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ENTROPY SIGNATURES OF TOPOLOGICAL PHASE TRANSITIONS

Y. M. Galperin [a,b], ***D. Grassano*** [c], ***V. P. Gusynin*** [d], ***A. V. Kavokin*** [e,f], ***O. Pulci*** [c], ***S. G. Sharapov*** [d], ***V. O. Shubnyi*** [g], ***A. A. Varlamov*** [e*]

[a] *Department of Physics, University of Oslo, P. O. Box 1048 Blindern 0316, Oslo, Norway*

[b] *Ioffe Physical Technical Institute 194021, St. Petersburg, Russia*

[c] *Departments of Physics and INFN, University of Rome Tor Vergata I-00133, Rome, Italy*

[d] *Bogolyubov Institute for Theoretical Physics, National Academy of Sciences of Ukraine 03680, Kiev, Ukraine*

[e] *SPIN-CNR, c/o Department of Civil Engineering and Computer Science Engineering, University of Rome Tor Vergata, I-00133, Rome, Italy*

[f] *Spin Optics Laboratory, St. Petersburg State University 198504, St. Petersburg, Russia*

[g] *Department of Physics, Taras Shevchenko National University of Kiev 03680, Kiev, Ukraine*

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Low-dimensional electronic structures are of a great interest because of their importance as the building blocks for quantum electronics. Another reason of such interest is that size quantization of the electronic states in low-dimensional systems leads to quantization of their thermodynamic and transport properties. The most famous are the integer [1] and fractional [2] quantum Hall effects in two-dimensional electron gas (2DEG) and conductance quantization of quasi-one-dimensional channels [3, 4].

In the recent decades, a new class of atomically thin two-dimensional (2D) crystals has come to the focus of numerous experimental and theoretical studies. Starting from the pioneering works on the gapless 2D semimetal, graphene, the physics of 2D crystals advances at a high pace. A variety of gapped 2D crystals has come into play, including, e. g., the transition metal dichalcogenides such as molybdenum or tungsten disulphites and diselenides.

One of the ways to describe the anomalies of the properties of low-dimensional electron systems appearing in the result of size quantization is the formalism of Lifshitz topological transitions [5]. In three dimensional bulk crystals, Lifshitz transitions are sometimes referred to as $2\frac{1}{2}$ order transitions. In contrast, in 2D crystals, this is no more universally valid, and particular cases need to be specifically analyzed. In accordance to the Ehrenfest terminology, the resonance of the electronic chemical potential with the energy level of size-quantization in a 2DEG with a parabolic spectrum should be interpreted as the second-order phase transition. The crossing points of the electronic chemical potential and the Landau level achieved by tuning the magnetic field perpendicular to the crystal plane may be identified as $1\frac{1}{2}$ order transitions. Such transitions are accompanied by the steps or logarithmic singulari-

* E-mail: varlamov@ing.uniroma2.it

ties in the electronic density of states (DOS), openings of the specific channels in the electron scattering, giant resonances in thermoelectric power [6], de Haas–van Alphen and Shubnikov–de Haas oscillations [7]. Manifestations of these phase transitions constitute an important part of the modern physics of 2D electronic systems.

In recent years, a new class of topological materials has been theoretically predicted and experimentally studied (see reviews [8, 9]). Topological insulators are characterized by bulk band gaps and gapless edges or surface states, that are protected by the time-reversal symmetry and characterized by a Z_2 topological order parameter. Novel group-IV graphene-like 2D crystals such as silicene, germanene, and stanene are examples of the 2D topological insulators proposed in Refs. [10, 11]. They attract an enhanced attention nowadays because of their high potential for applications in nanoelectronic devices of a new generation.

