

CONTENTS - *Continued*

PHYSICAL REVIEW B

THIRD SERIES, VOLUME 103, NUMBER 5

FEBRUARY 2021-1(I)

<i>Ab initio</i> study of the structural response to magnetic disorder and van der Waals interactions in FeSe (9 pages)	054506
Felix Lochner, Ilya M. Eremin, Tilmann Hickel, and Jörg Neugebauer	
 Motional quantum states of surface electrons on liquid helium in a tilted magnetic field (14 pages)	054507
A. A. Zadorozhko, J. Chen, A. D. Chepelianskii, and D. Konstantinov	
Planar Josephson Hall effect in topological Josephson junctions (16 pages)	054508
Oleksii Maistrenko, Benedikt Scharf, Dirk Manske, and Ewelina M. Hankiewicz	
Theoretical model for parallel SQUID arrays with fluxoid focusing (14 pages)	054509
K.-H. Müller and E. E. Mitchell	
Superconductivity at 1 K in Y-Au-Si quasicrystal approximants (5 pages)	054510
Takayuki Shiino, Girma Hailu Gebresenbut, Fernand Denoel, Roland Mathieu, Ulrich Häussermann, and Andreas Rydh	

ERRATA

Erratum: Measurement-induced quantum criticality under continuous monitoring [Phys. Rev. B 102 , 054302 (2020)] (6 pages)	059901(E)
Yohei Fuji and Yuto Ashida	
Erratum: Quasiclassical theory for interfaces with spin-orbit coupling [Phys. Rev. B 100 , 064502 (2019)] (1 page)	059902(E)
Morten Amundsen and Jacob Linder	

Coincidence inelastic neutron scattering for detection of two-spin magnetic correlations (<i>9 pages</i>)	054431
Yuehua Su, Shengyan Wang, and Chao Zhang	
Role of density-dependent magnon hopping and magnon-magnon repulsion in ferrimagnetic spin-(1/2, <i>S</i>) chains in a magnetic field (<i>12 pages</i>)	054432
W. M. da Silva and R. R. Montenegro-Filho	
First-principles study of the electronic and magnetic properties of Fe, Co, and Ni dimers adsorbed on polycyclic-aromatic-hydrocarbon molecules as well as the laser chirp effect on the ultrafast spin dynamics (<i>12 pages</i>)	054433
Meng-Lin Xie, Yu-Ting Zheng, Jing Liu, Wei Jin, Chun Li, Georgios Lefkidis, and Wolfgang Hübner	
First-principles study of an $S = 1$ quasi one-dimensional quantum molecular magnetic material (<i>10 pages</i>)	054434
Maher Yazback, Jie-Xiang Yu, Shuanglong Liu, Long Zhang, Neil S. Sullivan, and Hai-Ping Cheng	
Domain-wall dynamics in multisegmented Ni/Co nanowires (<i>11 pages</i>)	054435
V. O. Dolocan	
Cryogenic spin Seebeck effect (<i>7 pages</i>)	054436
Mehrdad Elyasi and Gerrit E. W. Bauer	
Classical spin order near the antiferromagnetic Kitaev point in the spin- $\frac{1}{2}$ Kitaev-Gamma chain (<i>16 pages</i>)	054437
Wang Yang, Alberto Nocera, Erik S. Sørensen, Hae-Young Kee, and Ian Affleck	
Robust edge states in magnetic soliton racetrack (<i>10 pages</i>)	054438
Z.-X. Li, Zhenyu Wang, Yunshan Cao, H. W. Zhang, and Peng Yan	
Confined magnetoelastic waves in thin waveguides (<i>14 pages</i>)	054439
Frederic Vanderveken, Jeroen Mulkers, Jonathan Leliaert, Bartel Van Waeyenberge, Bart Sorée, Odysseas Zografos, Florin Ciubotaru, and Christoph Adelman	
Angle-dependent thermodynamics of α -RuCl ₃ (<i>11 pages</i>)	054440
S. Bachus, D. A. S. Kaib, A. Jesche, V. Tsurkan, A. Loidl, S. M. Winter, A. A. Tsirlin, R. Valentí, and P. Gegenwart	
Superfluidity and superconductivity	
Superconducting ground state of the topological superconducting candidates Ti ₃ X ($X = \text{Ir, Sb}$) (<i>6 pages</i>)	054501
Manasi Mandal, Sajilesh K. P., Rajeswari Roy Chowdhury, D. Singh, P. K. Biswas, A. D. Hillier, and R. P. Singh	
Temperature dependence of London penetration depth anisotropy in superconductors with anisotropic order parameters (<i>8 pages</i>)	054502
V. G. Kogan and R. Prozorov	
Hund's superconductor Li(Fe,Co)As (<i>5 pages</i>)	054503
H. Miao, Y. L. Wang, J.-X. Yin, J. Zhang, S. Zhang, M. Z. Hasan, R. Yang, X. C. Wang, C. Q. Jin, T. Qian, H. Ding, H.-N. Lee, and G. Kotliar	
<i>Ab initio</i> simulation of non-Abelian braiding statistics in topological superconductors (<i>17 pages</i>)	054504
Takumi Sanno, Shunsuke Miyazaki, Takeshi Mizushima, and Satoshi Fujimoto	
Interorbital nematicity and the origin of a single electron Fermi pocket in FeSe (<i>16 pages</i>)	054505
Daniel Steffensen, Andreas Kreisel, P. J. Hirschfeld, and Brian M. Andersen	

