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Unraveling The Quantum Nature of Materials

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Abstract: *The fundamental interaction between electrons and atoms is described in quantum mechanics, which forms the basis of the physical description of all substances. While classical descriptions at the macroscopic level can often approximate these quantum effects, there has been an increasing focus in recent years on material systems where quantum effects persist across a broader spectrum of energy and length scales. Superconductors, graphene, topological insulators, Weyl semimetals, quantum spin liquids, and spin ices are examples of such materials. A considerable number of these entities obtain their characteristics through reduced dimensionality, specifically by confining electrons to two-dimensional surfaces. Furthermore, these materials often consist of electrons that cannot be regarded as independent particles due to their intense interactions; instead, they generate quasiparticles, which are collective excitations. However, it is worth noting that quantum-mechanical effects profoundly modify the properties of the material in every instance. This review provides an overview of the electronic characteristics of quantum materials as observed via the electron wavefunction. It investigates how the topology and entanglement of the material lead to an extensive range of quantum states and phases, which are more difficult to characterize classically than conventionally ordered states that are also influenced by quantum mechanics, including ferromagnetism.*

Keywords: Quantum Materials, Condensed Matter Physics, Electronic Structure.

I. INTRODUCTION

Recently, quantum physics in materials has undergone a paradigm change. Materials scientists and engineers have used quantum effects in various electronic devices for a long time, but their understanding of how subtle quantum effects govern the macroscopic has grown over the last decade.

There are two unique and outstanding quantum mechanics properties. Topological properties of quantum wave functions are one. Quantized vortices in superconductors are well-known. These vortices occur because the superconducting condensate must have a precisely defined phase, and gauge invariance controls how this phase links to magnetic flux. A topological invariant, such as the phase's winding number being an integer multiple of 2π around a vortex, is a constant attribute of a system despite incremental changes. In addition to superconductors, these quantities govern unique quasiparticle excitations and dissipationless transport in many other materials.

Quantum physics' non-local entanglement of some quantum states in teleportation operations with two photons separated by vast distances is another remarkable feature. In a singlet, the wavefunctions of its two spins are entangled because they are not exactly specified. Schrodinger said "the best possible knowledge of a whole does not necessarily include the best possible knowledge of all its parts". This highlights the unusual circumstance. Even in elementary substances, entanglement in a solid is confusing: the states of every 1023 electrons in a typical metal chunk are superimposed, so the many-body wavefunction encompassing the entire solid changes sign whenever two electrons are exchanged due to the fermion nature of electrons.

Fermi statistics, which need this antisymmetric entanglement, show that electrons with energies around the Fermi level strongly affect metal transport and thermodynamics. Many "conduction electrons" with tightly entangled wavefunctions survive. Quantum materials have unique entanglement or topological features, such as entanglement that exceeds Fermi statistics and topological processes like vortex generation. Due to electron entanglement in Cooper pairs and spin entanglement in complex magnets, traditional pictures cannot show them. Topology and entanglement create orderee states with phase transitions, which are different from normal states. Materials science is only beginning to study these complex quantum states.

Fermi statistics regulate electronic wavefunctions and are unchangeable. However, many quantum materials create quasiparticles, which may have characteristics different from their electrons. The Bogoliubov quasiparticles of a superconductor are complex superpositions of an undefined electric charge and a cavity. Topological quantum materials use exchange statistics to enable new emergent quasiparticles, even though they are fermions. Increasing experimental data reveals that bulk magnets dissipate magnons, conventional spin-wave excitation.

