Conformal field theory at the critical point of monolayer-bilayer phases of subvalent cations in honeycomb layered materials

Godwill Mbiti Kanyolo\textsuperscript{1,*} and Titus Masese\textsuperscript{2,3,†}

\textsuperscript{1}The University of Electro-Communications, Department of Engineering Science, 1-5-1 Choju-cho, Chofu, Tokyo 182-8585
\textsuperscript{2}Research Institute of Electrochemical Energy (RIECEN), National Institute of Advanced Industrial Science and Technology (AIST), 1-8-31 Midorigaoka, Ikeda, Osaka 563-8577, Japan
\textsuperscript{3}AIST-Kyoto University Chemical Energy Materials Open Innovation Laboratory (ChEM-OIL), Yoshidahonmachi, Sakyo-ku, Kyoto-shi 606-8501, Japan

The rather intriguing experimental result that a wide class of silver (Ag)-based layered materials form stable Ag bilayers is often explained in literature by the presence of argentophilic bonds between Ag cations, whose origin is traced not only to unconventional weak attractive interactions between $d^1$-$t_2g$ orbitals of monovalent Ag atoms but also to the formation of an empty orbital band of mainly Ag-5s orbital character near the Fermi level, capable of accommodating additional electrons, translating to anomalous subvalent states. However, the fact that each Ag bilayer consists of a pair of triangular sub-lattices suggests an unexplained bifurcation mechanism for the honeycomb lattice. On the other hand, it is well-known that the honeycomb lattice of graphene requires an additional degree of freedom to describe the orbital wave functions sitting in two different triangular sub-lattices, known as pseudo-spin. In this paper, we exploit the pseudo-spin degree of freedom in the Ag honeycomb lattice to propose a bifurcation mechanism for the Ag triangular sub-lattices, which ultimately requires conformal symmetry breaking within the context of an idealized model, resulting in a cation monolayer-bilayer phase transition in exemplars such as Ag$_2$M$_2$TeO$_6$ (where $M = $ Ni, Co, Cu, Mg, Zn). In this description, the critical point of the phase transition is described by Liouville conformal field theory. Our framework is consistent with the following necessary and sufficient conditions for the observation of stable bilayers of cations in layered materials: 1) observation of a pair of cation triangular sub-lattices of the honeycomb lattice; 2) a bond between the subvalent cation and an anion and; 3) existence of weakly attractive cation-cation interactions related to allowed cation subvalent states. Since other materials such as Ti$_2$MnTeO$_6$ share the aforementioned conditions with Ag-based systems, the theoretical framework herein also sheds light on the nature of their bilayer structure, with noteworthy applications in the vast field of analogue quantum gravity research.

I. INTRODUCTION

Whether a physical theory is particularly soluble or not is predicated on the number of conservation laws exhibited by the system.\cite{1, 2} In particular, since Noether’s theorem requires every continuous symmetry to guarantee a corresponding conservation law\cite{1}, highly-symmetric theories tend to be the most soluble. Consequently, physicists can often exploit continuous symmetries of the physical system to completely find the solutions of the theory, in what can be dubbed as ‘bootstrapping’ the theory in question.\cite{3}

At the heart of all physical quantum theories is group theory, which requires that each continuous internal symmetry (here labeled by a positive integer, $g \in \mathbb{N}$) be generated by a Hermitian quantum operator, $Q_g(t) = \exp(i\mathcal{H}t)Q_g(0)\exp(-i\mathcal{H}t) \equiv Q_g = Q_g^\dagger$ which must commute with the Hamiltonian, $\mathcal{H} = \mathcal{H}^\dagger$ of the system (the generator of time translations) to be considered a symmetry of the system, $i\partial_t Q_g(t) = [Q_g(t), \mathcal{H}] = 0$, thus satisfying Noether’s theorem. Consequently, conservation laws require $Q_g$ and $\mathcal{H}$ to be simultaneously diagonalizable (\textit{i.e.} operators that commute share common eigenstates), which in turn restricts the size of the irreducible representation of the Lie algebra of the group (Hilbert/Fock space \textit{etc}) to a subset spanned only by the eigenvectors $|Q_{g_1} \cdots Q_{g_2} \rangle_{g \neq g'}$ and their linear combinations, since only these states correspond to the eigenstates of the Hamiltonian. For instance, this implies that, physical systems that admit a Lie group of size, $N$ with a large number of generators often admit known solutions. Indeed, this is the philosophy exploited when embarking on solving matrix field theories in the large $N$ limit.\cite{4, 5}