(Continued)

Nonanalytic momentum dependence of spin susceptibility for Heisenberg magnets in the paramagnetic phase and its effect on critical exponents (<i>9 pages</i>)	054415
A. A. Katanin	
Optical Hall response in spin-orbit coupled metals: Comparative study of magnetic cluster monopole, quadrupole, and toroidal orders (<i>9 pages</i>)	054416
Tatsuki Sato, Yuma Umimoto, Yusuke Sugita, Yasuyuki Kato, and Yukitoshi Motome	
Tuning Dzyaloshinskii-Moriya interactions in magnetic bilayers with a ferroelectric substrate (<i>5 pages</i>)	054417
B. H. Zhang, Y. S. Hou, Z. Wang, and R. Q. Wu	
Unconventional U(1) to Z_q crossover in quantum and classical q -state clock models (<i>24 pages</i>)	054418
Pranay Patil, Hui Shao, and Anders W. Sandvik	
Avoided ferromagnetic quantum critical point in pressurized $\text{La}_5\text{Co}_2\text{Ge}_3$ (<i>7 pages</i>)	054419
Li Xiang, Elena Gati, Sergey L. Bud'ko, Scott M. Saunders, and Paul C. Canfield	
Role of impurity clusters for the current-driven motion of magnetic skyrmions (<i>13 pages</i>)	054420
M. Stier, R. Strobel, S. Krause, W. Häusler, and M. Thorwart	
Systematic survey of magnetic configurations in multilayer ferromagnet system with dipole-dipole interaction (<i>9 pages</i>)	054421
Taichi Hinokihara and Seiji Miyashita	
Noncoplanar multiple- Q spin textures by itinerant frustration: Effects of single-ion anisotropy and bond-dependent anisotropy (<i>36 pages</i>)	054422
Satoru Hayami and Yukitoshi Motome	
Pressure-tuned spin switching in compensated GdCrO_3 ferrimagnet (<i>7 pages</i>)	054423
I. Fita, R. Puzniak, and A. Wisniewski	
Pressure-induced large increase of Curie temperature of the van der Waals ferromagnet VI_3 (<i>14 pages</i>)	054424
J. Valenta, M. Kratochvílová, M. Míšek, K. Carva, J. Kaštil, P. Doležal, P. Opletal, P. Čermák, P. Proschek, K. Uhlířová, J. Prchal, M. J. Coak, S. Son, J-G. Park, and V. Sechovský	
Magnon valve effect and resonant transmission in a one-dimensional magnonic crystal (<i>7 pages</i>)	054425
Y. W. Xing, Z. R. Yan, and X. F. Han	
Spin transfer torque switching dynamics in CoFeB/MgO magnetic tunnel junctions (<i>10 pages</i>)	054426
A. Meo, S. Sampan-a-pai, P. B. Visscher, R. Chepulskyy, D. Apalkov, J. Chureemart, P. Chureemart, R. W. Chantrell, and R. F. L. Evans	
Phase transitions between helices, vortices, and hedgehogs driven by spatial anisotropy in chiral magnets (<i>8 pages</i>)	054427
Kotaro Shimizu, Shun Okumura, Yasuyuki Kato, and Yukitoshi Motome	
Skew scattering and side jump of spin wave across magnetic texture (<i>6 pages</i>)	054428
Jin Lan (兰金) and Jiang Xiao (萧江)	
Direct observation of topological Hall effect in Co/Pt nanostructured films (<i>9 pages</i>)	054429
M. V. Sapozhnikov, N. S. Gusev, S. A. Gusev, D. A. Tatarskiy, Yu. V. Petrov, A. G. Temiryazev, and A. A. Fraerman	
Mechanism of fast domain wall motion via current-assisted Bloch-point domain wall stabilization (<i>12 pages</i>)	054430
A. De Riz, J. Hurst, M. Schöbitz, C. Thirion, J. Bachmann, J. C. Toussaint, O. Fruchart, and D. Gusakova	

