

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 88, NUMBER 13

OCTOBER 2013-1(I)

Probing the anisotropic vortex lattice in the Fe-based superconductor KFe_2As_2 using small-angle neutron scattering (8 pages)	134524
H. Kawano-Furukawa, Lisa DeBeer-Schmitt, H. Kikuchi, A. S. Cameron, A. T. Holmes, R. W. Heslop, E. M. Forgan, J. S. White, K. Kihou, C. H. Lee, A. Iyo, H. Eisaki, T. Saito, H. Fukazawa, Y. Kohori, and J. L. Gavilano	

Doping evolution of Zhang-Rice singlet spectral weight: A comprehensive examination by x-ray absorption spectroscopy (5 pages)	134525
Y.-J. Chen, M. G. Jiang, C. W. Luo, J.-Y. Lin, K. H. Wu, J. M. Lee, J. M. Chen, Y. K. Kuo, J. Y. Juang, and Chung-Yu Mou	

COMMENTS

Comment on “First-principles study of the influence of (110)-oriented strain on the ferroelectric properties of rutile TiO_2 ” (5 pages)	136101
Keith Refson, Barbara Montanari, Pavlin D. Mitev, Kersti Hermansson, and Nicholas M. Harrison	
Reply to “Comment on ‘First-principles study of the influence of (110)-oriented strain on the ferroelectric properties of rutile TiO_2 ’ ” (3 pages)	136102
A. Grünebohm, C. Ederer, and P. Entel	

ERRATA

Publisher’s Note: Evolution of the Fermi surface of arsenic through the rhombohedral to simple-cubic phase transition: A Wannier interpolation study [Phys. Rev. B 88 , 134103 (2013)] (1 page)	139901(E)
Patricia K. Silas, Peter D. Haynes, and Jonathan R. Yates	
Erratum: Magnetic form factor, field map, and field distribution for a BCS type-II superconductor near its $B_{c2}(T)$ phase boundary [Phys. Rev. B 87 , 134508 (2013)] (1 page)	139902(E)
A. Maisuradze and A. Yaouanc	

Space group symmetry, spin-orbit coupling, and the low-energy effective Hamiltonian for iron-based superconductors (<i>34 pages</i>)	134510
Vladimir Cvetkovic and Oskar Vafek	
Toward engineered quantum many-body phonon systems (<i>7 pages</i>)	134511
Ö. O. Soykal and Charles Tahan	
In-plane spin excitation anisotropy in the paramagnetic state of NaFeAs (<i>6 pages</i>)	134512
Yu Song, Louis-Pierre Regnault, Chenglin Zhang, Guotai Tan, Scott V. Carr, Songxue Chi, A. D. Christianson, Tao Xiang, and Pengcheng Dai	
Magnetotransport properties of single-crystalline LaFeAsO (<i>7 pages</i>)	134513
C. A. McElroy, J. J. Hamlin, B. D. White, M. A. McGuire, B. C. Sales, and M. B. Maple	
Magnetostatics and optics of noncentrosymmetric metals (<i>7 pages</i>)	134514
V. P. Mineev	
Quasiparticle spectra of Abrikosov vortices in a uniform supercurrent flow (<i>4 pages</i>)	134515
C. Berthod	
Measuring the superconducting coherence length in thin films using a two-coil experiment (<i>5 pages</i>)	134516
John Draskovic, Thomas R. Lemberger, Brian Peters, Fengyuan Yang, Jaseung Ku, Alexey Bezryadin, and Song Wang	
✂ Bulk evidence for a time-reversal symmetry broken superconducting state in URu ₂ Si ₂ (<i>7 pages</i>)	134517
G. Li, Q. Zhang, D. Rhodes, B. Zeng, P. Goswami, R. E. Baumbach, P. H. Tobash, F. Ronning, J. D. Thompson, E. D. Bauer, and L. Balicas	
Microscopic coexistence of a two-component incommensurate spin density wave with superconductivity in underdoped NaFe _{0.983} Co _{0.017} As (<i>4 pages</i>)	134518
Sangwon Oh, A. M. Mounce, Jeongseop A. Lee, W. P. Halperin, C. L. Zhang, S. Carr, Pengcheng Dai, A. P. Reyes, and P. L. Kuhns	
Multiorbital and hybridization effects in the quasiparticle interference of the triplet superconductor Sr ₂ RuO ₄ (<i>8 pages</i>)	134519
Alireza Akbari and Peter Thalmeier	
Superconductivity in the Mn ₅ Si ₃ -type Zr ₅ Sb ₃ system (<i>5 pages</i>)	134520
B. Lv, X. Y. Zhu, B. Lorenz, F. Y. Wei, Y. Y. Xue, Z. P. Yin, G. Kotliar, and C. W. Chu	
✂ Evidence from tunneling spectroscopy for a quasi-one-dimensional origin of superconductivity in Sr ₂ RuO ₄ (<i>10 pages</i>)	134521
I. A. Firmo, S. Lederer, C. Lupien, A. P. Mackenzie, J. C. Davis, and S. A. Kivelson	
Propagating and annihilating vortex dipoles in the Gross-Pitaevskii equation (<i>10 pages</i>)	134522
Cecilia Rorai, K. R. Sreenivasan, and Michael E. Fisher	
Topological invariant for generic one-dimensional time-reversal-symmetric superconductors in class DIII (<i>5 pages</i>)	134523
Jan Carl Budich and Eddy Ardonne	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 88, NUMBER 13