On the other hand, quantum field theories (QFTs) in $d$-dimensional Minkowski space-time, $\eta_{\mu\nu}$ have space-time symmetries generated by $d+d(d-1)/2 = d(d+1)/2$ number of Poincaré group generators\cite{6, 7}, corresponding to $d$ translations, $p_\mu = -i\partial_\mu$ and $d(d-1)/2$ rotations and boosts, $M^\mu_\nu = ix^\nu \partial_\mu - ix^\mu \partial_\nu$, alongside the set of all internal symmetries, $\{Q_{g}\}$ which further constrain the representation space. For instance, the Coleman-Mandula theorem requires such QFTs with a mass (inverse-length) scale to have no internal symmetries with space-time indices\cite{8}, hence guaranteeing internal symmetries are strictly generated by space-time scalars. Nonetheless, relativistic QFTs with no mass scale offer a recourse
to circumventing this no-go theorem.[8, 9] As a result, the emergent conformal symmetry near critical points of physical systems where phase transitions occur[10], further augments the constraints on such theories known as conformal field theories (CFTs)[11], by introducing additional conformal symmetries (scale transformations, $D = ix^\mu \partial_\mu$ and special conformal transformations, $K_\mu = i(x^\alpha x^\mu \partial_\mu - 2x^\mu x^\alpha \partial_\alpha)$).[9, 11] Provided conformal symmetries are adhered to in calculations of quantum correlation functions, CFTs can be completely solved by conformal bootstrap.[3] The most famous examples are Liouville conformal field theory[12] and two-dimensional (2D) CFTs known as Virasoro minimal models[11], which have successfully been classified and completely solved.[13, 14]

On the other hand, layered materials tend to exhibit a myriad of intriguing crystalline symmetries and topological characteristics based on their 2D geometries and defects.[15, 16] Since the discovery of graphene-based systems[17] and layered materials[15] such as honeycomb layered materials[16], a great deal of experimental and theoretical studies has been dedicated to illuminating the role the honeycomb lattice plays in the dynamics of electron quasi-particles and spin degrees of freedom, enriching our understanding of phenomena in materials ranging from high-temperature superconductors and 2D quantum hall systems to topological insulators and Kitaev materials.[16, 18–20] Despite their crystal-structural versatility and compositional tuneability attracting interest in various realms of solid-state (electro)chemistry, materials science, condensed matter physics and pioneering the discovery of next generation energy storage materials[16, 21–26], theoretical and experimental studies centered on the honeycomb lattice have focused mainly on its effect on 2D electron and spin dynamics, thus rendering the behavior of larger particles such as positively-charged ions (cations) on the lattice understudied.

In previous works[16, 27], the present authors have suggested that a wide class of layered materials, where positively charged mobile cations are sandwiched between the layers of immobile ions forming adjacent series of slabs within a stable crystalline structure, are poised to exhibit emergent quantum geometries.[28] In a majority of these exemplars, cationic mobility can be traced to extremely weak Van der Waals bonds whose strength correlate with the large inter-layer distances between the slabs.[16, 29–32] Particularly, layered transition metal oxides display a wide swath of crystal structural versatility and composition tuneability, which renders these properties attractive in various realms of solid-state (electro)chemistry, materials science and condensed matter physics research.[16, 21–26] A specific class of layered transition metal oxides has recently emerged adopting, inter alia, chemical compositions embodied mainly by $A_M^2\text{MDO}_6$, $A_2M_2\text{DO}_6$ or $A_2M_2\text{DO}_6$ wherein $A$ represents an alkali-ion (Li, Na, K, etc.) or coinage metal ions such as Ag, whereas $M$ is mainly a transition metal species such as Co, Ni, Cu, Zn, etc. and $D$ depicts a pnictogen or chalcogen metal species such as Sb, Bi and Te.[33–55] In these materials, mobile $A$ cations are sandwiched between slabs entailing $M$ atoms coordinated with oxygen around $D$ atoms in a honeycomb lattice arrangement.[16]

