PHYSICAL REVIEW B™

For editorial and subscription correspondence, please see inside front cover
(ISSN: 2469-9950)

PERIODICALS
Postmaster send address changes to:

APS Subscription Services
P.O. Box 41
Annapolis Junction, MD 20701

THIRD SERIES, VOLUME 101, NUMBER 19 *CONTENTS* **MAY 2020-15(I)**

ARTICLES

Electronic structure and strongly correlated systems

Fermi surface of $PtCoO_2$ from quantum oscillations and electronic structure calculations *(9 pages)* 195101
F. Arnold, M. Naumann, H. Rosner, N. Kikugawa, D. Graf, L. Balicas, T. Terashima, S. Uji, H. Takatsu, S. Khim, A. P. Mackenzie, and E. Hassinger

Permutation cycles of hardcore Bose-Hubbard models on square and kagome lattices *(7 pages)* 195103
L. Shpani, F. Lingua, W. Wang (王巍), and B. Capogrosso-Sansone

Inverse design of broadband highly reflective metasurfaces using neural networks *(9 pages)* 195104
Eric S. Harper, Eleanor J. Coyle, Jonathan P. Vernon, and Matthew S. Mills

Quantum Hall phase and chiral edge states simulated by a coupled dipole method *(6 pages)* 195105
Minkyung Kim and Junsuk Rho

Drag viscosity of metals and its connection to Coulomb drag *(14 pages)* 195106
Yunxiang Liao and Victor Galitski

Stable and metastable kinetic ferromagnetism on a ring *(5 pages)* 195107
Ilya Ivantsov, Hernan B. Xavier, Alvaro Ferraz, and Evgenii Kochetov

Slow magnetic fluctuations and critical slowing down in $Sr_2Ir_{1-x}Rh_xO_4$ *(9 pages)* 195108
C. Tan, Z. F. Ding, J. Zhang, Z. H. Zhu, O. O. Bernal, P. C. Ho, A. D. Hillier, A. Koda, H. Luetkens, G. D. Morris, D. E. MacLaughlin, and L. Shu

Excitations with projected entangled pair states using the corner transfer matrix method *(12 pages)* 195109
Boris Ponsioen and Philippe Corboz

Magnetization plateaus of spin-$\frac{1}{2}$ system on a 5/7 skewed ladder *(8 pages)* 195110
Dayasindhu Dey, Sambunath Das, Manoranjan Kumar, and S. Ramasesha

Two-dimensional topological semimetals protected by symmorphic symmetries *(10 pages)* 195111
Wei Luo, Junyi Ji, Jinlian Lu, Xiuwen Zhang, and Hongjun Xiang

Pressure tuning of structural and magnetic transitions in $EuAg_4As_2$ *(8 pages)* 195112
Sergey L. Bud'ko, Li Xiang, Chaowei Hu, Bing Shen, Ni Ni, and Paul C. Canfield

Continuous momentum dependence in the dynamical cluster approximation *(10 pages)* 195114
Urs R. Hähner, Thomas A. Maier, and Thomas C. Schulthess

Copyright 2020 by American Physical Society

(Continued)

2469-9950(20200515)101:19;1-8

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 101, NUMBER 19** **MAY 2020-15(I)**

Short-range charge fluctuations in the two-dimensional Hubbard model *(8 pages)* 195115
Xinyang Dong and Emanuel Gull

Cupratelike electronic and magnetic properties of layered transition-metal difluorides from first-principles calculations *(5 pages)* 195116
Clark Miller and Antia Sanchez Botana

Topological and nontopological features of generalized Su-Schrieffer-Heeger models *(12 pages)* 195117
N. Ahmadi, J. Abouie, and D. Baeriswyl

Collective modes in excitonic insulators: Effects of electron-phonon coupling and signatures in the optical response *(17 pages)* 195118
Yuta Murakami, Denis Golež, Tatsuya Kaneko, Akihisa Koga, Andrew J. Millis, and Philipp Werner

Hybrid purification and sampling approach for thermal quantum systems *(9 pages)* 195119
Jing Chen and E. M. Stoudenmire

Absence of equilibrium edge currents in theoretical models of topological insulators *(9 pages)* 195120
Wei Chen

Symmetry-protected topological phases in a two-leg SU(N) spin ladder with unequal spins *(19 pages)* 195121
S. Capponi, P. Fromholz, P. Lecheminant, and K. Totsuka