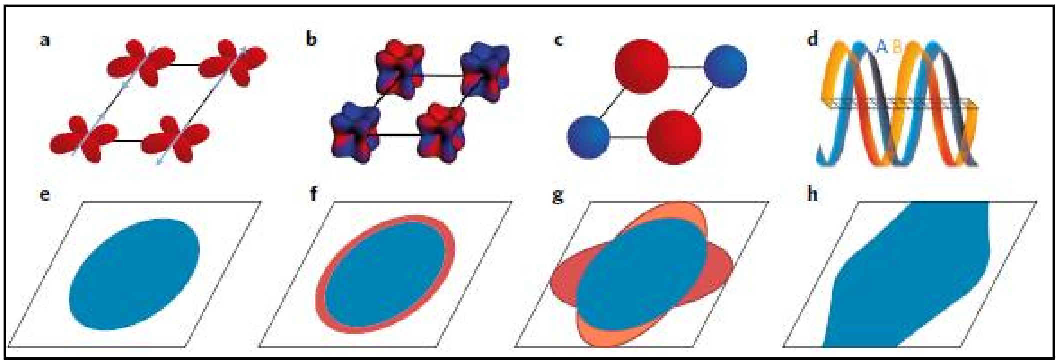

Figure 1 | A two-dimensional square lattice's electron configuration

There are real reasons for our incapacity to see the fascinating quantum beauty in nearby materials. Scattering from thermally stimulated lattice vibrations or random imperfections confuses electron quantum wavefunction phase. However, common metals like copper have unique quantum properties when chilled to a few Kelvin, when inelastic electron-lattice vibration scattering stops. Numerous physical observables exhibit quantum oscillations that are dependent on the magnetic field and have no classical counterpart if an external magnetic field generates circular orbits in electrons. Other basic metals like aluminum and lead have superconducting states at low temperatures, demonstrating quantum entanglement. The many-electron wavefunction reorganizes into a phase-coherent superposition of Cooper pairs6 due to effective electron attraction assisted by lattice vibrations. This re-entanglement affects just a fraction of electron states with energies around the Fermi level, but its macro-level manifestation—charge transfer without dissipation—illustrates the practical ramifications of quantum many-body physics. Topological considerations may also provide dissipationless transport like that seen in the very precise quantization of observables like the Josephson frequency quantum or Hall conductance.

Since 1986, when copper oxides showed high-temperature superconductivity, quantum materials research has grown. This discovery revealed that macroscopic quantum processes, including superconductivity, are not limited to very cold settings. This discovery inspired scientists to face one of the biggest challenges in modern physics: understanding coulomb interactions among conduction electrons, which occur far below the Fermi level and entangle both the spatial and spin components of a single electron's quantum state. Innovative applications and intellectual challenge sparked a vast research effort that has grown into many sectors. Hydrogen sulfide, a foul-smelling gas, transforms into a superconductor under high pressure with a record-setting transition temperature exceeding 200 K(8), and diamond, which exhibits quantum oscillations with several-second coherence times at room temperature due to electronic and nuclear spin entanglement at defect centers.

In recent years, topological quantum materials research has also grown significantly. Research into two-dimensional systems under very low temperature and severe magnetic field circumstances in the 1980s led to the idea of a new order based on electron wavefunction nontrivial topology. Theorists of that period developed topological tools that, twenty years later, allowed them to predict that even bulk materials may exist in topological states—the "topological insulators"—after adequate extension to zero field. Signatures also appear as electrical wavefunction entanglement. Entanglement in a bulk wavefunction may indicate if a boundary will exhibit a unique metallic edge state.

More topological states, including semimetals and strongly coupled states, are being found. Theorists believe 'quantum liquid' models have more complicated ground states than metals and superconductors. Experimentalists are nearing identifying quantum materials with these states. These liquids differ from ordinary phases in long-range entanglement

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due to topology. Thus, entanglement helps explain some of the differences between topological and superconducting states and normal matter. The interaction of topology and superconductivity is a hot study topic. This brief description doesn't capture the complexity of modern quantum materials research. We focus on two overarching properties of electronic quantum states that produce behaviors qualitatively distinct from the more basic quantum effects used in modern electronics. These are single-electron topological qualities. Bloch wavefunctions in materials and coulomb interactions between electrons that create entanglement beyond Fermi statistics. These processes might lead to the widespread use of quantum materials in device development.

Quantum collective phenomena

For years, solid state research has focused on the condensation of interacting electron systems into ground states with different collective order. Electronic correlation ideas are well-known in small molecule physics; review them before addressing recent improvements. Spin-1/2 and degenerate 1s-orbitals make up the hydrogen molecule's ground-state wavefunction, the simplest example. The spin-singleton ground state has symmetric atomic orbitals that accumulate negative charge between nuclei, reducing coulomb repulsion. Early quantum chemistry's inadequate computer resources allowed the modest contradiction with the spin-triplet state, which minimizes electron mutual coulomb repulsion and retains electron separation. The singlet molecule wavefunction cannot be represented as a product of single-electron states, proving that correlations entangle orbital and spin degrees of freedom. The eight-electron ground state of beryllium dimer surpasses current computers' processing power. The Be2 molecule has some peculiarities due to strong electron correlations in the nearly degenerate 2s and 2p valence orbitals of the fully occupied Be atoms, but this simple example shows that the computational power needed to analyze correlated-electron systems increases exponentially with electron number.