Of further interest are the dynamics of the cations within the aforementioned materials[27], since their diffusion contributes a net current when a sufficient external electric field arises in an electrode-electrolyte setup forming a cell or battery.[56] The polarity of the electric field defines the charging and discharging processes corresponding to cation extraction (de-intercalation) and cation insertion/reinsertion (intercalation) processes respectively. Experimental characterization and theoretical computations show that the diffusion paths are largely restricted to honeycomb pathways in honeycomb layered tellurides (for instance, $K_2\text{Ni}_2\text{TeO}_6$, $Na_2\text{Ni}_2\text{TeO}_6$ and $Na\text{K}2\text{TeO}_6$[57–59]) as shown in Figure 1, where locations of cations with highest occupation probability are found at specific sites correlated with honeycomb octahedral structures within the slabs. Thus, the Van der Waals forces initially localize the cations, forming a loosely-bound 2D honeycomb lattice where mobility of the cations is only possible when sufficient activation energy offset this localization leaving cationic vacancies.[60, 61] If the material had no vacancy defects to begin with, the number of cationic vacancies will correspond to the number of mobile cations. Thus, it is reasonable to expect that diffusion properties in the material can be completely captured either by the dynamics of the cations within the honeycomb lattice or by the dynamics of their vacancies.[16, 27] This corresponds to a gravity/CFT duality, where the lattice of cations exhibit conformal symmetries whereas the vacancies are topological defects tied to emergent quantum geometries.[62]

Considering emergent gravity to describe defects in crystals is not entirely a novel idea.[63–68] For instance, it has long been proposed that considering finite torsion (non-symmetric Christoffel symbols/affine connection, $\Gamma^\rho_{\mu\nu} \neq \Gamma^\rho_{\nu\mu}$) within the context of Einstein-Cartan theory ought to capture various intriguing aspects related to disclinations and dislocations within crystals.[63–67] Moreover, it has been further argued that Einstein gravity can still emerge in a crystal whose kinetic energy order terms are restricted to second-order in derivatives[68] in accordance with Lovelock’s theorem.[69] Herein, we shall concern ourselves with Einstein gravity with a torsion-free connection, $\Gamma^\rho_{\mu\nu} = \Gamma^\rho_{\nu\mu}$ where topological defects can still be non-vanishing even for torsion-free manifolds as long as higher order derivatives of the Gauss-Bonnet type[69] are present in the crystal.

Moreover, we shall focus on a description of bosonic cations with vacancies as topological defects. In particular, when the cations are bosons, a Fermi level does not exist, implying that a particle-hole picture, where the particle and the vacancy carry separate pieces of information is precluded. Thus, the vacancies cannot be treated as holes, but an equivalent description for the dynam-
ics of the cations carrying the same (thermodynamic) information. Consequently, a Bose-Einstein condensate of the cations\cite{27} avails a prime avenue for an emergent geometric description of such vacancies as topological defects within a theory of diffusion on the honeycomb lattice in the context of emergent quantum geometry. Conversely, describing the diffusion in layered materials comprising fermionic cations such as $^6$Li with this approach would pose some significant challenge. Nonetheless, since their magnetic moment is readily traceable in nuclear magnetic resonance experiments, the fermionic cations are typically introduced in meager amounts via doping techniques in order to improve resolution.\cite{70,71}

Consequently, their overall effects on the diffusion properties are expected to be negligible. Nonetheless, if the vacancies are treated as holes it is expected that this particle-hole symmetry is rather befitting to cationic Majorana modes \textit{e.g.} with twist defects\cite{72-74} which could be exploited to incorporate fermionic behavior in the formalism.\cite{75} Another approach dealing with fermionic degrees of freedom is a pairing mechanism, which transforms pairs of fermions into bosons\cite{76}, hence preserving the bosonic description.\cite{27} Meanwhile, the honeycomb lattice can be shown to exhibit modular symmetries generated by $Q \in \text{SL}_2(\mathbb{Z})/\mathbb{Z}_2 \equiv \text{PSL}_2(\mathbb{Z})$, elements of the special linear group, $\text{SL}_2(\mathbb{Z})/\mathbb{Z}_2$ up to a sign in the cyclic group, $\mathbb{Z}_2$\cite{62}, suggesting a link between the theory of cations on the honeycomb lattice and conformal field theory.\cite{77} On the other hand, it is well-known that the honeycomb lattice of graphene requires an additional degree of freedom to describe the orbital wave functions sitting in two different triangular sub-lattices, known as pseudo-spin.\cite{78}