Magnetic phase diagram and magnetoelastic coupling of $NiTiO_3$ *(8 pages)* 195122
K. Dey, S. Sauerland, J. Werner, Y. Skourski, M. Abdel-Hafiez, R. Bag, S. Singh, and R. Klingeler

Emergence of quasiparticle multiplets in curium *(8 pages)* 195123
Li Huang, Ruofan Chen, and Haiyan Lu

Spin-wave study of entanglement and Rényi entropy for coplanar and collinear magnetic orders in two-dimensional quantum Heisenberg antiferromagnets *(11 pages)* 195124
Dag-Vidar Bauer and J. O. Fjærestad

DFT + DMFT study of spin-charge-lattice coupling in covalent $LaCoO_3$ *(12 pages)* 195125
Hyowon Park, Ravindra Nanguneri, and Anh T. Ngo

Gauge theories for the thermal Hall effect *(17 pages)* 195126
Haoyu Guo, Rhine Samajdar, Mathias S. Scheurer, and Subir Sachdev

Majorana zero modes in a quantum wire platform without Rashba spin-orbit coupling *(13 pages)* 195127
Ömer M. Aksoy and John R. Tolsma

Doped NiO: The mottness of a charge transfer insulator *(15 pages)* 195128
Friederike Wrobel, Hyowon Park, Changhee Sohn, Haw-Wen Hsiao, Jian-Min Zuo, Hyeondeok Shin, Ho Nyung Lee, P. Ganesh, Anouar Benali, Paul R. C. Kent, Olle Heinonen, and Anand Bhattacharya

Influence of finite temperature exchange-correlation effects in hydrogen *(13 pages)* 195129
Kushal Ramakrishna, Tobias Dornheim, and Jan Vorberger

Non-Abelian topology of nodal-line rings in $\mathcal{PT}$-symmetric systems *(29 pages)* 195130
Apoorv Tiwari and Tomáš Bzdušek

Unified structure for exact towers of scar states in the Affleck-Kennedy-Lieb-Tasaki and other models *(17 pages)* 195131
Daniel K. Mark, Cheng-Ju Lin, and Olexei I. Motrunich

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 101, NUMBER 19** **MAY 2020-15(I)**

Evidence for an orbital dependent Mott transition in the ladders of $(La, Ca)_xSr_{14-x}Cu_{24}O_{41}$ derived by electron energy loss spectroscopy *(8 pages)* 195132
Friedrich Roth, Alexandre Revcolevschi, Bernd Büchner, Martin Knupfer, and Jörg Fink

Antichiral edge states in Heisenberg ferromagnet on a honeycomb lattice *(12 pages)* 195133
Dhiman Bhowmick and Pinaki Sengupta

Entanglement as geometry and flow *(12 pages)* 195134
Sudipto Singha Roy, Silvia N. Santalla, Javier Rodríguez-Laguna, and Germán Sierra

Unveiling charge density wave quantum phase transitions by x-ray diffraction *(5 pages)* 195135
F. B. Carneiro, L. S. I. Veiga, J. R. L. Mardegan, R. Khan, C. Macchiutti, A. López, and E. M. Bittar

Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model assisted by machine learning *(10 pages)* 195136
Kazuya Shinjo, Shigetoshi Sota, Seiji Yunoki, and Takami Tohyama

Understanding plasmon dispersion in nearly free electron metals: Relevance of exact constraints for exchange-correlation kernels within time-dependent density functional theory *(9 pages)* 195137
Niraj K. Nepal, Santosh Adhikari, Bimal Neupane, Shiqi Ruan, Santosh Neupane, and Adrienn Ruzsinszky

Emergent conservation laws and nonthermal states in the mixed-field Ising model *(12 pages)* 195138
Jonathan Wurtz and Anatoli Polkovnikov

Signatures of bosonic excitations in high-harmonic spectra of Mott insulators *(12 pages)* 195139
Markus Lysne, Yuta Murakami, and Philipp Werner

Tunable spin/charge Kondo effect at a double superconducting island connected to two spinless quantum wires *(22 pages)* 195140
Domenico Giuliano, Luca Lepori, and Andrea Nava

Approximating power of machine-learning ansatz for quantum many-body states *(9 pages)* 195141
Artem Borin and Dmitry A. Abanin