In order to study the peculiar electronic properties of both classical semiconductor quantum wells and novel 2D crystals, one needs an experimental technique that would be sensitive to the peculiarities of the electronic band structure. Traditional methods, such as optical transmission, sometimes fail to detect the variations of the electronic DOS in the far-infrared and terahertz spectral ranges [12, 13], while electronic conductivity measurements, even at ultra-low temperatures, provide only an indirect information on the band and spin structure of the studied material.

Recently, a promising tool for the band structure studies with use of the electronic transport measurements has been proposed and successfully tested on a 2D electron gas with a parabolic dispersion [14]. This method, based on the measurements of recharging currents in a planar capacitor geometry, gives access to the entropy per particle $s \equiv (\partial S/\partial n)_T$ (S is the entropy per unit volume and n is the electron density) at temperature T, which we shall express in energy units. This characterization technique is based on the Maxwell relation that links the temperature derivative of the chemical potential in the system, μ, to the entropy per particle:

$$s = (\partial S/\partial n)_T = -(\partial \mu/\partial T)_n.$$

The modulation of the sample temperature changes the chemical potential and, hence, causes recharging of the gated structure, where the 2DEG and the gate act as two plates of a capacitor. Therefore, $(\partial \mu/\partial T)_n$ may be directly obtained in this experiment from the measured recharging current.

The entropy per particle is an important characteristic *per se* of any many-body system. It also governs the thermoelectric and thermomagnetic properties of the system entering explicitly the expressions for the Seebeck and Nernst–Ettingshausen coefficients [15, 16]. In the present Review, we address theoretically this major thermodynamic quantity — entropy per particle — of quasi-2DEGs in various solid state systems. We specifically focus on the behavior of entropy in the vicinity of topological transitions of different types.

The review is based on the papers [17–20] and organized as follows. We start with general expressions for the entropy per particle. Then we provide the general equations that link the entropy per particle with DOS, chemical potential, and temperature. We consider the specific case of a 2DEG characterized by parabolic energy subbands, as it is the case, e. g., in semiconductor quantum wells. We show that the quantization of the energy spectrum of quasi-2DEG with a parabolic dispersion into subbands leads to a very specific quantization of the entropy: s exhibits sharp maxima as the chemical potential μ passes through the bottoms of size quantization subbands (E_j). The value of the entropy in the N-th maximum depends only on the size-quantization quantum number corresponding to this maximum, N:

$$s|_{\mu=E_n} \equiv \left(\frac{\partial S}{\partial n}\right)_{T,\,\mu=E_n} = \frac{\ln 2}{N-1/2}\,. \qquad (1)$$

In the absence of scattering this result is independent of the shape of the transverse potential that confines 2DEG and of the material parameters including the electron effective mass and dielectric constant. We reveal the quantization of entropy per electron at resonances of the chemical potential and electron quantization levels and discuss the accuracy of the obtained expression for the quantized entropy in the presence of disorder and electron-electron interactions.

After that, we calculate the entropy per particle in the vicinity of topological transitions in various 2D electronic systems. In contrast to the case of a 2DEG with a parabolic energy spectrum in double-gapped Dirac materials, the entropy per particle demonstrates characteristic spikes once the chemical potential passes through the band edges. We consider specific cases of the gapped graphene and silicene. We show that studies of the entropy per particle shed light on multiple

otherwise hidden peculiarities of the electronic band structure of novel 2D crystals.

Then, we focus on monoatomically thin layers of transition metal dichalcogendes. This class of structures is characterized by significant energy gaps that can be tuned by application of external fields and strain. This results in a peculiar band-structure that finds its unique signature in the entropy-per-particle dependence on the chemical potential. Particularly, we study the strain effect on the entropy per particle dependence on the chemical potential and show that it may be very prominent even at elevated temperatures.

