PHYSICAL REVIEW B **THIRD SERIES, VOLUME 103, NUMBER 15** **APRIL 2021-15(I)**

Determining the optimum thickness for high harmonic generation from nanoscale thin films: An *ab initio* computational study *(11 pages)* 155426
Shunsuke Yamada and Kazuhiro Yabana

Wigner wave packets: Transmission, reflection, and tunneling *(22 pages)* 155427
Kevin L. Jensen, Joel L. Lebowitz, Jeanne M. Riga, Donald A. Shiffler, and Rebecca Seviour

Phonon-mediated tunneling into a two-dimensional electron gas on the Be(0001) surface *(7 pages)* 155428
Hermann Osterhage, Roland Wiesendanger, and Stefan Krause

Dynamical polarization function and plasmons in monolayer XSe (X = In, Ga) *(8 pages)* 155429
Ma Zhou

Magnon dispersion in bilayers of two-dimensional ferromagnets *(8 pages)* 155430
Lara C. Ortmanns, Gerrit E. W. Bauer, and Yaroslav M. Blanter

Tunneling magnetoresistance and spin-valley polarization in magnetic silicene superlattices *(12 pages)* 155431
J. G. Rojas-Briseño, M. A. Flores-Carranza, P. Villasana-Mercado, S. Molina-Valdovinos, and I. Rodríguez-Vargas

Effects of temperature on strain engineering and transition-metal adatom magnetization in phosphorene: *Ab initio* molecular dynamics studies *(14 pages)* 155432
Shuchao Zhang and Hong Sun

Anomalous Floquet tunneling in uniaxially strained graphene *(14 pages)* 155433
Yonatan Betancur-Ocampo, Parisa Majari, Diego Espitia, François Leyvraz, and Thomas Stegmann

Thermal rectification through a nonlinear quantum resonator *(28 pages)* 155434
Bibek Bhandari, Paolo Andrea Erdman, Rosario Fazio, Elisabetta Paladino, and Fabio Taddei

Role of coherence in quantum-dot-based nanomachines within the Coulomb blockade regime *(17 pages)* 155435
Federico D. Ribetto, Raúl A. Bustos-Marún, and Hernán L. Calvo

ERRATA

Erratum: Crystal-field theory of Co^{2+} in doped ZnO [Phys. Rev. B **74**, 155201 (2006)] *(1 page)* . . . . . 159901(E)
R. O. Kuzian, A. M. Daré, P. Sati, and R. Hayn

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 103, NUMBER 15** **APRIL 2021-15(I)**

Electron-electron interactions and weak antilocalization in few-layer $ZrTe_5$ devices *(8 pages)* 155408
Zhijian Xie, Xinjian Wei, Shimin Cao, Yu Zhang, Shili Yan, G. D. Gu, Qiang Li, and Jian-Hao Chen

Gauge invariance of light-matter interactions in first-principle tight-binding models *(12 pages)* 155409
Michael Schüler, Jacob A. Marks, Yuta Murakami, Chunjing Jia, and Thomas P. Devereaux

Moiré edge states in twisted bilayer graphene and their topological relation to quantum pumping *(9 pages)* 155410
Manato Fujimoto and Mikito Koshino

CoN_4C_2: Two-dimensional cobalt carbonitride with a flat-band feature *(6 pages)* 155411
Dapeng Liu, Panjun Feng, Miao Gao, and Xun-Wang Yan

Effect of local geometry on magnetic property of nitric oxide on Au(110)-(1×2) *(8 pages)* 155412
H. Koshida, H. Okuyama, S. Hatta, T. Aruga, and E. Minamitani

Time-dependent forces between a swift electron and a small nanoparticle within the dipole approximation *(11 pages)* 155413
J. Castrejón-Figueroa, J. Á. Castellanos-Reyes, C. Maciel-Escudero, A. Reyes-Coronado, and R. G. Barrera

Thermally assisted Pauli spin blockade in double quantum dots *(7 pages)* 155414
M. Kondo, S. Miyota, W. Izumida, S. Amaha, and T. Hatano

Theory for linear and nonlinear planar Hall effect in topological insulator thin films *(7 pages)* 155415
Wen Rao, Yong-Long Zhou, Yong-jia Wu, Hou-Jian Duan, Ming-Xun Deng, and Rui-Qiang Wang

Transition metal dichalcogenide monolayers in an ultrashort optical pulse: Femtosecond currents and anisotropic electron dynamics *(9 pages)* 155416
S. Azar Oliaei Motlagh, Vadym Apalkov, and Mark I. Stockman

