Discrete scale invariance of the quasi-bound states at atomic vacancies in a topological material

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Recently, log-periodic quantum oscillations have been detected in the topological materials zirconium pentatelluride (ZrTe5) and hafnium pentatelluride (HfTe5), displaying an intriguing discrete scale invariance (DSI) characteristic. In condensed materials, the DSI is considered to be related to the quasi-bound states formed by massless Dirac fermions with strong Coulomb attraction, offering a feasible platform to study the long-pursued atomic-collapse phenomenon. Here, we demonstrate that a variety of atomic vacancies in the topological material HfTe5 can host the geometric quasi-bound states with a DSI feature, resembling an artificial supercritical atom collapse. The density of states of these quasi-bound states is enhanced, and the quasi-bound states are spatially distributed in the “orbitals” surrounding the vacancy sites, which are detected and visualized by low-temperature scanning tunneling microscope/spectroscopy. By applying the perpendicular magnetic fields, the quasi-bound states at lower energies become wider and eventually invisible; meanwhile, the energies of quasi-bound states move gradually toward the Fermi energy (E_F). These features are consistent with the theoretical prediction of a magnetic field–induced transition from supercritical to subcritical states. The direct observation of geometric quasi-bound states sheds light on the deep understanding of the DSI in quantum materials.

atomic collapse state | discrete scale invariance | topological material | scanning tunneling microscope

One of the most striking and challenging issues in fundamental physics is the observation of the supercriticality phenomenon in ultra-heavy nuclei, which does not exist in nature. The atomic wave function will collapse when the nuclear charge parameter exceeds a critical value Z_c (1–4). Unfortunately, the very large Z_c makes it almost impossible for atoms to satisfy the supercritical condition that β = Z/α exceeds a critical value of order unity, where α = 1/137 is the fine structure constant. Recently, the Dirac materials with massless or massive Dirac fermions analogous to high-energy relativistic particles have provided new platforms for related investigations. Moreover, the supercritical regime guarantees the existence of a geometric series of quasi-bound states showing a dramatic discrete scale invariance (DSI) property (5, 6). The DSI induces log-periodic corrections to scaling and has been rarely demonstrated in quantum systems other than cold atom gas (7–14). In condensed materials, the atomic collapse states were observed in graphene by scanning tunneling microscope/spectroscopy (STM/S) experiments (15, 16), and further STM/S studies of graphene reported the two quasi-bound states indicating a signature of DSI (17). In addition, the DSI feature has been clearly detected in the topological materials zirconium pentatelluride (ZrTe5) and hafnium pentatelluride (HfTe5) by the observation of log-periodic quantum oscillations involving up to five oscillating cycles in magnetoresistance (MR) under ultrahigh magnetic fields (B) (18–20). The underlying mechanism can be attributed to the discrete scale–invariant quasi-bound states composed of relativistic quasi-particles and non-relativistic quasi-particles (or charge impurity) in Dirac materials (18, 21). Thus, Dirac materials can serve as promising systems to uncover the DSI characteristic in quantum systems that satisfy the supercritical collapse condition. Direct imaging of the quasi-bound states responsible for the appearance of the DSI feature in topological systems is certainly of particular importance because it has not been presented.

ZrTe5 and HfTe5 are predicted to be quantum-spin Hall insulators in the 2-dimensional (2D) limit, and the 3-dimensional (3D) crystals are located near the phase boundary between weak and strong topological insulators (TIs) (22, 23). However, previous experimental results about these materials have presented a large diversity. Some angle-resolved photoemission spectroscopy (ARPES) (24, 25) and magneto-infrared spectroscopy studies show that ZrTe5 is a Dirac semi-metal (26). Negative MR and the anomalous Hall effect also support the massless Dirac band structure of ZrTe5 (27–29). Recently, more electrical transport, ARPES, and STM results suggest that ZrTe5 and HfTe5 are TIs with a small gap (30–35). The small Fermi surface and ultralow carrier density of ZrTe5 and

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HfTe$_5$ guarantee the supercritical Coulomb attraction due to the weak screening effect (18), which makes them promising platforms to explore the quasi-bound states with DSI.