OCTOBER 2013-1(I)

⁵⁵ Mn NMR study of quaternary half-metallic ferromagnetic Co ₂ Mn _{1-x} Fe _x Si Heusler compounds (8 pages)	134424
S. Wurmehl, A. Alfonsov, J. T. Kohlhepp, H. J. M. Swagten, B. Koopmans, M. Wójcik, B. Balke, V. Ksenofontov, C. G. F. Blum, and B. Büchner	
Possible spin-orbit driven spin-liquid ground state in the double perovskite phase of Ba ₃ YIr ₂ O ₉ (5 pages)	134425
Tusharkanti Dey, A. V. Mahajan, R. Kumar, B. Koteswararao, F. C. Chou, A. A. Omrani, and H. M. Ronnow	
Antiferromagnetism in UO ₂ thin epitaxial films (10 pages)	134426
Z. Bao, R. Springell, H. C. Walker, H. Leiste, K. Kuebel, R. Prang, G. Nisbet, S. Langridge, R. C. C. Ward, T. Gouder, R. Caciuffo, and G. H. Lander	
Exchange parameters and adiabatic magnon energies from spin-spiral calculations (8 pages)	134427
Adam Jacobsson, Biplab Sanyal, Marjana Ležaić, and Stefan Blügel	
Unconventional magnetic ground state in Yb ₂ Ti ₂ O ₇ (6 pages)	134428
R. M. D'Ortenzio, H. A. Dabkowska, S. R. Dunsiger, B. D. Gaulin, M. J. P. Gingras, T. Goko, J. B. Kycia, L. Liu, T. Medina, T. J. Munsie, D. Pomaranski, K. A. Ross, Y. J. Uemura, T. J. Williams, and G. M. Luke	
Interface states in CoFe ₂ O ₄ spin-filter tunnel junctions (5 pages)	134430
Pavel V. Lukashev, J. D. Burton, Alexander Smogunov, Julian P. Velev, and Evgeny Y. Tsymbal	
Superfluidity and superconductivity	
Photoemission and muon spin relaxation spectroscopy of the iron-based Rb _{0.77} Fe _{1.61} Se ₂ superconductor: Crucial role of the cigar-shaped Fermi surface (7 pages)	134501
J. Maletz, V. B. Zabolotnyy, D. V. Evtushinsky, A. N. Yaresko, A. A. Kordyuk, Z. Shermadini, H. Luetkens, K. Sedlak, R. Khasanov, A. Amato, A. Krzton-Maziopa, K. Conder, E. Pomjakushina, H.-H. Klauss, E. D. L. Rienks, B. Büchner, and S. V. Borisenko	
Absence of structural transition in M _{0.5} IrTe ₂ (M = Mn, Fe, Co, Ni) (7 pages)	134502
J.-Q. Yan, B. Sapiro, A. S. Sefat, H. Yang, H. B. Cao, H. D. Zhou, B. C. Sales, and D. G. Mandrus	
Resistivity of Ba(Fe _{1-x} Co _x) ₂ As ₂ : Evidence for a broad composition range of non-Fermi-liquid behavior (5 pages)	134503
G. N. Tam, B. D. Faeth, J. S. Kim, and G. R. Stewart	
Weyl phases in point-group symmetric superconductors (9 pages)	134504
Vasudha Shivamoggi and Matthew J. Gilbert	
Theory of quasiparticle scattering interference on the surface of topological superconductors (10 pages)	134505
Johannes S. Hofmann, Raquel Queiroz, and Andreas P. Schnyder	
Restoring phase coherence in a one-dimensional superconductor using power-law electron hopping (9 pages)	134506
Alejandro M. Lobos, Masaki Tezuka, and Antonio M. García-García	
<i>p</i> -wave pairing in a two-component Fermi system with unequal population: Weak-coupling BCS to strong-coupling BEC regimes (6 pages)	134507
Renyuan Liao, Florentin Popescu, and Khandker Quader	
Impurity-induced subgap bound states in alkali-doped iron chalcogenide superconductors (7 pages)	134508
Shantanu Mukherjee, Maria N. Gastiasoro, and Brian M. Andersen	
Changes in the self-energy and <i>d</i> -wave pairing strength with doping in overdoped La _{2-x} Sr _x CuO ₄ (5 pages)	134509
Thomas Dahm and D. J. Scalapino	