Probing non-Hermitian phase transitions in curved space via quench dynamics *(10 pages)* 155417
Ygor Pará, Giandomenico Palumbo, and Tommaso Macrì

Dark-bright excitons mixing in alloyed InGaAs self-assembled quantum dots *(15 pages)* 155418
Michał Zieliński

Quantum network approach to spin interferometry driven by Abelian and non-Abelian fields *(13 pages)* 155419
A. Hijano, T. L. van den Berg, D. Frustaglia, and D. Bercioux

Quench dynamics of a correlated quantum dot sandwiched between normal-metal and superconducting leads *(14 pages)* 155420
K. Wrześniewski, B. Baran, R. Taranko, T. Domański, and I. Weymann

Effects of domain walls in bilayer graphene in an external magnetic field *(18 pages)* 155422
Nico S. Baßler and Kai Phillip Schmidt

Harnessing the photonic local density of states in graphene moiré superlattices *(6 pages)* 155423
W. J. M. Kort-Kamp, F. J. Culchac, F. S. S. Rosa, C. Farina, Rodrigo B. Capaz, and F. A. Pinheiro

Conductance suppression by nonmagnetic point defects in helical edge channels of two-dimensional topological insulators *(15 pages)* 155424
Vladimir A. Sablikov and Aleksei A. Sukhanov

Topological microelectromechanical systems *(5 pages)* 155425
Motohiko Ezawa

(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 103, NUMBER 15** **APRIL 2021-15(I)**

Magnetization energy current in the axial magnetic effect *(8 pages)* 155202
Atsuo Shitade and Yasufumi Araki

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

Superradiantlike dynamics of nuclear spins by nonadiabatic electron shuttling *(17 pages)* 155301
Yinan Fang, Ying-Dan Wang, Rosario Fazio, and Stefano Chesi

Polariton spin jets through optical control *(9 pages)* 155302
L. Pickup, J. D. Töpfer, H. Sigurdsson, and P. G. Lagoudakis

Geometric response of quantum Hall states to electric fields *(11 pages)* 155303
YingKang Chen, Guodong Jiang, and Rudro R. Biswas

Landau level spectroscopy of the PbSnSe topological crystalline insulator *(11 pages)* 155304
Kristupas Kazimieras Tikuišis, Jan Wyzula, Lukáš Ohnoutek, Petr Cejpek, Klára Uhlířová, Michael Hakl, Clément Faugeras, Karel Výborný, Akihiro Ishida, Martin Veis, and Milan Orlita

Maximization and minimization of interfacial thermal conductance by modulating the mass distribution of the interlayer *(9 pages)* 155305
Lina Yang, Xiao Wan, Dengke Ma, Yi Jiang, and Nuo Yang

Origin of the $\nu = 1/2$ fractional quantum Hall effect in wide quantum wells *(28 pages)* 155306
Tongzhou Zhao, William N. Faugno, Songyang Pu, Ajit C. Balram, and J. K. Jain

Surface physics, nanoscale physics, low-dimensional systems

Dirac states in the noncentrosymmetric superconductor BiPd *(7 pages)* 155401
Arindam Pramanik, Ram Prakash Pandeya, Denis V. Vyalikh, Alexander Generalov, Paolo Moras, Asish K. Kundu, Polina M. Sheverdyaeva, Carlo Carbone, Bhanu Joshi, A. Thamizhavel, S. Ramakrishnan, and Kalobaran Maiti

Plasmonic modes at inclined edges of anisotropic two-dimensional materials *(14 pages)* 155402
Alexey A. Sokolik, Oleg V. Kotov, and Yurii E. Lozovik

Fano resonance enhanced multiphoton photoemission from single plasmonic nanostructure excited by femtosecond laser *(7 pages)* 155403
Guiqi Wang, Xiaowei Song, Meiling Jiang, Peng Lang, Boyu Ji, Zheyu Fang, and Jingquan Lin

Polariton topological transition effects on radiative heat transfer *(13 pages)* 155404
Cheng-Long Zhou, Xiao-Hu Wu, Yong Zhang, Hong-Liang Yi, and Mauro Antezza

Quantifying the interplay between fine structure and geometry of an individual molecule on a surface *(13 pages)* 155405
Manuel Steinbrecher, Werner M. J. van Weerdenburg, Etienne F. Walraven, Niels P. E. van Mullekom, Jan W. Gerritsen, Fabian D. Natterer, Danis I. Badrtdinov, Alexander N. Rudenko, Vladimir V. Mazurenko, Mikhail I. Katsnelson, Ad van der Avoird, Gerrit C. Groenenboom, and Alexander A. Khajetoorians