**Results**

**Atomic-resolved STM image and small energy gap of HfTe$_5$ surface.** The HfTe$_5$ crystal shows an orthorhombic layered structure (36) and contains 2D sheets of HfTe$_5$ in the $a$-$c$ plane that stack along the $b$ axis via interlayer van der Waals interactions, as shown in Fig. 1A. Each 2D sheet consists of alternating prismatic HfTe$_3$ chains along the $a$ axis that are linked by parallel zigzag Te chains. The prism of HfTe$_3$ is formed by a dimer of Te and an apical Te atom surrounding an Hf atom. HfTe$_5$ is easily cleavable along the $a$–$c$ plane and exhibits a quasi-1-dimensional (1D) preference along the $a$ axis. Fig. 1B shows the atomically resolved topography of such a cleaved HfTe$_5$ surface, in which 1D chains of Te dimers can be well identified. The lattice constants along both the $a$ and $c$ axis can be directly measured from STM images, which are 3.93 Å and 13.5 Å, respectively, in good agreement with the crystal structure of HfTe$_5$ (22). The local density of states (from spectroscopic measurement) obtained at the surface terrace are plotted in Fig. 1C at 77 K and Fig. 1D at 4.2 K. The $dI/dV$ spectrum at 77 K shows a small energy gap developed around the Fermi energy ($E_F$). Further $I/V$ and $dI/dV$ spectroscopic measurements are performed at 4.2 K and repeated more than 40 times at different surface locations, as shown in Fig. 1D. An energy gap of approximately 16.5 meV is identified with the top of the valence band and the bottom of the conductance band located at $\sim -1.5$ and $\sim +15$ meV, respectively. The observation of the TI gap in HfTe$_5$ is generally consistent with previous STM/ARPES work (37, 38). The size of the gap observed on the HfTe$_5$ surface agrees well with the density-functional theory calculation on our Te-flux grown HfTe$_5$ samples (30). Note that the previously reported gap values by STS measurement (31, 33) on the ZrTe$_5$ surface are much larger than the value of HfTe$_5$ reported here, which could be due to the difference of the samples.

**Surface defects and the calculated charges.** On the cleaved (010) surface of HfTe$_5$, there are a number of surface defects.

![Image of HfTe5 structure and STM images](https://doi.org/10.1073/pnas.2204804119)
These surface defects provide natural, static charge centers for generating the long-range Coulomb attraction considering the low carrier density in HfTe₅ (19). In our HfTe₅ sample, a very small gap around $E_F$ is detected (Fig. 1D), which indicates that our samples are TIs, consistent with previous photoemission reports (37). Theoretically, the small gap has little influence on the formation of quasi-bound states showing the DSI feature (19) and the quasi-bound states can be attributed to the Dirac fermions from the bulk massive Dirac bands (Fig. 1C, Inset). In this situation, the Weyl equation with Coulomb attraction generating the long-range Coulomb attraction considering the central charge, and the fine structure constant $\alpha = \frac{e^2}{\hbar c}$ is larger than 1 due to the small Fermi velocity $v_F$ in Dirac materials compared with the speed of light in the vacuum (18, 24, 26, 30, 39–41). Previous transport studies have reported that the fine structure constant $\alpha$ is approximately 4.9 in our HfTe₅ samples (19). The so-called supercritical condition ($Z_\alpha$ surpassing the angular momenta $m$) can be readily matched in this material and further gives rise to a quasi-bound–states solution in the system (5, 6). If one only considers the lowest angular momentum channel with $m = 1$, then the charge number $Z$ of defects has to be larger than 0.20 to result in the quasi-bound states with DSI. Such a DSI property of the quasi-bound states, composed of charge defects and hole carriers in our HfTe₅, is supposed to give rise to log-periodic density of states (DOS) peaks above $E_F$, which can be detected by differential tunneling spectroscopy, namely the $dI/dV$ spectrum.