(Continued)

CONTENTS - Continued

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 88, NUMBER 13

OCTOBER 2013-1(I)

Simulating rare switching events of magnetic nanostructures with forward flux sampling (9 pages)	134409
Christoph Vogler, Florian Bruckner, Bernhard Bergmair, Thomas Huber, Dieter Suess, and Christoph Dellago	
Magnetoelastic coupling in $\text{La}_{0.7}\text{Ca}_{0.3}\text{MnO}_3/\text{BaTiO}_3$ ultrathin films (12 pages)	134410
A. Alberca, N. M. Nemes, F. J. Mompean, T. Fehér, F. Simon, J. Tornos, C. Leon, C. Munuera, B. J. Kirby, M. R. Fitzsimmons, A. Hernando, J. Santamaria, and M. Garcia-Hernandez	
Phase transitions in three-dimensional loop models and the CP^{n-1} sigma model (15 pages)	134411
Adam Nahum, J. T. Chalker, P. Serna, M. Ortuño, and A. M. Somoza	
Decoupled phase of frustrated spin- $\frac{1}{2}$ antiferromagnetic chains with and without long-range order in the ground state (8 pages)	134412
Manoranjan Kumar and Z. G. Soos	
Classical modeling of ultrafast coherent magneto-optical experiments (11 pages)	134413
Y. Hirschberger and P.-A. Hervieux	
Spin-driven bond order in a $\frac{1}{5}$ -magnetization plateau phase in the triangular lattice antiferromagnet CuFeO_2 (5 pages)	134414
Taro Nakajima, Noriki Terada, Setsuo Mitsuda, and Robert Bewley	
Thermal and spin-transfer-torque excitation of precessional modes in magnetic tunnel junction nanopillars with symmetric interfaces and a thick free layer (7 pages)	134415
P. Gangmei, A. Neudert, M. K. Marcham, R. J. Hicken, M. A. Gubbins, X. Cao, R. R. Lamberton, and A. B. Johnston	
Neutron scattering and muon spin relaxation measurements of the noncentrosymmetric antiferromagnet CeCoGe_3 (10 pages)	134416
M. Smidman, D. T. Adroja, A. D. Hillier, L. C. Chapon, J. W. Taylor, V. K. Anand, R. P. Singh, M. R. Lees, E. A. Goremychkin, M. M. Koza, V. V. Krishnamurthy, D. M. Paul, and G. Balakrishnan	
Kondo effect and spin quenching in high-spin molecules on metal substrates (5 pages)	134417
D. Jacob, M. Soriano, and J. J. Palacios	
Coupling of the local defect and magnetic structure of wüstite Fe_{1-x}O (8 pages)	134418
Paul J. Saines, Matthew G. Tucker, David A. Keen, Anthony K. Cheetham, and Andrew L. Goodwin	
Exact solution for a quantum spin- $\frac{1}{2}$ Ising-Heisenberg orthogonal-dimer chain with Heisenberg intradimer and Ising interdimer interactions (9 pages)	134419
Taras Verkholyak and Jozef Strečka	
Magnetic responses of randomly depleted spin ladders (23 pages)	134420
Arthur Lavarélo, Guillaume Roux, and Nicolas Laflorencie	
Saturation field entropies of antiferromagnetic Ising models: Ladders and the kagome lattice (5 pages)	134421
Vipin Kerala Varma	
Anomalous Hall effect as the response of the orbital momentum to the gradient of electrochemical potential (5 pages)	134422
Pavel Sřředa	
Local and chemical environment dependence of the magnetic properties of CoRh core-shell nanoparticles (11 pages)	134423
L. E. Díaz-Sánchez, J. Dorantes-Dávila, and G. M. Pastor	