Metal-to-metal transition and heavy-electron state in $Nd_4Ni_3O_{10-\delta}$ *(10 pages)* 195142
Bai-Zhuo Li, Cao Wang, P. T. Yang, J. P. Sun, Ya-Bin Liu, Jifeng Wu, Zhi Ren, J.-G. Cheng, Guang-Ming Zhang, and Guang-Han Cao

Orbital corner states on breathing kagome lattices *(7 pages)* 195143
Xiancong Lu, Ying Chen, and Huanyang Chen

Topological properties of Mo_2C and W_2C superconductors *(6 pages)* 195144
Ning-Ning Zhao, Peng-Jie Guo, Xiao-Qin Lu, Qiang Han, Kai Liu, and Zhong-Yi Lu

Evidence for pseudo–Jahn-Teller distortions in the charge density wave phase of $1T$-$TiSe_2$ *(6 pages)* 195145
A. Wegner, J. Zhao, J. Li, J. Yang, A. A. Anikin, G. Karapetrov, K. Esfarjani, D. Louca, and U. Chatterjee

Magnetic structure of Cd-doped $CeIrIn_5$ *(6 pages)* 195146
K. Beauvois, N. Qureshi, R. Tsunoda, Y. Hirose, R. Settai, D. Aoki, P. Rodière, A. McCollam, and I. Sheikin

Non-Bloch band theory of non-Hermitian Hamiltonians in the symplectic class *(12 pages)* 195147
Kohei Kawabata, Nobuyuki Okuma, and Masatoshi Sato

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B THIRD SERIES, VOLUME 101, NUMBER 19 MAY 2020-15(I)

Semiconductors I: bulk

Examining the validity of the two-dimensional conical model to describe the three-dimensional $ZrTe_5$ *(8 pages)* 195201
Yi-Xiang Wang and Fuxiang Li

Spin pump induced inverse spin Hall effect observed in Bi-doped *n*-type Si *(7 pages)* 195202
A. A. Ezhevskii, D. V. Guseinov, A. V. Soukhorukov, A. V. Novikov, D. V. Yurasov, and N. S. Gusev

Understanding semiconductor valence mass *(10 pages)* 195203
Monique Combescot and Shiue-Yuan Shiau

Temperature-dependent photoluminescence in Ge: Experiment and theory *(22 pages)* 195204
José Menéndez, Christian D. Poweleit, and Sean E. Tilton

Semiconductors II: surfaces, interfaces, microstructures, and related topics

Perfect quantum cloaking of tilted cylindrical nanocavities *(8 pages)* 195301
Constantinos Valagiannopoulos

Excitonic complexes in InAs/InP nanowire quantum dots *(12 pages)* 195302
Michał Zieliński

From fractional solitons to Majorana fermions in a paradigmatic model of topological superconductivity *(7 pages)* 195303
N. Traverso Ziani, C. Fleckenstein, L. Vigliotti, B. Trauzettel, and M. Sassetti

Optical and electronic properties of low-density InAs/InP quantum-dot-like structures designed for single-photon emitters at telecom wavelengths *(14 pages)* 195304
P. Holewa, M. Gawełczyk, C. Ciostek, P. Wyborski, S. Kadkhodazadeh, E. Semenova, and M. Syperek

Two-dimensional CP_3 monolayer and its fluorinated derivative with promising electronic and optical properties: A theoretical study *(8 pages)* 195305
Moumita Kar, Ritabrata Sarkar, Sougata Pal, and Pranab Sarkar

Anticorrelation of compressibility and resistivity in a microwave-irradiated two-dimensional electron system *(5 pages)* 195306
Jian Mi, Long Zhang, Jianli Wang, Saeed Fallahi, Geoffrey C. Gardner, M. J. Manfra, and Chi Zhang

Density functional calculations for structures and energetics of atomic steps and their implication for surface morphology on Si-face SiC polar surfaces *(10 pages)* 195307
Kaori Seino and Atsushi Oshiyama

Mixed-strategy approach to band-edge analysis and modeling in semiconductors *(15 pages)* 195308
Amrah Canul, Dinesh Thapa, Jesse Huso, Leah Bergman, Richard Vaughan Williams, and Ruprecht Machleidt

Topological states in generalized electric quadrupole insulators *(11 pages)* 195309
Chang-An Li and Shu-Shan Wu