The variety of surface defects could provide a fertile playground to study the supercritical ($Z_\alpha > m$) and subcritical ($Z_\alpha < m$) phenomena in this intriguing material. To understand the defect-induced DSI effects, we systematically investigate the surface defects observed in experiments, rationalized by employing density-functional theory (DFT) calculations to estimate the local charge of the defect. As shown in Fig. 2A, the pristine HfTe₅ is first calculated. HfTe₅ has two kinds of Te atoms. Three Te atoms are in the HfTe₃ prism, and two Te atoms connect in-between two HfTe₃ prisms. We name the top Te atoms in the HfTe₃ prism, the bottom Te atom in the HfTe₃ prism, and the Te atoms connecting two adjacent HfTe₃ prisms as $Te_\alpha$, $Te_\beta$, and $Te_\gamma$, respectively. For the pristine surface, the HfTe₅ cell is neutral and the net charge is zero. Then we calculate the structures, simulated images, and charges for three different surface vacancies experimentally observed with a number of theoretically predicted defect structures, as shown in Fig. 2B–D. For defect I, a single $Te_\alpha$ vacancy could induce a net charge of 0.16 e (Fig. 2B). The surface $Te_\alpha$ vacancies are carefully introduced to best fit the experimental STM image. More theoretically examined structures are listed in SI Appendix, Table S1. For defects with larger net charges, the Hf vacancy should be included; in particular, for defect II, with the largest net charge, two Hf vacancies are introduced (Fig. 2C). To validate the proposed structures of these defects, the simulated STM images are also calculated and presented with the experimental STM image for each defect. The simulated STM images of the pristine surface and three surface vacancies are in good consistency with the experiments.

The observation of DSI quasi-bound states at atomic vacancies. Fig. 3 summarizes high-resolution STM images and corresponding STS spectra for the pristine surface without defects

Fig. 2. Structures, charges, and simulated images for pristine HfTe₅ and three different surface vacancies. (A) Pristine HfTe₅ marked with two types of Te atoms with different coordination, top Te atoms in HfTe₃ prism ($Te_\alpha$) and bottom Te atom in HfTe₃ prism ($Te_\beta$). (B–D) Structures, experimental/simulated STM images, and calculated charges for three theoretically predicted surface defects. For the side view of the structures (top, A–D), only the HfTe₃ chain containing the vacancy is shown; the vacant atoms are labeled as yellow balls. For the top view, the Te atoms in the HfTe₃ chain and the zigzag Te chain are labeled as brown and gray balls, respectively.
(A) and three different surface defects (vacancies 1–3) with possible configurations, e.g., vac. 1, single Te vacancy (B); vac. 2, 2Hf + 1Te vacancy (C); and vac. 3, Hf vacancy (D), respectively. For the pristine surface (Fig. 3A and SI Appendix, Fig. S1A) and the 1Tet vacancy (Fig. 3B and SI Appendix, Fig. S1B), dI/dV spectra taken at 4.2 K show the clean curve without any extra peaks above $E_F$ in both linear and log-scaled plots. Clearly, the local charge of 1Tet vacancy ($Z$) is only 0.165 electrons, which does not meet the supercritical condition $Z \geq 0.20$ electrons in HfTe$_5$. The charges of vac. 2 and vac. 3, estimated at approximately 0.972 and 0.776, respectively, are much larger than the supercritical condition. Indeed, the dI/dV spectra of these defects show a series of DOS peaks above $E_F$ (Fig. 3C and D). The differences of the height of resonance peaks and the overall background between Fig. 3C (vac. 2) and Fig. 3D (vac. 3) may be attributed to the local inhomogeneity and distinct kinds of vacancies as well as the charges. Theoretically, the energy of the quasi-bound states satisfies DSI when the Dirac point is chosen as the zero point (18). However, in our HfTe$_5$ sample, a very small gap around $E_F$ is detected. Consequently, the Dirac point is absent in the STS and the energy of the Dirac point should be replaced by the middle position of the gap $E_M$ (about 8 meV above the Fermi energy), which is very close to $E_F$. The log-scaled dI/dV spectra as a function of $E_E$ are plotted in Fig. 3C and D, which show clear log periodicity and DSI of the quasi-bound states. The ratio $\lambda$ of $E_{n+1}$ vs. $E_n$ is $\lambda = \exp(\pi/s_0)$ (18), where $s_0 = \sqrt{(Z \cdot \alpha)^2 - 1}$. At approximately 10 mV, the resonance peaks slightly deviate from the log periodicity, which may be induced by the influence of the energy gap. Based on the data at vac. 2 ($E_E > 30$ mV) as shown in Fig. 3C, the scale factor $\lambda = 1.9$ gives the effective charge $Z \sim 1$ of vac. 2, which is consistent with the charge value (0.972) from ab initio calculation. Furthermore, the value of $\lambda$ is consistent with the previous MR measurements on our HfTe$_5$ samples (19), wherein the scale factor of the characteristic magnetic fields $\lambda_B = \frac{B_{B+1}}{B_n}$ is approximately 3.7 and then $\lambda_E = \lambda^{1/s_0} = \sqrt{\lambda_B} \sim 1.92$. The $\lambda$ value of the DSI spectrum at vac. 3 shown in Fig. 3D gives an estimation of charge value of approximately 1, which agrees roughly with the