Finally, we show that a specific resonant feature in the entropy per electron dependence on the chemical potential may be considered as a fingerprint of the transition between topological and trivial insulator phases in germanene. The entropy per electron in a honeycomb 2D crystal of germanene subjected to the external electric field is obtained from the *ab initio* calculation of the density of electronic states and the Maxwell relation. We demonstrate that, in agreement to the recent prediction of the analytical model, strong spikes in the entropy per particle dependence on the chemical potential appear at low temperatures. They are observed at the values of the applied bias both below and above the critical value that corresponds to the transition between the topological insulator and trivial insulator phases, while the giant resonant feature in the vicinity of zero chemical potential is strongly suppressed at the topological transition point, in the low temperature limit. In a wide energy range, the van Hove singularities in the electronic density of states manifest themselves as zeros in the entropy per particle dependence on the chemical potential.

In conclusion, in our paper, we have considered several examples of 2D electronic systems undergoing topological transitions of various types. We demonstrated that the entropy experiences quantized steps at the points of Lifshitz transitions in a 2DEG with a parabolic energy spectrum. In contrast, in doubled-gapped Dirac materials, the entropy per particle shows characteristic spikes once the chemical potential passes through the band edges. The transition from a topological to trivial insulator phase in germanene is manifested by the disappearance of a strong zero-energy resonance in the entropy per particle dependence on the chemical potential. We conclude that studies of the entropy per particle shed light on multiple otherwise hidden peculiarities of the electronic band structure of novel 2D crystals.

The goal of this review is to attract attention of the scientific community to the surprising behavior of the entropy per particle in the vicinity of topological transitions in various 2D systems and to stimulate its further experimental and theoretical studies.

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REFERENCES

1. K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980).

2. D. C. Tsui, H. L. Stormer, and A. C. Gossard, Phys. Rev. Lett. **48**, 1559 (1982).

3. D. A. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J. E. F. Frost, D. G. Hasko, D. C. Peacock, D. A. Ritchie, and G. A. C. Jones, J. Phys. C **21**, L209 (1988).

4. B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, and C. T. Foxon, Phys. Rev. Lett. **60**, 848 (1988).

5. I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **38**, 1569 (1960) [Sov. Phys. JETP **11**, 1130 (1960)].

6. Y. M. Blanter, A. V. Pantsulaya, and A. A. Varlamov, Phys. Rev. B **45**, 6267 (1992).

7. Y. M. Blanter, M. I. Kaganov, A. V. Pantsulaya, and A. A. Varlamov, Phys. Rep. **245**, 159 (1994).

8. M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).

9. X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).

10. C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).

11. B. A. Bernevig and S.-C. Zhang, Phys. Rev. Lett. **96**, 106802 (2006.)

12. F. Bechstedt, L. Matthes, P. Gori, and O. Pulci, Appl. Phys. Lett. **100**, 261906 (2012).

13. L. Stille, C. J. Tabert, and E. J. Nicol, Phys. Rev. B **86**, 195405 (2012).

14. A. Y. Kuntsevich, Y. V. Tupikov, V. M. Pudalov, and I. S. Burmistrov, Nature Comm. **6**, 7298 (2015).

15. A. A. Varlamov and A. V. Kavokin, Europhys. Lett. **103**, 47005 (2013).

16. C. Goupil, W. Seifert, K. Zabrocki, E. Müller, and G. J. Snyder, Entropy **13**, 1481 (2011).

17. A. A. Varlamov, A. V. Kavokin, and Y. M. Galperin, Phys. Rev. B **93**, 155404 (2016).

18. V. Y. Tsaran, A. Kavokin, S. Sharapov, A. Varlamov, V. Gusynin, Sci. Rep. **7**, 10271 (2017).

19. V. O. Shubnyi, V. P. Gusynin, S. G. Sharapov, and A. A. Varlamov, Low Temp. Phys./Fiz. Nizk. Temp. **44**, 721 (2018).

20. D. Grassano, O. Pulci, V. O. Shubnyi, S. G. Sharapov, V. P. Gusynin, A. V. Kavokin, and A. A. Varlamov, Phys. Rev. B **97**, 205442 (2018).