Solid state scientists have overcome these obstacles in decades of theory-practice research. After moving beyond a qualitative knowledge of electronic ordering phenomena, theory may now be used to change and generate electronic correlation characteristics. This breakthrough applies to metals, where electrons are delocalized and coulomb correlations are effectively screened, and Mott insulators, where electrons are strongly localized around atomic sites. In the 1950s, researchers devised semi-empirical principles for Mott insulators' effective spin-spin amplitude and direction. The magnetic ordering patterns and interactions of transition metal complexes with localized electrons in the third-dimensional atomic shell may now be properly computed. Normal Mott-insulator LaMnO3 is present. Ab initio methods approximate electronic correlations more precisely. To compute element transition temperatures from Pb to MgB2 in conventional superconductors with weakly correlated electrons, ab initio methods have been extended.

Novel magnets. Nevertheless, even these ostensibly established domains of quantum materials research have witnessed unexpected advancements in recent times. Among these is the revelation that Mott insulators featuring 4d and 5d valence electrons manifest a wholly distinct form of magnetic interaction in comparison to their widely recognized counterparts with 3d electrons. The relativistic spin-orbit coupling of the valence electrons in these materials is analogous to the strength of the correlation; consequently, the magnetic moments generated by the spin and orbital motion of the electrons are securely immobilized. The magnetic interactions that result from the entangled spin-orbit wavefunctions are significantly hindered, even in the simplest honeycomb lattice configurations implemented in stoichiometric quantum materials like RuCl3, Li2IrO3, and Na2IrO3. The resonant X-ray scattering data presented in provide direct evidence of the existence of these interactions within a honeycomb iridate. 'Spin liquid' ground states—solid-state equivalents of liquid helium in which quantum fluctuations destroy crystalline order even at zero temperatures—offer a novel approach to realizing model Hamiltonians, given that frustration impedes the formation of conventional magnetic order.

Over the last decade, magnetic Mott insulators have also evolved into a model platform for studying electronic correlations in the vicinity of quantum phase transitions that are controlled at zero temperature by an external parameter. Two instances of quantum transitions that distinguish conventional antiferromagnetic order from non-magnetic ground states composed of singlets are illustrated in Figure 3. At the interface where these two radically distinct types of order converge, the ground-state wavefunction becomes entangled on a macroscopic scale. Recent findings from neutron scattering experiments have unveiled the manifestation of bosonic quasiparticles at quantum critical sites for magnetism. Standard magnets demonstrate clearly defined spin waves that govern the magnetization's direction. However, the longitudinal modes responsible for modulating the magnetization's amplitude are typically encountered at significantly higher energies and are frequently intermingled with multimagnon excitations. However, in close proximity to the quantum critical point, longitudinal magnons exhibit a diminished magnitude, and neutron data indicate that they are safeguarded against decay into transverse spin waves in certain areas of momentum space. Thus, the dynamics of the Higgs mode can be investigated in a novel condensed-matter environment. As depicted in Figure 3, the quantitative comparison between neutron scattering data and theoretical work on insulating model magnets lays the groundwork for investigation into the impact of quantum-critical correlations on the characteristics of a significantly broader category of quantum materials, such as superconductors and metals.