**Fig. 3.** High-resolution STM images and the corresponding dI/dV spectra plotted in both linear and log scales, for the pristine HfTe$_5$ surface (A); vac. 1, single Te vacancy (B); vac. 2, 2Hf + 1Te vacancy (C); and vac. 3, Hf vacancy (D). a.u., arbitrary unit. $E_M$ is the middle position of the gap ($\sim$8 meV above $E_F$). The dI/dV spectra shown here were measured at 4.2 K with parameters of $V_B = 300$ mV, $I_T = 300$ pA, and the magnitude of the bias modulation for the lock-in technique is 2.5 mV. All data were measured >10 times to check the reproducibility.
calculated charge of $-0.776$. Note that the calculated net charge is slightly lower than the expected values, which may be due to the limited size of the simulation model and the definition of the defect charge.

In previous works on graphene, highly charged impurities, e.g., Ca dimers created by tip manipulation (15), single atomic vacancy created by applying voltage pulses, or He ion beam sputtering (16, 17), served as the superheavy atomic nucleus, and two atomic collapse states were measured by tunneling spectroscopy. More atomic collapse states are still desired to make the DSI feature unambiguous. In the crystalline topological material HfTe$_5$, intriguingly, we detect four remarkable quasi-bound states by STS > 19 meV (outside the small band gap $\sim$6.5 meV) in different vacancies with the similar charge showing almost the same $\lambda$ values. Furthermore, in another HfTe$_5$ sample, dI/dV peaks at log-periodic energies are also detected at an atomic vacancy (vac. 4) with an effective charge of $Z \sim 0.62$, which is lower than $Z \sim 1$ at vac. 2 and vac. 3 (SI Appendix, Fig. S2). The discrete scale–invariant quasi-bound states at vacancies with different charges in different samples further support the emergence of geometric quasi-bound states at the atomic scale in HfTe$_5$.

**Spatial and magnetic field dependence of the quasi-bound states.** To further characterize the spatial dependence of the quasi-bound states that appear for the artificial nuclei, we performed dI/dV mapping at a series of resonance energies around vac. 2 (Fig. 4A, e.g., +21, +41, +76, and +136 mV). The defects are randomly distributed, and we find that vac. 2 is relatively far away from others. As shown in Fig. 4A, Top, the vacancy is located in the middle and there is no other defect along the $a$ axis in the field of view. Furthermore, the intensity of the resonance extends outward from the vacancy center to a distance $> 6$ nm with decreasing energies. The DOS is distributed mainly on the left and right sides of the vacancy, which may be due to the anisotropy of the Fermi velocity in the $a$–$c$ plane (40). Furthermore, dI/dV maps at +76 mV and +136 mV display more symmetric DOS distribution around the vacancy than dI/dV maps at +21 mV and +61 mV. The asymmetric distribution could be due to the distant defects.

![Diagram](image_url)