(Continued)

Homogenization and design of acoustic Willis metasurfaces (<i>11 pages</i>)	054306
Hussein Esfahlani, Yarden Mazor, and Andrea Alù	
Magnetism	
Anomalous thermal properties and spin crossover of ferromagnesite (Mg,Fe)CO ₃ (<i>10 pages</i>)	054401
Han Hsu, Christian P. Crisostomo, Wenzhong Wang, and Zhongqing Wu	
Spintronic properties of topological surface Dirac electrons with hexagonal warping (<i>17 pages</i>)	054402
Yusuke Imai, Terufumi Yamaguchi, Ai Yamakage, and Hiroshi Kohno	
Laser-induced torques in spin spirals (<i>8 pages</i>)	054403
Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov	
Symmetry-protected topological phases beyond groups: The q -deformed bilinear-biquadratic spin chain (<i>12 pages</i>)	054404
Thomas Quella	
Chiral phase transition and thermal Hall effect in an anisotropic spin model on the kagome lattice (<i>7 pages</i>)	054405
F. A. Gómez Albarracín, H. D. Rosales, and P. Pujol	
Total helicity of electromagnetic fields and matter (<i>9 pages</i>)	054406
Ivan Fernandez-Corbaton	
Band structure tuning of Heusler compounds: Spin- and momentum-resolved electronic structure analysis of compounds with different band filling (<i>15 pages</i>)	054407
S. Chernov, C. Lidig, O. Fedchenko, K. Medjanik, S. Babenkov, D. Vasilyev, M. Jourdan, G. Schönhense, and H. J. Elmers	
Magnetic and electronic phases of U ₂ Rh ₃ Si ₅ (<i>11 pages</i>)	054408
J. Willwater, N. Steinki, D. Menzel, R. Reuter, H. Amitsuka, V. Sechovský, M. Vališka, M. Jaime, F. Weickert, and S. Süllo	
Intrinsic spin-dynamical properties of two-dimensional half-metallic FeX ₂ ($X = \text{Cl, Br, I}$) ferromagnets: Insight from density functional theory calculations (<i>11 pages</i>)	054409
Ram Krishna Ghosh, Ashna Jose, and Geetu Kumari	
Comprehensive study of the global phase diagram of the J - K - Γ model on a triangular lattice (<i>13 pages</i>)	054410
Shi Wang, Zhongyuan Qi, Bin Xi, Wei Wang, Shun-Li Yu, and Jian-Xin Li	
Revealing thermally driven distortion of magnon dispersion by spin Seebeck effect in Gd ₃ Fe ₅ O ₁₂ (<i>6 pages</i>)	054411
B. Yang, S. Y. Xia, H. Zhao, G. Liu, J. Du, Ka Shen, Zhiyong Qiu, and D. Wu	
Effects of exchange distortion and spin rotation in the magnetic Kagome Lattice (<i>16 pages</i>)	054412
A. A. Coker, A. Saxena, and J. T. Haraldsen	
Evidence for linear dependence of exchange bias on pinned uncompensated spins in an Fe/FeO bilayer (<i>5 pages</i>)	054413
Jiajun Guo, Xiaonan Zhao, Zhijian Lu, Peng Shi, Yufeng Tian, Yanxue Chen, Shishen Yan, Lihui Bai, and Michael Harder	
Prediction of a Heusler alloy with switchable metal-to-half-metal behavior (<i>7 pages</i>)	054414
Vasilij D. Buchelnikov, Vladimir V. Sokolovskiy, Olga N. Miroshkina, Danil R. Baigutlin, Mikhail A. Zagrebin, Bernardo Barbiellini, and Erkki Lähderanta	