In this paper, we are interested in 2D honeycomb materials whose cationic dynamics exploit aforementioned gravity/CFT duality. We shall specifically consider the conditions that lead to the pairing of pseudo-spin states of cations in the honeycomb sub-lattices of honeycomb layered tellurates such as Ag$_2$M$_2$TeO$_6$ (where $M$ is a transition metal (such as Co, Ni, Cu and Zn)) or alkali-earth metal (such as Mg), or a combination of multiple transition metals), layered binary and ternary oxides such as Ag$_6$O$_2$ (or equivalently as Ag$_3$O) and Ag$_2$MO$_2$ ($M = \text{Co, Cr, Ni, Cu, Fe, Mn, Rh}$), Ag$_3$Ni$_2$O$_4$, and layered halides such as Ag$_2$F \cite{79-90}, requires conformal symmetry breaking (via breaking of scale invariance), resulting in a cation monolayer-bilayer phase transition. In this description, we find that 2D Liouville conformal field theory exists at the critical point of the phase transition\cite{10,12}, which is shown to be dual to 1 + 3 dimensional Anti-de Sitter (AdS) space-time.\cite{91}

Our framework is consistent with the following necessary and sufficient conditions for the observation of stable bilayers of cations in layered materials: 1) observation of a pair of cation triangular sub-lattices of the honeycomb lattice; 2) a bond between the subvalent cation and an anion and; 3) existence of weakly attractive cation-cation interactions related to allowed cation subvalent states. Since other materials such as Tl$_2$MnTeO$_6$\cite{92} share the aforementioned conditions with Ag-based systems, the theoretical framework herein is consistent with their monolayer-bilayer phase transition.

Hereafter, we shall set Planck’s constant, the speed of electromagnetic waves in the material, $\hbar$, Boltzmann’s constant, $k_B$ and the elementary charge of the cations to unity, $\hbar = e = k_B = q_e = 1$, and employ Einstein summation convention for all raised and lowered indices unless explicitly stated otherwise.

II. IDEALIZED MODEL OF CATIONIC DIFFUSION

A. Candidate materials

We shall introduce the idealized model of cationic diffusion\cite{16,27}, which lays the groundwork for our formalism thereafter. The idealized model applies to a wide class of layered materials, where positively charged mobile cations are sandwiched between the layers of immobile ions forming adjacent series of slabs within a stable crystalline structure as exemplified in Figure 1. In a majority of these exemplars, the mobility and diffusion of the cations can be traced to extremely weak chemical bonds whose strength is correlated with the strength of emergent forces such as Van der Waals interactions and the inter-layer distance between the slabs,\cite{16,29-32} \textit{viz.},

(a) Layered transition metal oxides such as $A_xMO_2$ (where $A = \text{Li, Na, K, Ag, etc.}$, $M$ is a transition metal or a combination of multiple transition metals and $0 < x < 1$), $A_yV_2O_5$ (where $0 < y < 2$), $D_xV_3O_5$ (where $D = \text{Mg, Ca, Al, Ag}$ and Ca$_3$Co$_4$O$_9$;\cite{30,32,56,93-99}

(b) Layered metal (di)chalcogenides such as $A_x\text{TiS}_2$ and $A_x\text{CrS}_2$ (where $0 < x < 1$);\cite{100-102}

(c) Graphite intercalation compounds such as LiC$_6$, KC$_8$, RbC$_8$ and CsC$_8$, including their intermediate compositions, for instance, KC$_{12n}$ ($n > 1$), LiC$_{6n}$ ($n > 1$) and LiC$_9n$ ($n \geq 2$);\cite{31,103-106}