**Fig. 4.** Spatial distribution and magnetic field dependence of the quasi-bound states. (A) Topographic image (Top) and four dI/dV maps taken at a series of resonance energies of +21, +41, +76, and +136 mV for vac. 2. (B) The peak intensity of each quasi-bound state drawing from the dI/dV maps is plotted with lateral distances (black dots). The red curves are the fitting with the radius $R_n$ (the distance from the center of the vacancy) of each quasi-bound state. (C) Semiclassical picture of the orbits of the supercritical states. The radii exhibit the DSI of these states. (D) dI/dV curves for vac. 3 at the magnetic field from 0 T to 7 T. The energies of quasi-bound states are indicated by black arrows, which are identified by the Gaussian peak fitting (SI Appendix, Fig. S5). The gray dashed lines are guides to the eye. (E) The energies of quasi-bound states versus the magnetic fields. The peak positions and error bars of the quasi-bound states are determined by the Gaussian peak fitting of the dI/dV curves at different magnetic fields. (F) The energies of the quasi-bound states plotted on the log scale versus the index. The gray dashed line is highlighting the DSI property at 0 T.
(SI Appendix, Fig. S3), especially for the lower-energy quasi-bound states (e.g., +21 mV) showing larger radii. We draw out the intensity of each quasi-bound state from the dI/dV maps and plot them with lateral distances in Fig. 4B, which can be fitted with the radius \( R_0 \) (the distance from the center of the vacancy) for each quasi-bound state (see SI Appendix for more details). Due to the influence from other defects in the vicinity, the uncertainties of radii at lower energies (+21 mV and +41 mV) are relatively large, and a precisely log-periodic relation is hard to determine. However, the spatial distribution of quasi-bound states still shows a log-periodic trend, especially for the quasi-bound states at high energies (+76 mV and +136 mV). The radii of quasi-bound states at +76 mV and +136 mV are estimated to be approximately 25 Å and 15 Å, respectively. The ratio between these two radii is approximately 1.7, which is close to the energy ratio of differential conductance peaks (\( \lambda_B = E_B/E_0 \sim 1.9 \)). In addition, if the dielectric constant of \( \text{HfTe}_5 \) is of order 10 \( \epsilon_0 \) (42), where \( \epsilon_0 \) is the vacuum dielectric constant, the deduced \( R_0 \) values at +76 mV and +136 mV from the relation \( R_0 \sim \frac{E}{\lambda_B \epsilon_0} \) (18) are 23 Å and 12 Å, which agree with the experimental results. These spatial properties of quasi-bound states further support the realization of quasi-bound states with DSI.

The evolution of dI/dV spectra under magnetic fields is further investigated. Theoretically, the quasi-bound states with DSI are predicted to be converted into subcritical states with increasing magnetic fields (43) (see SI Appendix for more details). During the transition, the energy of the quasi-bound state gradually approaches the Fermi energy and the corresponding resonance peak becomes wider (SI Appendix, Fig. S4). The experimental results are shown in Fig. 4 D–F. The dI/dV curve of vac. 3 presents four quasi-bound states at 0 T that are determined by the Gaussian peak fitting (SI Appendix, Fig. S5A) and labeled as ‘\( E_1, E_2, E_3, \) and ‘\( E_4 \). As the magnetic field is increased, the resonance peak of the first quasi-bound state (\( n = 1 \)) becomes wider at 1 T with a larger error bar and is hard to distinguish at 2 T (SI Appendix, Fig. S5 B and C), in accordance with the magnetic field–induced broadening effect in the transition. A similar magnetic field–induced broadening effect is also observed for the second quasi-bound state (\( n = 2 \)) when the applied magnetic field is increased from 0 T to 2 T, and the second quasi-bound state is almost indistinguishable at 3 T (SI Appendix, Fig. S5D). Note that when the magnetic field is increased from 1 T to 2 T, the energy of the second quasi-bound state shown in Fig. 4 E and F becomes smaller (approaching the Fermi energy) and deviates the log periodicity (dashed line in Fig. 4F), which is also consistent with the magnetic field–induced transition scenario (43). Furthermore, the resonance peak broadening and the energy shift to the Fermi energy with increasing magnetic fields are reproduced at vac. 2, as shown in SI Appendix, Figs. S6 and S7.

When the magnetic field \( B \geq 3 \) T, only two quasi-bound states at higher energy (>60 meV) are distinguishable, as shown in Fig. 4 D–F. The scale factor \( \lambda \) of vac. 3 is approximately \( \lambda = E_3/E_{n=1} \sim 2.0 \). Therefore, the ratio between the characteristic fields \( B_n/E_{n=1} \) should be \( \lambda^2 \sim 4 \) (19). Considering that the second quasi-bound state is indistinguishable at 3 T, it is expected that the resonance peak of the third quasi-bound state should disappear at \( B > 12 \) T, which exceeds the maximum magnetic field of our facilities.