Quantum Monte Carlo simulation of BEC-impurity tunneling *(6 pages)* 155406
A. S. Popova, V. V. Tiunova, and A. N. Rubtsov

Tunneling processes between Yu-Shiba-Rusinov bound states *(15 pages)* 155407
A. Villas, R. L. Klees, G. Morrás, H. Huang, C. R. Ast, G. Rastelli, W. Belzig, and J. C. Cuevas

(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 103, NUMBER 15** **APRIL 2021-15(I)**

Modeling multiorbital effects in Sr_2IrO_4 under strain and a Zeeman field *(12 pages)* 155147
Lena Engström, T. Pereg-Barnea, and William Witczak-Krempa

Observation of topological Dirac fermions and surface states in superconducting $BaSn_3$ *(7 pages)* 155148
K. Huang, A. Y. Luo, C. Chen, G. N. Zhang, X. L. Liu, Y. W. Li, F. Wu, S. T. Cui, Z. Sun, Chris Jozwiak, Aaron Bostwick, Eli Rotenberg, H. F. Yang, L. X. Yang, G. Xu, Y. F. Guo, Z. K. Liu, and Y. L. Chen

Trigonal warping, satellite Dirac points, and multiple field tuned topological transitions in twisted double bilayer graphene *(16 pages)* 155149
Priyanka Mohan, Unmesh Ghorai, and Rajdeep Sensarma

Hidden wave function of twisted bilayer graphene: The flat band as a Landau level *(8 pages)* 155150
Fedor K. Popov and Alexey Milekhin

Dynamics of local magnetic moments induced by itinerant Weyl electrons *(16 pages)* 155151
Predrag Nikolić

Spinorial formulation of the *GW*-BSE equations and spin properties of excitons in two-dimensional transition metal dichalcogenides *(20 pages)* 155152
Margherita Marsili, Alejandro Molina-Sánchez, Maurizia Palummo, Davide Sangalli, and Andrea Marini

Nonmagnetic-magnetic transition and magnetically ordered structure in SmS *(5 pages)* 155153
S. Yoshida, T. Koyama, H. Yamada, Y. Nakai, K. Ueda, T. Mito, K. Kitagawa, and Y. Haga

Spin and charge order in doped spin-orbit coupled Mott insulators *(12 pages)* 155154
Mehdi Biderang, Alireza Akbari, and Jesko Sirker

Gap generation and flat band catalysis in dice model with local interaction *(12 pages)* 155155
E. V. Gorbar, V. P. Gusynin, and D. O. Oriekhov

Parquet approximation and one-loop renormalization group: Equivalence on the leading-logarithmic level *(20 pages)* 155156
Jan Diekmann and Severin G. Jakobs

Moiré superlattice on the surface of a topological insulator *(24 pages)* 155157
Jennifer Cano, Shiang Fang, J. H. Pixley, and Justin H. Wilson

Testing the Green's function coupled cluster singles and doubles impurity solver on real materials within the framework of self-energy embedding theory *(12 pages)* 155158
Chia-Nan Yeh, Avijit Shee, Sergei Iskakov, and Dominika Zgid

Quarter-filled Kane-Mele Hubbard model: Dirac half metals *(6 pages)* 155159
S. Mellaerts, R. Meng, V. Afanasiev, J. W. Seo, M. Houssa, and J.-P. Locquet

Fractionalized quantum criticality in spin-orbital liquids from field theory beyond the leading order *(18 pages)* . . . 155160
Shouryya Ray, Bernhard Ihrig, Daniel Kruti, John A. Gracey, Michael M. Scherer, and Lukas Janssen

Thermal effects in non-Fermi liquid superconductivity *(21 pages)* 155161
Jeremias Aguilera Damia, Mario Solís, and Gonzalo Torroba

Semiconductors I: bulk

Quantum transport properties of β-Bi_4I_4 near and well beyond the extreme quantum limit *(7 pages)* 155201
Peipei Wang, Fangdong Tang, Peng Wang, Haipeng Zhu, Chang-Woo Cho, Junfeng Wang, Xu Du, Yonghong Shao, and Liyuan Zhang

(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 103, NUMBER 15** **APRIL 2021-15(I)**

Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals *(17 pages)* 155127
F. Sarcinella, E. Fabiano, L. A. Constantin, and F. Della Sala

Electron-phonon hydrodynamics *(26 pages)* 155128
Xiaoyang Huang and Andrew Lucas

Homotopical characterization of non-Hermitian band structures *(11 pages)* 155129
Zhi Li and Roger S. K. Mong