Quantum Hall effects of exciton condensate in topological flat bands *(7 pages)* 195310
Tian-Sheng Zeng, D. N. Sheng, and W. Zhu

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B THIRD SERIES, VOLUME 101, NUMBER 19 MAY 2020-15(I)

Surface physics, nanoscale physics, low-dimensional systems

Tuning electronic and magnetic properties of the graphone/Ni(111) interface by oxygen intercalation: A first-principles prediction *(11 pages)* 195401
Niharika Joshi, C. Gaurav, Nirmalya Ballav, and Prasenjit Ghosh

Quantum teleportation of single-electron states *(12 pages)* 195403
Edvin Olofsson, Peter Samuelsson, Nicolas Brunner, and Patrick P. Potts

Tunneling into a Luttinger liquid coupled to acoustic phonons out of equilibrium *(19 pages)* 195404
P. A. Nosov, R. A. Niyazov, and D. N. Aristov

Superconducting proximity effect in a transparent van der Waals superconductor-metal junction *(13 pages)* 195405
Jing Li, Han-Bing Leng, Hailong Fu, Kenji Watanabe, Takashi Taniguchi, Xin Liu, Chao-Xing Liu, and Jun Zhu

Manipulating Berry curvature in hBN/bilayer graphene commensurate heterostructures *(8 pages)* 195406
Afsal Kareekunnan, Manoharan Muruganathan, and Hiroshi Mizuta

Annihilation mechanism of excitons in a MoS_2 monolayer through direct Förster-type energy transfer and multistep diffusion *(9 pages)* 195407
Kwang Jin Lee, Wei Xin, and Chunlei Guo

Heat transport in carbon nanotubes: Length dependence of phononic conductivity from the Boltzmann transport equation and molecular dynamics *(11 pages)* 195408
Daniel Bruns, Alireza Nojeh, A. Srikantha Phani, and Jörg Rottler

Flexural modes of graphene resonators derived from the reactive empirical bond-order potential *(10 pages)* 195409
Yisen Wang and Liang Huang

Structure-specific mode-resolved phonon coherence and specularity at graphene grain boundaries *(7 pages)* 195410
Zhun-Yong Ong, Georg Schusteritsch, and Chris J. Pickard

Towards more general constitutive relations for metamaterials: A checklist for consistent formulations *(23 pages)* 195411
Fatima Z. Goffi, Karim Mnasri, Michael Plum, Carsten Rockstuhl, and Andrii Khrabustovskyi

Topological Dirac nodal loops in nonsymmorphic hydrogenated monolayer boron *(11 pages)* 195412
N. T. Cuong, I. Tateishi, M. Cameau, M. Niibe, N. Umezawa, B. Slater, K. Yubuta, T. Kondo, M. Ogata, S. Okada, and I. Matsuda

Coverage-dependent electronic and optical properties of H- or F-passivated Si/Ag(111) from first principles *(10 pages)* 195413
A. Ugolotti, G. P. Brivio, and Guido Fratesi

One-photon absorption by inorganic perovskite nanocrystals: A theoretical study *(15 pages)* 195414
T. P. T. Nguyen, S. A. Blundell, and C. Guet

Proximity-induced spin-orbit splitting in graphene nanoribbons on transition-metal dichalcogenides *(16 pages)* 195416
Yohanes S. Gani, Eric J. Walter, and Enrico Rossi

Theory of exciton-electron scattering in atomically thin semiconductors *(13 pages)* 195417
Christian Fey, Peter Schmelcher, Atac Imamoglu, and Richard Schmidt

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 101, NUMBER 19** **MAY 2020-15(I)**

Persistent spin textures and currents in wurtzite nanowire-based quantum structures *(16 pages)* 195418
Michael Kammermeier, Adrian Seith, Paul Wenk, and John Schliemann

Large RKKY coupling from multiple scattering in armchair graphene nanoribbons *(12 pages)* 195419
Van Minh Nguyen and C. S. Chu

Transport properties of coupled Majorana bound states in the Coulomb blockade regime *(14 pages)* 195420
Johan Ekström, Patrik Recher, and Thomas L. Schmidt

Majorana-like localized spin density without bound states in topologically trivial spin-orbit coupled nanowires *(16 pages)* 195421
Lorenzo Rossi, Fabrizio Dolcini, and Fausto Rossi