(Continued)

Structural and electronic properties of solid molecular hydrogen from many-electron theories (<i>7 pages</i>)	054111
Ke Liao, Tong Shen, Xin-Zheng Li, Ali Alavi, and Andreas Grüneis	
Origin of large negative electrocaloric effect in antiferroelectric PbZrO ₃ (<i>8 pages</i>)	054112
Pablo Vales-Castro, Romain Faye, Miquel Vellvehi, Youri Nouchokgwe, Xavier Perpiñà, J. M. Caicedo, Xavier Jordà, Krystian Roleder, Dariusz Kajewski, Amador Perez-Tomas, Emmanuel Defay, and Gustau Catalan	
Multiple structural components and their competition in the intermediate state of antiferroelectric Pb(Zr,Ti)O ₃ (<i>10 pages</i>)	054113
Zheyi An, Hiroko Yokota, Nan Zhang, Marek Paściak, Jan Fábry, Miloš Kopecký, Jiří Kub, Guanjie Zhang, A. M. Glazer, T. R. Welberry, Wei Ren, and Zuo-Guang Ye	
Dynamical topology in ferroelectric nanostructures by $\frac{1}{2}[1\bar{1}0](110)$ dislocations in SrTiO ₃ (<i>7 pages</i>)	054114
Kairi Masuda, Takahiro Shimada, and Takayuki Kitamura	
Sb-5s lone pair dynamics and collinear magnetic ordering in Ba ₂ FeSbSe ₅ (<i>7 pages</i>)	054115
Stefan Maier, Michael W. Gaultois, Nami Matsubara, Wesley Surta, Francoise Damay, Sylvie Hebert, Vincent Hardy, David Berthebaud, and Franck Gascoin	
Inhomogeneous, disordered, and partially ordered systems	
Compositional ordering in relaxor ferroelectric Pb(BB')O ₃ : Nearest neighbor approach (<i>6 pages</i>)	054201
J. Zhang, L. Liu, A. A. Bokov, N. Zhang, D. Wang, Z.-G. Ye, and C.-L. Jia	
Anomalous low-energy properties in amorphous solids and the interplay of electric and elastic interactions of tunneling two-level systems (<i>11 pages</i>)	054202
Alexander Churkin, Shlomi Matityahu, Andrii O. Maksymov, Alexander L. Burin, and Moshe Schechter	
Phase transitions in a non-Hermitian Aubry-André-Harper model (<i>12 pages</i>)	054203
Stefano Longhi	
First-principles study of the anomalous Hall effect based on exact muffin-tin orbitals (<i>9 pages</i>)	054204
Lei Wang (王蕾), Tai Min, and Ke Xia	
Dynamics, dynamical systems, lattice effects:	
Development of semiempirical equation of state of binary functionally graded materials and its influence on generation of ramp compression: Comparison with bilayer graded density impactors (<i>24 pages</i>)	054301
Aditi Ray and Anuradha Singla	
Limits of the quasiharmonic approximation in MgO: Volume dependence of optical modes investigated by infrared reflectivity and <i>ab initio</i> calculations (<i>10 pages</i>)	054302
Eugenio Calandrini, Lorenzo Paulatto, Daniele Antonangeli, Fei He, Ricardo P. S. M. Lobo, Francesco Capitani, Jean-Blaise Brubach, Pascale Roy, Laetitia Vincent, and Paola Giura	
Analog time machine in a photonic system (<i>7 pages</i>)	054303
D. D. Solnyshkov and G. Malpuech	
Dynamic properties of a polaron coupled to dispersive optical phonons (<i>9 pages</i>)	054304
J. Bonča and S. A. Trugman	
Prethermal quasiconserved observables in Floquet quantum systems (<i>9 pages</i>)	054305
Chao Yin, Pai Peng (彭湃), Xiaoyang Huang, Chandrasekhar Ramanathan, and Paola Cappellaro	