Excitonic insulators. Recent discoveries in the study of metals containing weakly correlated electrons that are highly delocalized have also been unexpected. A notable aspect of the study is a series of experiments conducted on semimetals, such as TiSe2 and Ta2NiSe5, which, when cooled, endure phase transitions into insulating ground states. Experimental evidence indicates that excitons are generated as a result of coulomb attraction between electrons and holes in small pockets near the Fermi level, thereby inducing this transition. The condensation of excitons into an insulating many-body ground state can be conceptually likened to the superconducting transition that arises from the formation of Cooper pairs between two electrons. However, in the zero-temperature limit, this process leads to conductivity of zero as opposed to an infinite amount. Insights into a concealed correlation between these two antithetical ordering phenomena have been presented in recent experiments, which demonstrate that doping or moderate hydrostatic pressure induces the formation of a superconducting phase in TiSe2. This observation prompts an inquiry into the degree to which the standard theory of lattice-mediated attraction between electrons can account for the superconductivity observed in TiSe2 and similar materials. Alternatively, it raises the question of whether collective electronic modes resulting from coulomb correlations are more significant. Ongoing research is concerned with determining whether the superconductivity observed in SrTiO3, a material that has traditionally been classified as an electron-phonon superconductor, is in fact propelled by plasmons or quantum-critical ferroelectric soft modes. The emergence of the capability to manipulate the dimensionality and density of the electron system in complex materials such as TiSe2, SrTiO3, heterostructures, and exfoliated layers, presents novel prospects for testing these predictions.

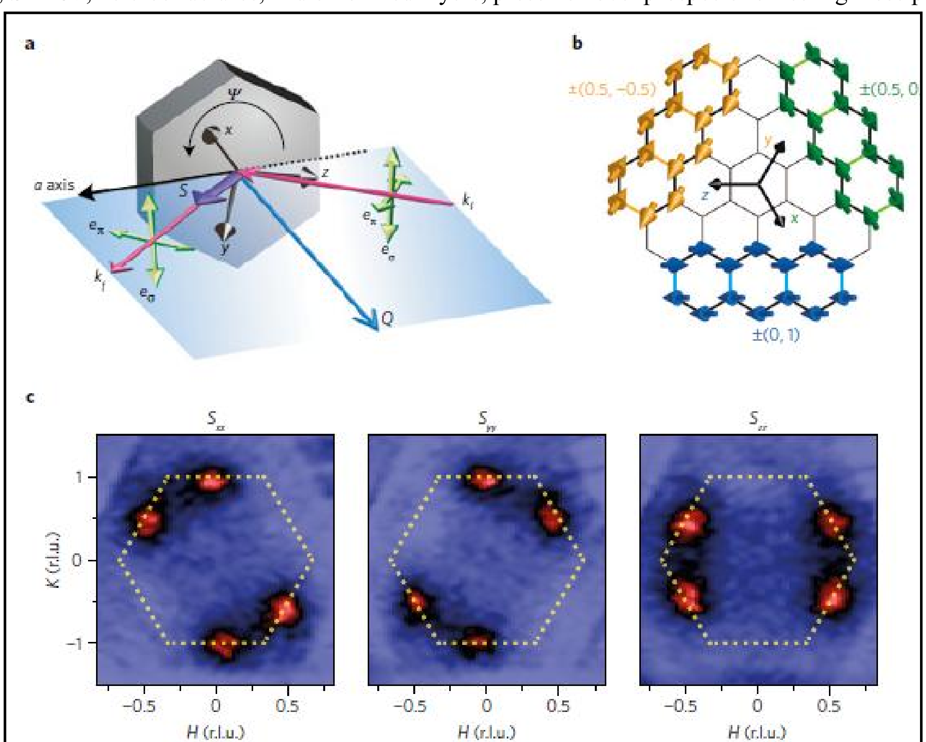

Figure 2 | Scattering of resonant X-rays by a Kitaev magnet.

Unconventional superconductors. Subsequent to the identification of high-temperature superconductivity in chalcogenides and iron pnictides, research has established a framework for the systematic investigation of electronically driven superconductivity and its interaction with various types of electronic order. The correlation strength in these materials is moderate, meaning it is analogous to the bandwidth of a single electron but insufficient to induce Mott localization. Electronic correlations are evident in the form of pervasive and powerful antiferromagnetic spin fluctuations. These fluctuations have been extensively documented as having a significant impact on superconductivity.

These developments have been fueled in part by experimental observations on iron-based superconductors. While the present methods fail to provide exact predictions of the temperatures at which superconductivity begins to flow and there are still unanswered significant inquiries, there are valid grounds to anticipate ongoing advancements by methodically refining the experimental and theoretical methodology, in a manner similar to that which conventional magnets and superconductivity research has been approached.