(Continued)

Direct measurements of thermodynamic functions and electrical resistivity of fluid tungsten over a wide range of densities (<i>8 pages</i>)	134203
V. N. Korobenko and A. D. Rakhel	
Typical versus averaged overlap distribution in spin glasses: Evidence for droplet scaling theory (<i>13 pages</i>)	134204
Cécile Monthus and Thomas Garel	
Structural evolution and kinetics in Cu-Zr metallic liquids from molecular dynamics simulations (<i>10 pages</i>)	134205
Logan Ward, Dan Miracle, Wolfgang Windl, Oleg N. Senkov, and Katharine Flores	
Breakdown of self-averaging in the Bose glass (<i>5 pages</i>)	134206
Anthony Hegg, Frank Krüger, and Philip W. Phillips	
Coarse-grained kinetic Monte Carlo simulation of diffusion in alloys (<i>17 pages</i>)	134207
Thomas Garnier and Maylise Nastar	
Dynamics, dynamical systems, lattice effects:	
Nonequilibrium thermal transport in the quantum Ising chain (<i>6 pages</i>)	134301
Andrea De Luca, Jacopo Viti, Denis Bernard, and Benjamin Doyon	
Magnetism	
Magnetic ground state of the $M_{n+1}AX_n$ -phase nitride Cr_2GaN (<i>7 pages</i>)	134401
Z. Liu, T. Waki, Y. Tabata, K. Yuge, H. Nakamura, and I. Watanabe	
<i>Ab initio</i> calculation of the effective on-site Coulomb interaction parameters for half-metallic magnets (<i>10 pages</i>)	134402
Ersoy Şaşıoğlu, Iosif Galanakis, Christoph Friedrich, and Stefan Blügel	
Exchange interactions and local-moment fluctuation corrections in ferromagnets at finite temperatures based on noncollinear density-functional calculations (<i>19 pages</i>)	134403
Marjana Ležaić, Phivos Mavropoulos, Gustav Bihlmayer, and Stefan Blügel	
 Evolution of incommensurate spin order with magnetic field and temperature in the itinerant antiferromagnet GdSi (<i>8 pages</i>)	134404
Yejun Feng, D. M. Silevitch, Jiyang Wang, A. Palmer, Nayoon Woo, J.-Q. Yan, Z. Islam, A. V. Suslov, P. B. Littlewood, and T. F. Rosenbaum	
Evolution of the electronic structure of HoB_4 with temperature (<i>5 pages</i>)	134405
Deepnarayan Biswas, Nishaina Sahadev, Ganesh Adhikary, Geetha Balakrishnan, and Kalobaran Maiti	
Magnonic band gaps in waveguides with a periodic variation of the saturation magnetization (<i>5 pages</i>)	134406
Florin Ciubotaru, Andrii V. Chumak, Björn Obry, Alexander A. Serga, and Burkard Hillebrands	
Interface characterization of $\text{Co}_2\text{MnGe}/\text{Rh}_2\text{CuSn}$ Heusler multilayers (<i>8 pages</i>)	134407
Ronny Knut, Peter Svedlindh, Oleg Mryasov, Klas Gunnarsson, Peter Warnicke, D. A. Arena, Matts Björck, Andrew J. C. Dennison, Anindita Sahoo, Sumanta Mukherjee, D. D. Sarma, Sari Granroth, Mihaela Gorgoi, and Olof Karis	
Palmer-Chalker correlations in the XY pyrochlore antiferromagnet $\text{Er}_2\text{Sn}_2\text{O}_7$ (<i>8 pages</i>)	134408
Solene Guitteny, Sylvain Petit, Elsa Lhotel, Julien Robert, Pierre Bonville, Anne Forget, and Isabelle Mirebeau	