(Continued)

ARTICLES

Structure, structural phase transitions, mechanical properties, defects

- Giant magnetocaloric effect driven by first-order magnetostructural transition in cosubstituted Ni-Mn-Sb Heusler compounds: Predictions from *ab initio* and Monte Carlo calculations (12 pages) 054101
Sheuly Ghosh and Subhradip Ghosh
- Structural and vibrational study of $\text{Zn}(\text{IO}_3)_2$ combining high-pressure experiments and density-functional theory (12 pages) 054102
A. Liang, C. Popescu, F. J. Manjon, P. Rodriguez-Hernandez, A. Muñoz, Z. Hebboul, and D. Errandonea
- Disorder effects in $\text{LaAlO}_3:\text{Ho}^{3+}$ single crystals revealed by optical spectra (11 pages) 054103
K. N. Boldyrev, N. M. Abishev, I. E. Mumdzi, S. I. Nikitin, P. J. Deren, B. Z. Malkin, and M. N. Popova
- Second-order nonlinear optical and linear ultraviolet-visible absorption properties of the type-II multiferroic candidates $\text{RbFe}(\text{AO}_4)_2$ ($A = \text{Mo, Se, S}$) (14 pages) 054104
Rachel Owen, Elizabeth Drueke, Charlotte Albunio, Austin Kaczmarek, Wencan Jin, Dimuthu Obeysekera, Sang-Wook Cheong, Junjie Yang, Steven Cundiff, and Liuyan Zhao
- Tailoring submicrometer periodic surface structures via ultrashort pulsed direct laser interference patterning (15 pages) 054105
F. Fraggelakis, G. D. Tsididis, and E. Stratakis
- Breaking of inversion symmetry in NdGaO_3 (14 pages) 054106
Binoy Krishna De, Vivek Dwij, Mayanak K. Gupta, Ranjan Mittal, Himal Bhatt, V. R. Reddy, and V. G. Sathe
- Machine learning metadynamics simulation of reconstructive phase transition (9 pages) 054107
Qunchao Tong, Xiaoshan Luo, Adebayo A. Adeleke, Pengyue Gao, Yu Xie, Hanyu Liu, Quan Li, Yanchao Wang, Jian Lv, Yansun Yao, and Yanming Ma
- Anisotropic elasticity drives negative thermal expansion in monocrystalline SnSe (8 pages) 054108
Ashoka Karunaratne, Prakash Parajuli, Gautam Priyadarshan, Sriparna Bhattacharya, Rahul Rao, Pai-Chun Wei, Yang-Yuan Chen, Joseph R. Gladden, and Apparao M. Rao
- Ultrafast formation of domain walls of a charge density wave in SmTe_3 (6 pages) 054109
M. Trigo, P. Giraldo-Gallo, J. N. Clark, M. E. Kozina, T. Henighan, M. P. Jiang, M. Chollet, I. R. Fisher, J. M. Glowina, T. Katayama, P. S. Kirchmann, D. Leuenberger, H. Liu, D. A. Reis, Z. X. Shen, and D. Zhu
- Stress correlations in frictional granular media (10 pages) 054110
Anaël Lemaître, Chandana Mondal, Itamar Procaccia, and Saikat Roy