Conclusion

In conclusion, in quantum materials, two quasi-bound states in graphene were revealed by STM/S indicating the existence of DSI, and transport measurements of topological materials showed a clear feature of DSI by detecting the log-periodic quantum oscillations in MR. The underlying quasi-bound states showing DSI call for more direct experimental evidence. Here, the STS results clearly demonstrate the geometric quasi-bound states around a variety of atomic vacancies in the topological material \( \text{HfTe}_5 \). Four geometric quasi-bound states in different charge vacancies constitute the unambiguous evidence and a clean example for the realization of quasi-bound states with DSI in condensed matter. This work provides a promising platform for studying supercritical atomic collapse with a relativistic effect in quantum systems.

Materials and Methods

Theoretical model and method. To explore the possible atomic structures of the charged defects, we apply first-principles simulations to optimize the defect structures and calculate the defect charges. The simulations are performed using the plane-wave method, with the projector-augmented wave pseudopotentials (44) and the Perdew-Burke-Ernzerhof exchange-correlation functional (45) as implemented in the Vienna Ab initio Simulation Package (VASP) code (46, 47).

In the calculations, only the gamma point is sampled in the Brillouin zone, and the energy cutoff of the plane-wave basis is 300 eV.

To explore the defect structures, the simulation model is constructed as a single \( \text{HfTe}_5 \) layer in the \( a \)-\( c \)-plane, containing 6 \times 4 unit cells (total of 144 atoms), and each unit cell includes 1 Hf atom and 5 Te atoms. The periodic boundary conditions are considered in the \( a \) and \( c \) directions, while in the \( b \) direction, a 20 Å vacuum layer is added. The defect structures are designed as a complex of atomic vacancies with up to 2 Hf vacancies and 3 Te vacancies. The charge of the defect is calculated by summing the charges of all atoms in one or two \( \text{HfTe}_5 \) unit cells after removing the certain atoms; the atomic charge is obtained by Bader analysis (48) on the charge density obtained by the first-principles method. For the comparison with experiments, the STM images of the defects are also simulated theoretically and are obtained by the profile of the partial charge density contributed by relevant electronic states (within 1.0 eV above the Fermi energy).

Sample information. Single-crystal \( \text{HfTe}_5 \) used in our experiments were grown by the self-Te-flux method as described in a previous report (30). The samples in this work are of the same batch as that in references (19), (20), and (35). Typical sizes of the \( \text{HfTe}_5 \) samples are approximately 15 mm \( \times \) 0.3 mm \( \times \) 0.1 mm (length \( \times \) width \( \times \) height). The longest direction of the sample is always along the crystallographic \( a \) axis, and a large \( a \)-\( c \) plane can be obtained by exfoliation. The structure and composition of the \( \text{HfTe}_5 \) crystals were analyzed by powder X-ray diffraction, transmission electron microscopy, and scanning electron microscopy with energy-dispersive X-ray spectroscopy (19, 30, 35). The carrier density and the mobility of the \( \text{HfTe}_5 \) samples at 2 K are estimated to be 1.4 \( \times \) 10\(^{12} \) cm\(^{-2} \) and 1.84 \( \times \) 10\(^{3} \) cm\(^2\)V\(^{-1}\)s\(^{-1} \), respectively, by electrical transport measurements (30).

STM characterization. \( \text{HfTe}_5 \) is a layered material with van der Waals interlayer coupling (22). Therefore, a large atomically flat surface is conveniently obtained by exfoliation, which is suitable for STM measurements. Our STM experiments were carried out on an ultrahigh vacuum commercial STM system (Unisoku) that can reach a temperature of 400 mK by using a single-shot He cryostat. The base pressure for experiments was 2.0 \( \times \) 10\(^{-10} \) Torr. \( \text{HfTe}_5 \) samples were cleaved in situ at 78 K and then transferred into STM. The bias voltage was applied on the samples. The STS data were obtained by a standard lock-in method that applied an additional small alternating-current voltage with a frequency of 973.0 Hz. The dI/dV spectra were collected by disrupting the feedback loop and sweeping the direct-current bias voltage. WSXm software was used for the post-process of all STM data (49).

Data, Materials, and Software Availability. All study data are included in the article and/or SI Appendix.

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T. H. Boyer, Unfamiliar trajectories for a relativistic particle in a Kepler or Coulomb potential. Am. J. Phys. 72, 992–997 (2004).