Anisotropy of the spin-polarized edge current in monolayer transition metal dichalcogenide zigzag nanoribbons *(13 pages)* 195422
J. H. Correa, A. C. Dias, L. Villegas-Lelovsky, Jiyong Fu, Leonor Chico, and Fanyao Qu

Thermodynamic uncertainty relation in atomic-scale quantum conductors *(9 pages)* 195423
Hava Meira Friedman, Bijay K. Agarwalla, Ofir Shein-Lumbroso, Oren Tal, and Dvira Segal

Phase diagrams of single-layer two-dimensional transition metal dichalcogenides: Landau theory *(15 pages)* 195424
Anna N. Morozovska, Eugene A. Eliseev, Kevin D. Stubbs, Rama Vasudevan, Yunseok Kim, and Sergei V. Kalinin

Effective continuum model for relaxed twisted bilayer graphene and moiré electron-phonon interaction *(13 pages)* 195425
Mikito Koshino and Nguyen N. T. Nam

Density functionals combined with van der Waals corrections for graphene adsorbed on layered materials *(11 pages)* 195426
Hong Tang, Shah Tanvir ur Rahman Chowdhury, Jianmin Tao, and John P. Perdew

Entropic quantum machine *(8 pages)* 195427
Ryoko Hatakeyama and Akira Shimizu

Decoherence dynamics of Majorana qubits under braiding operations *(10 pages)* 195428
Hon-Lam Lai and Wei-Min Zhang

Many-body effects, orbital mixing, and cyclotron resonance in bilayer graphene *(12 pages)* 195429
K. Shizuya

Overlapping Andreev states in semiconducting nanowires: Competition of one-dimensional and three-dimensional propagation *(12 pages)* 195430
Viktoriia Kornich, Hristo S. Barakov, and Yuli V. Nazarov

Interparticle coulombic decay in coupled quantum dots: Enhanced energy transfer via bridge assisted mechanisms *(6 pages)* 195431
Hicham Agueny, Maxime Pesche, Bastien Lutet-Toti, Tsveta Miteva, Axel Molle, Jérémie Caillat, and Nicolas Sisourat

Landau level phases in bilayer graphene under pressure at charge neutrality *(13 pages)* 195432
Brett R. Green and Jorge O. Sofo

Fate of quantum anomalous Hall effect in the presence of external magnetic fields and particle-hole asymmetry *(16 pages)* 195433
Jan Böttcher, Christian Tutschku, and Ewelina M. Hankiewicz

(Continued)

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).

PHYSICAL REVIEW B **THIRD SERIES, VOLUME 101, NUMBER 19** **MAY 2020-15(I)**

Partially embedded Pb chains on a vicinal Si(113) surface *(7 pages)* 195434
L. Żurawek, M. Kopciuszyński, M. Dachniewicz, M. Stróżak, M. Krawiec, M. Jałochowski, and R. Zdyb

Enhanced topological protection in planar quasi-one-dimensional channels with periodically modulated width *(18 pages)* 195435
Benjamin D. Woods and Tudor D. Stanescu

Nanomechanics of a hydrogen molecule suspended between two equally charged tips *(13 pages)* 195436
W. Schattke, T. Frederiksen, M. A. Van Hove, and R. Díez Muiño

First-principles study of the excitonic effect on two-photon absorption of semiconductors: Theory and application to MoS_2 and WS_2 monolayers *(9 pages)* 195437
You-Zhao Lan and Xiao-Hu Bao

Programable two-qubit gates in capacitively coupled flopping-mode spin qubits *(8 pages)* 195438
Jorge Cayao, Mónica Benito, and Guido Burkard

Role of quantum confinement and interlayer coupling in CrI_3-graphene magnetic tunnel junctions *(7 pages)* 195439
Jonathan J. Heath, Marcio Costa, Marco Buongiorno-Nardelli, and Marcelo A. Kuroda

COMMENTS

Comment on "Study of counterintuitive transport properties in the Aubry-André-Harper model via entanglement entropy and persistent current" *(4 pages)* 197101
Francisco M. Fernández, Diego R. Alcoba, Alicia Torre, Luis Lain, Ofelia B. Oña, and Elias Ríos

Comment on "Electron states for gapped pseudospin-1 fermions in the field of a charged impurity" *(3 pages)* 197102
R. Van Pottelberge

The editors and referees of PRB find these papers to be of particular interest, importance, or clarity. Please see our Announcement Phys. Rev. B 77, 130001 (2008).