Field tensor network states *(6 pages)* 155130
Anne E. B. Nielsen, Benedikt Herwerth, J. Ignacio Cirac, and Germán Sierra

High-throughput search for magnetic topological materials using spin-orbit spillage, machine learning, and experiments *(11 pages)* 155131
Kamal Choudhary, Kevin F. Garrity, Nirmal J. Ghimire, Naween Anand, and Francesca Tavazza

Correlation driven metallic and half-metallic phases in a band insulator *(15 pages)* 155132
Soumen Bag, Arti Garg, and H. R. Krishnamurthy

Enhancing superconductivity of $Lu_5Rh_6Sn_{18}$ by atomic disorder *(16 pages)* 155133
A. Ślebarski, M. Fijałkowski, M. M. Maśka, J. Deniszczyk, P. Zajdel, B. Trump, and A. Yakovenko

Local topological markers in odd dimensions *(13 pages)* 155134
Joseph Sykes and Ryan Barnett

Population control bias and importance sampling in full configuration interaction quantum Monte Carlo *(14 pages)* 155135
Khaldoon Ghanem, Niklas Liebermann, and Ali Alavi

Structural chirality of β-Mn *(8 pages)* 155136
S. W. Lovesey

Evolution of electronic states during change from a Mott commensurate to a nearly commensurate state in Nb-substituted $1T$-TaS_2 observed by scanning tunneling microscopy and spectroscopy *(6 pages)* 155137
S. Ohta, S. Kobayashi, S. Moroi, A. Nomura, and H. Sakata

Effects of energy extensivity on the quantum phases of long-range interacting systems *(12 pages)* 155139
T. Botzung, D. Hagenmüller, G. Masella, J. Dubail, N. Defenu, A. Trombettoni, and G. Pupillo

Type-II fractons from coupled spin chains and layers *(14 pages)* 155140
Dominic J. Williamson and Trithep Devakul

Electronic structures, charge transfer, and charge order in twisted transition metal dichalcogenide bilayers *(6 pages)* 155142
Yang Zhang, Tongtong Liu, and Liang Fu

One-dimensional model for deconfined criticality with $\mathbb{Z}_3 \times \mathbb{Z}_3$ symmetry *(24 pages)* 155143
Brenden Roberts, Shenghan Jiang, and Olexei I. Motrunich

Extremely large magnetoresistance from electron-hole compensation in the nodal-loop semimetal ZrP_2 *(8 pages)* 155144
J. Bannies, E. Razzoli, M. Michiardi, H.-H. Kung, I. S. Elfimov, M. Yao, A. Fedorov, J. Fink, C. Jozwiak, A. Bostwick, E. Rotenberg, A. Damascelli, and C. Felser

(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 103, NUMBER 15** **APRIL 2021-15(I)**

Transmission in a Fano-Anderson chain with a topological defect *(12 pages)* 155111
Ritu Nehra, Ajith Ramachandran, Sebastian Wüster, and Auditya Sharma

Accidental and symmetry-protected bound states in the continuum in a photonic-crystal slab: A resonant-state expansion study *(11 pages)* 155112
Sam Neale and Egor A. Muljarov

First-principles identification of topological crystalline insulators with C_2 rotation anomaly *(8 pages)* 155113
Zhipeng Cao, Feng Tang, Di Wang, and Xiangang Wan

Variety of scenarios for magnetic exchange response in topological insulators *(16 pages)* 155114
I. A. Nechaev and E. E. Krasovskii

Orbital-selective coherence-incoherence crossover and metal-insulator transition in Cu-doped NaFeAs *(8 pages)* 155115
S. L. Skornyakov, V. I. Anisimov, and I. Leonov

Crystal, local atomic, and local electronic structures of $YbFe_2Zn_{20-x}Cd_x$ ($0 \leqslant x \leqslant 1.4$): A multiband system with possible coexistence of light and heavy fermions *(8 pages)* 155116
A. Fahl, R. Grossi, D. Rigitano, M. Cabrera-Baez, M. A. Avila, C. Adriano, and E. Granado

Electronic structure and topological phases of the magnetic layered materials $MnBi_2Te_4$, $MnBi_2Se_4$, and $MnSb_2Te_4$ *(9 pages)* 155118
Ping Li, Jiangying Yu, Ying Wang, and Weidong Luo

Linkage between scattering rates and superconductivity in doped ferropnictides *(8 pages)* 155119
J. Fink, E. D. L. Rienks, M. Yao, R. Kurleto, J. Bannies, S. Aswartham, I. Morozov, S. Wurmehl, T. Wolf, F. Hardy, C. Meingast, H. S. Jeevan, J. Maiwald, P. Gegenwart, C. Felser, and B. Büchner