W. Greiner, B. Müller, J. Rafelski, Quantum Electrodynamics of Strong Fields (Springer-Verlag, Berlin, 1985).

Y. B. Zeldovich, V. S. Popov, Electronic structure of superheavy atoms. Sov. Phys. Usp. 14, 673–694 (1972).

I. Pomeranchuk, Y. Smorodinsky, On the energy levels of systems with \( Z > 137 \). J. Phys. USSR 9, 97–100 (1945).

A. V. Shytov, M. I. Katsnelson, L. S. Levitov, Atomic collapse and quasi-Rydberg states in graphene. Phys. Rev. Lett. 99, 246402 (2007).

Y. Nosaka, Vacuum polarization of graphene with a supercritical Coulomb impurity: Low-energy universality and discrete scale invariance. Phys. Rev. B Condens. Matter Mater. Phys. 90, 165414 (2014).

V. Efimov, Energy levels arising from resonant two-body forces in a three-body system. Phys. Lett. B 33, 563–564 (1970).

E. Braaten, H. W. Hammer, Universality in few-body systems with large scattering length. Phys. Rep. 428, 259–390 (2006).

P. Naidon, S. Endo, I. Pomeranchuk, Y. Smorodinsky, On the energy levels of systems with \( Z > 137 \). Phys. Rev. Lett. 112, 190401 (2014).

R. Pires et al., Observation of Efimov resonances in a mixture with extreme mass imbalance. Phys. Rev. Lett. 112, 250404 (2014).

S. K. Tung, K. Jiménez-García, J. Johannsen, C. V. Parker, C. Chin, Geometric scaling of Efimov states in a \( ^{40}\text{K}^{2}\text{S}^{16}\text{O} \) mixture. Phys. Rev. Lett. 113, 240402 (2014).

M. Kunitski et al., Three-body physics. Observation of the Efimov state of the helium trimer. Science 340, 551–555 (2013).

Y. Wang et al., Observing atomic collapse resonances in artificial nuclei on graphene. Science 340, 734–737 (2013).

J. Miao et al., Realization of a tunable artificial atom at a supercritically charged vacuum in graphene. Nat. Phys. 12, 545–549 (2016).

O. Ovdat, J. Man, Y. Jiang, E. Y. Andrei, E. Akkermans, Observing a scale anomaly and a universal quantum phase transition in graphene. Nat. Commun. 8, 507 (2017).

H. Wang et al., Discovery of log-periodic oscillations in ultraquantum topological materials. Sci. Adv. 4, eaau5066 (2018).

H. Wang et al., Log-periodic quantum magneto-oscillations and discrete-scale invariance in topological material HSE11. Nat. Sci. Rev. 6, 914–920 (2019).

Y. Liu et al., Tunable discrete scale invariance in transition-metal pentatelluride flakes. npj Quantum Mater. 5, 58 (2020).

H. Liu, H. Jiang, Z. Wang, R. Joynt, C. X. Xie, Discrete scale invariance in topological semimetals. arXiv [Preprint] (2018). https://arxiv.org/abs/1807.02459. Accessed 21 September 2022.

H. M. Weng, X. Dai, Z. Fang, Transition-metal pentatelluride \( \text{ZrTe}_2 \), and HfSe\(_2\): A paradigm for large-gap quantum spin Hall insulators. Phys. Rev. X 4, 011002 (2014).

Z. Fan, O. F. Liang, Y. B. Chen, S. H. Yao, J. Zhou, Transition between strong and weak topological insulator in \( \text{ZrTe}_2 \), and HfSe\(_2\). Sci. Rep. 7, 45667 (2017).

O. Li et al., Chiral magnetic effect in \( \text{ZrTe}_2 \). Nat. Phys. 12, 550–554 (2016).

L. Shen et al., Spectroscopic evidence for the gapless electronic structure in bulk \( \text{ZrTe}_2 \). J. Electron Spectrosc. Relat. Phenom. 219, 45–52 (2017).

Y. Wang et al., Log-periodic quantum magneto-oscillations and discrete-scale invariance in topological material HfSe\(_2\). Nat. Sci. Rev. 6, 914–920 (2019).

H. Wang et al., Discovery of log-periodic oscillations in ultraquantum topological materials. Sci. Adv. 4, eaau5066 (2018).

26. R. Y. Chen et al., Magnetotransistor spectroscopy of Landau levels and Zeeman splitting of three-dimensional massless Dirac fermions in \( \text{ZrTe}_2 \). Phys. Rev. Lett. 115, 176405 (2020).