Notwithstanding these progressions, comprehending electron systems that are strongly correlated in the vicinity of the Mott metal–insulator transition continues to be a formidable obstacle in contemporary physics. The transition induces a substantial re-entanglement of the many-electron wavefunction, which encompasses spatial and spin degrees of freedom and extends to the very bottom of the conduction band. The two-dimensional Hubbard model, which is considered the most basic model intended to represent this transition, has thus far evaded a comprehensive solution through analytical or numerical means, despite significant advancements in comprehending its phase behavior.

A variety of spontaneously broken rotational and translational symmetries and modulated structures with "intertwined" order parameters result from the interaction between short-range and long-range interactions near the metal–insulator transition. The intricate charge and spin textures that result bear some resemblance to partially ordered structures observed in classical liquid crystals. However, the quantum phase winding across these textures generates unprecedented phenomena that lack equivalents in classical physics. An example of this is the spontaneous decoupling of superconducting sheets in three-dimensional materials through the phase-coherent superposition of charge order and superconductivity. Additionally, this phenomenon can induce unconventional vortex excitations, although the veracity of this prediction remains to be determined. Thermodynamic and transport characteristics can be significantly influenced by quantum phase transitions between modulated structures that are induced by external electric and magnetic fields, doping, pressure, and recent experiments on high-temperature superconductors.

The comprehension and regulation of the impact that doping-induced disorder and lattice strain have on these transitions, as well as the overall mesoscale properties of correlated-electron systems, continue to be significant obstacles in the field of quantum materials research. This is primarily due to the fact that these electronically inhomogeneous states offer ample opportunities for diverse applications due to their considerable vulnerability to external parameters.

However, the identification of high-temperature superconductivity has demonstrated that from a chaotic mixture of strongly correlated electrons, exquisitely robust, homogeneous many-electron states can emerge. Significant advancements have been achieved in the examination of unconventional superconductivity and other ordering phenomena observed in copper oxides, in addition to related states in ruthenates, heavy-fermion intermetallics, organic conductors, and other correlated-electron substances.

However, basic questions about collective dynamics remain the focus of modern science. Does their entanglement include electrons on neighboring lattice sites in close proximity, or is it connected to quantum phase transitions between diverse types of collective order and hence critical? What is the effect of these considerations on unusual normal-state features like the temperature-linear resistivity seen in many quantum materials? Researchers are using unique experimental methods to study these and other questions. These methods include transport and thermodynamics in magnetic fields up to 100 T, novel spectroscopies like resonant inelastic X-ray scattering, and pump-probe methods that produce coherent states that deviate significantly from equilibrium. Ingenious computational schemes include machine-learning algorithms and ab initio methods, which provide direct insight into this collaboration, should speed up the controlled manipulation of highly coupled electron systems. This will enable theory-driven creation of quantum materials with collective electrical order that can tolerate thermal decoherence above room temperature.

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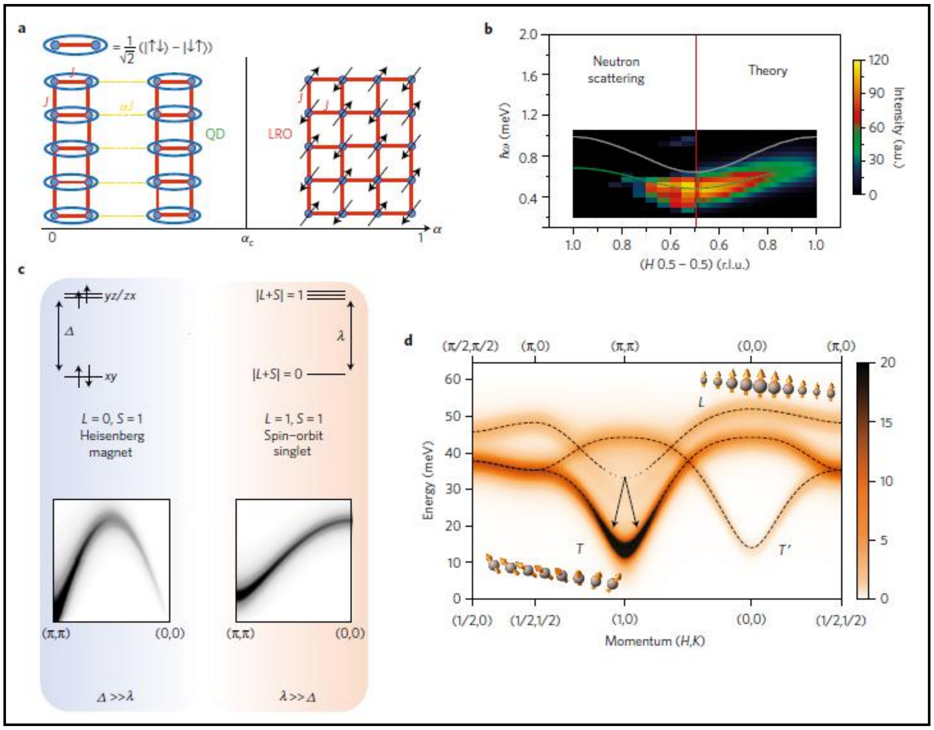