(Continued)

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

Shock-induced plasticity in tantalum single crystals: Interatomic potentials and large-scale molecular-dynamics simulations (17 pages) 134101

R. Ravelo, T. C. Germann, O. Guerrero, Q. An, and B. L. Holian

Point defect modeling in materials: Coupling *ab initio* and elasticity approaches (7 pages) 134102

Céline Varvenne, Fabien Bruneval, Mihai-Cosmin Marinica, and Emmanuel Clouet

Evolution of the Fermi surface of arsenic through the rhombohedral to simple-cubic phase transition: A Wannier interpolation study (9 pages) 134103

Patricia K. Silas, Peter D. Haynes, and Jonathan R. Yates

☞ Designer spin systems via inverse statistical mechanics (14 pages) 134104

Robert A. DiStasio, Jr., Étienne Marcotte, Roberto Car, Frank H. Stillinger, and Salvatore Torquato

Monte Carlo investigations on surface elastic energy of spin-crossover solids: Direct access to image pressure and the Eshelby constant (10 pages) 134105

Kamel Boukheddaden

☞ Paraelectric and ferroelectric states in a model for relaxor ferroelectrics (9 pages) 134106

G. G. Guzmán-Verri, P. B. Littlewood, and C. M. Varma

Multidomains made of different structural phases in multiferroic BiFeO₃: A first-principles-based study (7 pages) 134107

Dawei Wang, Ekhard K. H. Salje, Shao-Bo Mi, Chun-Lin Jia, and L. Bellaiche

Stress-induced anisotropic diffusion in alloys: Complex Si solute flow near a dislocation core in Ni (6 pages) 134108

Thomas Garnier, Venkateswara R. Manga, Dallas R. Trinkle, Maylise Nastar, and Pascal Bellon

Influence of defects on extreme ultraviolet laser ablation of LiF (9 pages) 134109

Yaroslav Cherednikov, Nail A. Inogamov, and Herbert M. Urbassek

Inhomogeneous, disordered, and partially ordered systems

☞ Solute drag by vacancies in body-centered cubic alloys (16 pages) 134201

Thomas Garnier, Maylise Nastar, Pascal Bellon, and Dallas R. Trinkle

Refinement of the equation of state of α -uranium (7 pages) 134202

A. Dewaele, J. Bouchet, F. Occelli, M. Hanfland, and G. Garbarino