27. G. L. Zheng et al., Transport evidence for the three-dimensional Dirac semimetal phase in \( \text{ZrTe}_2 \). Phys. Rev. B 93, 115414 (2016).

28. Y. Jiang et al., Anomalous Hall effect in \( \text{ZrTe}_2 \). Nat. Phys. 14, 451 (2018).

29. I. G. et al., Unconventional Hall effect induced by Berry curvature. Nat. Sci. Rev. 7, 1879–1885 (2020).

30. E. H. Wang et al., Chiral anomaly and ultrahigh mobility in crystalline \( \text{HfTe}_2 \). Phys. Rev. B 93, 165127 (2016).

31. Y. Liu et al., Evidence for topological edge states in a large energy gap near the step edges on the surface of \( \text{ZrTe}_2 \). Phys. Rev. X 4, 021017 (2016).

32. G. Marzoni et al., Evidence for a strong topological insulator phase in \( \text{ZrTe}_2 \). Phys. Rev. Lett. 117, 236401 (2016).

33. S. B. Li et al., Experimental observation of topological edge states at the surface step edge of the topological insulator \( \text{ZrTe}_2 \). Phys. Rev. Lett. 116, 176603 (2016).

34. Y. Zhang et al., Electronic evidence of temperature-induced Lifshitz transition and topological nature in \( \text{ZrTe}_2 \). Nat. Commun. 8, 15512 (2017).

35. Y. Liu et al., Induced anomalous Hall effect of massive Dirac fermions in \( \text{ZrTe}_2 \) and \( \text{HfSe}_2 \). Phys. Rev. B 103, L020110 (2021).

36. H. Follwag, A. Kjekshus, Structural properties of \( \text{ZrTe}_2 \) and \( \text{HfSe}_2 \) as seen by powder diffraction. Solid State Commun. 60, 91–93 (1986).

37. Y. Zhang et al., Temperature-induced Lifshitz transition in topological insulator candidate \( \text{HfTe}_2 \). Sci. Bull. (Beijing) 62, 955–956 (2017).

38. S. Liu et al., Experimental observation of conductive edge states in weak topological insulator candidate \( \text{HfTe}_2 \). Appl. Mater. 6, 121111 (2018).

39. H. Chi et al., Lifshitz transition mediated external transport anomaly in bulk \( \text{ZrTe}_2 \). New J. Phys. 19, 015005 (2017).

40. G. Galitski et al., Unconventional Hall response in the quantum limit of \( \text{HfTe}_2 \). Nat. Commun. 11, 5926 (2020).

41. N. Zhang et al., Magnetotransport signatures of Weyl physics and discrete scale invariance in the elemental semiconductor tellurium. Prog. Natl. Acad. Sci. U.S.A. 117, 11337–11343 (2020).

42. J. P. Jay Gers, M. J. Aubin, J. G. Caron, The electron mobility and the static dielectric constant of \( \text{CdS}_{0.6} \) at 4.2 K. Solid State Commun. 21, 771–774 (1977).

43. H. Li, H. Liu, R. Joynt, X. C. Xie, Evolution with magnetic field of discrete scale invariant superconducting states in graphene. arXiv [Preprint] (2021). https://arxiv.org/abs/2109.05403. Accessed 21 September 2022.

44. P. E. Böschl, Projector augmented-wave method. Phys. Rev. B Condens. Matter 50, 17953–17979 (1994).

45. J. P. Pendle, K. Burke, M. Emzerhof, Generalized gradient approximation made simple. Phys. Rev. Lett. 77, 3865–3868 (1996).

46. G. Kresse, J. Hafner, Ab initio molecular dynamics for liquid metals. Phys. Rev. B Condens. Matter 47, 558–561 (1993).

47. G. Kresse, J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set. Phys. Rev. B Condens. Matter 54, 11169–11186 (1996).

48. W. Tang, E. Sanville, G. Henkelman, A grid-based Bader analysis algorithm without lattice bias. J. Phys. Condens. Matter 21, 084204 (2009).

49. I. Horcas et al., WSXM: A software for scanning probe microscopy and a tool for nanotechnology. Rev. Sci. Instrum. 78, 013705 (2007).