Figure 3 | Scattering of neutrons by Higgs modes.

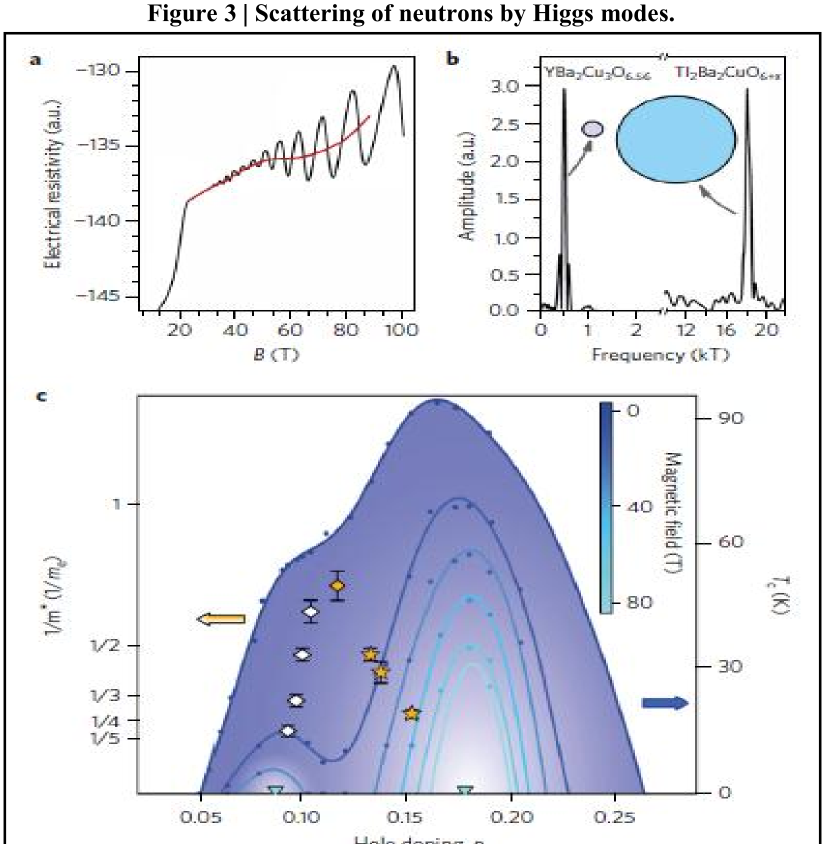

Figure 4 | Extreme-temperature superconductors exhibit quantum oscillations and quantum criticality.

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Novel electron wavefunction phenomena caused by geometry the simplest topological phases, based on single-electron wavefunction geometry, have seen a huge renaissance in the recent decade. These phases are based on the 1980-discovered integer quantum Hall effect (IQHE). It shows that two-dimensional electron systems under high magnetic fields may have very accurate transport quantization. It won the 2016 Nobel Prize in Physics and has been crucial to several recent advances in this area.

Topological insulators. Instead of a magnetic field, spin-orbit coupling creates nontrivial electronic topology, creating "topological insulators." Spin-orbit coupling has time-reversal symmetry, unlike magnetic fields, which makes numerous important differences. In two dimensions, a topological insulator phase contains quantum Hall effect-like edge states. Edge states may enable a quantized spin Hall effect at certain boundaries. The edge states are protected against backscattering by time-reversal symmetry, not an energy gap. "Chern insulators" may act as quantum Hall layer arrays. However, bulk materials have a three-dimensional topological insulator phase. Metallic surface states exist, and in the most basic implementation, the surface harbors a solitary 'Dirac cone' of electrons, which resembles the cones in the electronic structure of graphene shown in Figure. The 3D topological insulator supports the quantized magnetoelectric effect which may have been identified in recent terahertz optical experiments. A 3D topological insulator doped with magnets creates a quantum anomalous Hall state, similar to the IQHE but driven by spin–orbit coupling rather than orbital magnetic fields.

