. DeLong, B. Ilic, K. Chung, and P. J. Hesketh	
Dependence of activation energy upon magnetic field and temperature in YBa ₂ Cu ₃ O _{7-δ} epitaxial thin film	608
Xu Xiaojun, Fu Lan, Wang Liangbin, Zhang Yuheng, Fang Jun, Cao Xiaowen, Li Kebin, and Sekine Hisashi	
Vortex structure for a <i>d</i> + <i>is</i> -wave superconductor	613
Qunqing Li, Z. D. Wang, and Qiang-Hua Wang	
Strong interaction of correlated electrons with phonons: A diagrammatic approach	619
V. A. Moskalenko, P. Entel, and D. F. Digor	
Magnetic field and pressure dependence of T_c and T_N in TbSr ₂ Cu _{2.7} Mo _{0.3} O _{7-δ}	636
H. L. Tsay, Y. C. Chen, S. S. Weng, C. F. Chang, and H. D. Yang	
Magnetic penetration depth in superconducting La _{2-x} Sr _x CuO ₄ films	641
Kathleen M. Paget, Sabyasachi Guha, Marta Z. Cieplak, Igor E. Trofimov, Stefan J. Turneaure, and Thomas R. Lemberger	
Optical absorptivity of La _{1.87} Sr _{0.13} CuO ₄ below the superconducting plasma edge	647
J. T. Birmingham, S. M. Grannan, P. L. Richards, J. Kircher, M. Cardona, and A. Wittlin	

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 59, NUMBER 1

1 JANUARY 1999-I

Low-frequency spin dynamics as probed by ^{63}Cu and ^{199}Hg NMR in $\text{HgBa}_2\text{CuO}_{4+\delta}$ superconductors with different oxygen content	654
A. A. Gippius, E. V. Antipov, W. Hoffmann, K. Lüders, and G. Buntkowsky	
Quasiparticle bands in the extended t - J model: Application to $\text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4$	661
Jan Bala	

COMMENTS

Comment on “Crossover exponents in percolating superconductor–nonlinear-conductor mixtures”	668
Lei Gao, Wen-Gang Lu, and Zhen-Ya Li	
Comment on “Observation of vortex-lattice melting in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ by Seebeck-effect measurements”	671
M. Ausloos, H. Bougrine, M. Houssa, and M. Pekala	
Reply to “Comment on ‘Observation of vortex-lattice melting in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ by Seebeck-effect measurements’ ”	674
H. Ghamlouch, M. Aubin, R. Gagnon, and L. Taillefer	
Cumulative Author Index	677