Dissecting Mott and charge-density wave dynamics in the photoinduced phase of $1T$-TaS_2 *(7 pages)* 155120
Alberto Simoncig, Matija Stupar, Barbara Ressel, Tanusree Saha, Primoz Rebernik Ribic, and Giovanni De Ninno

Local electronic structure of dilute hydrogen in β-MnO_2 *(9 pages)* 155121
H. Okabe, M. Hiraishi, A. Koda, S. Takeshita, K. M. Kojima, I. Yamauchi, T. Ohsawa, N. Ohashi, H. Sato, and R. Kadono

Parameters of Tomonaga-Luttinger liquid in a quasi-one-dimensional material with Coulomb interactions *(12 pages)* 155122
Piotr Chudzinski

Spin diffusion and spin conductivity in the two-dimensional Hubbard model *(8 pages)* 155123
Martin Ulaga, Jernej Mravlje, and Jure Kokalj

Symmetry analysis of tensors in the honeycomb lattice of edge-sharing octahedra *(13 pages)* 155124
Franz G. Utermohlen and Nandini Trivedi

Topological nature of the Kondo insulator SmB_6 and its sensitiveness to Sm vacancy *(6 pages)* 155125
W. K. Park, J. A. Sittler, L. H. Greene, W. T. Fuhrman, J. R. Chamorro, S. M. Koohpayeh, W. A. Phelan, and T. M. McQueen

Charge and anion ordering in the quasi-one-dimensional organic conductor $(TMTTF)_2NO_3$ *(8 pages)* 155126
Olga Iakutkina, Lena Nadine Majer, Guilherme Gorgen Lesseux, Gabriele Untereiner, and Martin Dressel

(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™

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 103, NUMBER 15 *CONTENTS* **APRIL 2021-15(I)**

ARTICLES

Electronic structure and strongly correlated systems

Hydrodynamic sound and plasmons in three dimensions *(9 pages)* 155101
Shao-Kai Jian and Sankar Das Sarma

Thermopower across the phase diagram of the cuprate $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$: Signatures of the pseudogap and charge density wave phases *(9 pages)* 155102
C. Collignon, A. Ataei, A. Gourgout, S. Badoux, M. Lizaire, A. Legros, S. Licciardello, S. Wiedmann, J.-Q. Yan, J.-S. Zhou, Q. Ma, B. D. Gaulin, Nicolas Doiron-Leyraud, and Louis Taillefer

Abelian parton state for the $\nu = 4/11$ fractional quantum Hall effect *(6 pages)* 155103
Ajit C. Balram

Quantum quasi Monte Carlo algorithm for out-of-equilibrium Green functions at long times *(16 pages)* 155104
Corentin Bertrand, Daniel Bauernfeind, Philipp T. Dumitrescu, Marjan Maček, Xavier Waintal, and Olivier Parcollet

Fermiology and electron-phonon coupling in the 2*H* and 3*R* polytypes of NbS_2 *(7 pages)* 155105
Zakariae El Youbi, Sung Won Jung, Christine Richter, Karol Hricovini, Cephise Cacho, and Matthew D. Watson

Proposal for methods to measure the octupole susceptibility in certain cubic Pr compounds *(11 pages)* 155106
M. E. Sorensen and I. R. Fisher

Spatial locality of electronic correlations in LiFeAs *(6 pages)* 155107
Minjae Kim, Hu Miao, Sangkook Choi, Manuel Zingl, Antoine Georges, and Gabriel Kotliar

Lattice symmetry and emergence of antiferromagnetic quantum Hall states *(7 pages)* 155108
Morad Ebrahimkhas, Mohsen Hafez-Torbati, and Walter Hofstetter

Ubiquitous suppression of the nodal coherent spectral weight in Bi-based cuprates *(9 pages)* 155109
M. Zonno, F. Boschini, E. Razzoli, S. K. Y. Dufresne, M. Michiardi, M. X. Na, T. M. Pedersen, S. Gorovikov, S. Gonzalez, G. Di Santo, L. Petaccia, M. Schneider, D. Wong, P. Dosanjh, Y. Yoshida, H. Eisaki, R. D. Zhong, J. A. Schneeloch, G. D. Gu, A. K. Mills, S. Zhdanovich, G. Levy, D. J. Jones, and A. Damascelli

Stripe order in the doped Hubbard model on the honeycomb lattice *(6 pages)* 155110
Xu Yang, Hao Zheng, and Mingpu Qin

Copyright 2021 by American Physical Society

(Continued)

2469-9950(20210415)103:15;1-6

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).