Semimetals with topology. Recent study has focused on topological semimetals, which have two forms. Thouless, Kohmoto, Nightingale, and den Nijs (TKNN) developed an alternative IQHE picture around the same time as the textbook picture, based on Landau levels and more directly applicable to an electron moving in a crysta. As stated in this paper, the integer quantum Hall effect is connected to nontrivial topological features of crystal electron Bloch states. Haldane then demonstrated the integer quantum Hall effect in a simple crystal model with a zero average magnetic field. Haldane and Thouless used graphene's massless electrons to bulk materials. In solid states, Dirac's original equation for a massless fermion in three dimensions describes a point where four bands intersect; the effective Bloch Hamiltonian has four-by-four matrices that resemble those in the 3D Dirac equation. The first Dirac semimetals were discovered in the previous several years, and more research continues. Another example is Dirac quasiparticles, which often develop around gap function nodes in superconductors.

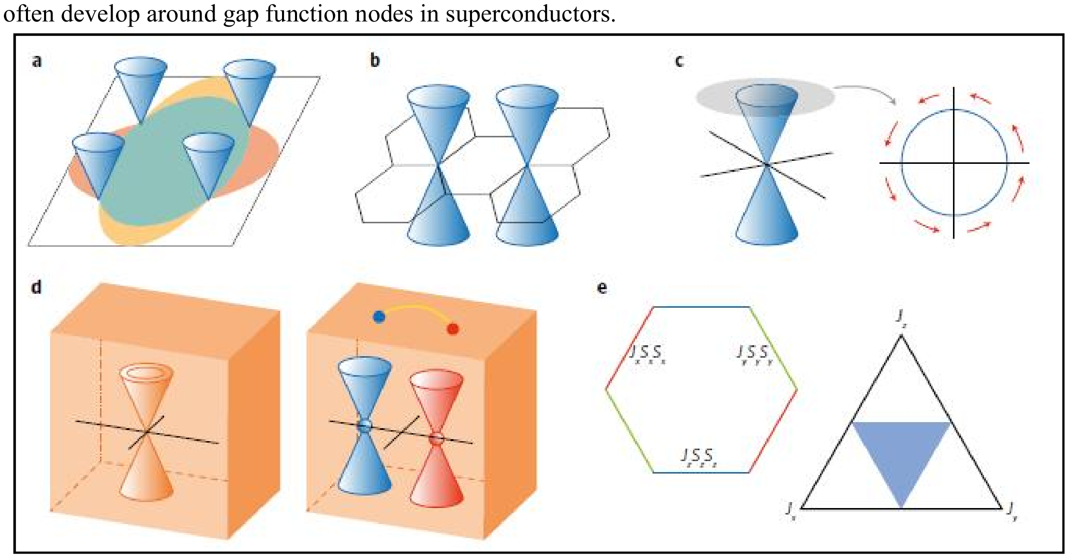

Figure 5 | Instances of fermions lacking mass in quantum materials.

Hermann Weyl discovered soon after Dirac's equation was developed that a massless particle may have a constant "handedness," allowing the equation to be split into two halves. Majorana's alternate approach of decomposing the Dirac equation is discussed later. Substances that contradict time-reversal or inversion symmetry may have degenerate points spanning two bands. Weyl points during phase transitions between conventional and topological insulators have been shown to have topological relevance. The Chern numbers addressed previously in the IQHE are intimately related

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to topological numbers for Weyl points. The Nielsen–Ninomiya theorem from particle physics also explains why materials have zero Weyl points.

Although theorists had been discussing Weyl semimetals since the 1930s, their experimental discovery was largely facilitated by new topological tools: Fermi arc surface states, and the detection of these arcs in photoemission provided substantial evidence that the phase had been successfully identified. Dirac and Weyl semimetals may enable many transport and optical phenomena.

Interplay of many-body physics and topology

A few years after the integer quantum Hall effect was discovered, two-dimensional electron vapors under a strong magnetic field showed an even more unusual electron state99. The fractional quantum Hall effect (FQHE) cannot be described by nearly independent electrons like the IQHE. An incompressible quantum liquid with exceptional properties results from strong Coulomb repulsion. For example, an electron supplied at 1/3 filling to the FQHE state separates into three quasiparticles with e/3 charges.

The surprising fractional statistics of quasiparticles in this intricate liquid suggest they are neither fermionic nor bosonic. Quantum physics textbooks classify point particle statistics in three dimensions as odd (fermionic) or even (bosonic) permutation group representations. Forward-thinking theoretical work revealed in 1976 that two-dimensional particles might have several statistics101. In two dimensions, the "braiding"—the mechanism by which the exchange occurred—becomes crucial, and statistics are classed using braid group representations rather than permutation group representations.

We will cover odd statistics here since the FQHE and topological superconductors have made them an important topic of study. The braid group is more complex than the permutation group. FQHE states have been shown to realize "Abelian" and "non-Abelian" statistics. The term "Abelian" refers to "commutative," because in a state with Abelian statistics, such as the FQHE state at 1/3, each braiding operation causes a phase component that impacts the state, not necessarily ±1.

That may seem challenging, yet very high-quality FQHE data revealed novel plateaus that were inexplicable to any known Abelian state. Theorists documented non-Abelian statistics wavefunctions103. When a system has many quasiparticles, a braiding acts as a unitary matrix on a degenerate subspace of states. Due of the large number of braiding matrix options, braiding quasiparticles may operate as a universal quantum computer104 in certain FQHE situations.

Topology superconductivity. This area was mysterious until it was proven that even a simple superconducting wavefunction may allow non-Abelian statistics105, like the classic theory of Bardeen, Cooper, and Schrieffer3. If the superconductor exhibits pairing symmetry (px + ipy), ordinary vortex cores capture Majorana zero modes with non-Abelian statistics. Most Majorana mode searches concentrate on "materials," not FQHE states. Our objective is to find a solid material that superconducts and sustains Majorana modes independently. One chemical extensively studied in this context106 is Sr2RuO4. This material would provide a new quantum computing strategy in addition to its interest in non-Abelian statistics.

Blending basic materials into a heterojunction that allows Majorana zero modes is another option. One material is standard s-wave superconductors, while the other is a topological insulator or semiconductor with spin-orbit coupling in a magnetic field. The heterojunction's non-superconducting component is defined by the single Fermi surface sheet, including spin.

Several promising experiments suggest Majorana zero modes may cause zero-bias peaks in tunnelling, although braiding has not been proved. A phase of superfluid helium, a topological superfluid of neutral atoms with zero modes and surface states, gives "exis-tence proof" of topological superconducting states. Fractional quasiparticles may also occur in materials without mobile electrons.

whisk liquids. One may question what causes unusual connected FQHE situations in the half filled Landau level. When considering just kinetic energy, a partly full Landau level has a high degeneracy, suggesting no energy barrier for interactions. Interactions turn noninteracting states into complex superpositions.

Magnetic frustration creates another useful solid degeneracy. When magnetic interaction energy cannot be diminished simultaneously, a magnet gets frustrated. In basic interaction models, many have degenerate ground states. Further interactions or remains of earlier contacts may build superpositions of the first degenerate spin configurations. Quantum spin liquids with fractional excitations, half-integer spin instead of integer spin of traditional magnons, and topological order like FQHE states in frustrated magnetism models come from this process.

The frustrated magnetism group has long explored quantum spin liquids, and many types have been found. Chiral spin liquids are closely related to simple FQHE states. Quantum dimer models use Z2 spin liquids to approximate cuprate superconductor singlet correlations. Herbert Smithite may have this spin liquid in the nearest-neighbor Heisenberg model on the kagome lattice.

Few topics are as intriguing as gapless spin liquids. Topological order may be rigid in states with an energy gap above the ground state subspace. There are explicit models with gapless spin liquid ground states, however it is harder to establish order. A famous example on the honeycomb lattice (Fig. 5) by Kitaev helped explain inelastic neutron scattering on $RuCl_3$. The newest numerical studies reveal that the kagome lattice antiferromagnet may be a gapless state, showing that fundamental Hamiltonians may allow multiple topological orderings.

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