(d) Layered polyion-based compounds comprising pyrophosphates such as Na$_2$Co$_2$P$_2$O$_7$ and K$_2$M$_2$P$_2$O$_7$ ($M = \text{Co, Ni, Cu}$), pyrovanadates such as K$_2$Mn$_2$V$_2$O$_7$ and Rb$_2$MnV$_2$O$_7$, oxyphosphates such as NaVOPO$_4$ and LiVOPO$_4$, layered KVOPO$_4$, diphosphates such as Na$_3$V(P$_2$O$_7$)$_2$, fluorophosphates such as Na$_2$FePO$_4$F, hydroxysulphates such as LiFeSO$_4$OH and oxysilicates such as Li$_2$VOSiO$_4$;\cite{107-115}

(e) Honeycomb layered oxides mainly entailing compositions such as $A_2MDO_6$, $A_2MD_2DO_6$ or $A_3M_2D_5O_6$ wherein $A$ represents an alkali-ion (Li, Na, K, etc.) or coinage metal ions such as Ag, whereas $M$ is mainly a transition metal species such as Ni, Cu, Zn, Co, etc. or Mg (and/or a combination of multiple transition
metals) and $D$ depicts a pnictogen or chalcogen metal species such as Sb, Bi, Te, amongst others.[33–55]

These materials are poised to exhibit emergent quantum geometries commensurate with 2D Liouville theory.[12, 27, 62]

**B. Cationic vacancies as topological defects**

In particular, the radial distribution function (pair correlation function) for the cations, $g(r)$ is the conditional probability density that a cation will be found at position $r$ at each inter-layer, relative to another cation within the same inter-layer. Equivalently, it is the average density of a cation at $r$ relative to a tagged particle.[116] This requires that the 2D number density given by,

$$\rho_{2D}(r) = \rho_0 g(r)$$

(1a)

is normalized as[117],

$$\int_{A} d^2 r \rho_{2D}(r) = \nu - 1,$$

(1b)

where $\nu$ is the number of cations within the inter-layer, $\rho_0$ is the bulk number density and the integration is performed over some emergent 2D Euclidean manifold, $A$ at each inter-layer. Moreover, the normalization given by, $\nu - 1$ instead of simply $\nu$, is understood to arise from excluding the contribution of the reference cation, as per the definition of the pair correlation function given above.

Meanwhile, the coordinate, $\vec{x} = (\vec{r}, z)$ tracks the average diffusion path of the center of mass of the cations and hence is taken to obey the Langevin equation[118],

$$\frac{d^2 \vec{x}}{dt^2} = -\vec{p}(t) - \vec{\eta}(t),$$

(2)

where $t$ is the proper length on the 2D manifold, $A$ with the metric,

$$dt^2 = g_{ab} dr^a dr^b,$$

(3)

$\vec{\eta}(t)$ is the acceleration and $\vec{p} = m d\vec{x}(t)/dt$ is the center of mass momentum acting as the friction component with $m$ the average effective mass of the cations and $1/m$ plays the role of a mean time between collisions, assumed to be equivalent in all slabs due to translation invariance along the unit vector, $\vec{n} = (0, 0, 1)$ normal to the slabs (where the unit vector points in the $z$ direction). This guarantees that in the continuum limit, the 3D crystal admits not only a time-like leading to energy conservation, but also a $z$-like Killing vector, which leads to momentum conservation in the $z$ direction.[27]

In fact, the additional constraint $mdz/dt = p_z = 0$ restricts cationic motion within the $x - y$ plane, which in turn allows one to effectively set $z = 0$ without loss of generality. We thus have, $\vec{x} = (\vec{r}, 0)$ where $\vec{r} = (x, y)$. Thus, it turns out that eq. (2) is the analogue of the Gauss-Bonnet theorem[119] on the manifold, $A$ as illustrated in Figure 2,

$$\chi(A) = \frac{1}{2π} \int_{A} \frac{1}{2} \frac{d^2 r}{\sqrt{\det(g_{ab})}} K + \frac{1}{2π} \int_{\partial A} k_g(t) dt,$$

(4)

where $\chi(A)$ is the Euler characteristic and,

$$\frac{1}{2π} \int_{\partial A} \vec{p} \cdot d\vec{x} = -\chi \in \mathbb{Z},$$

(5a)

interpreted as the old quantum condition[120, 121], while the geodesic and Gaussian curvatures respectively are given by,

$$k_g(t) = \frac{d^2 \vec{x}(t)}{dt^2} \cdot \frac{d\vec{x}(t)}{dt},$$

(5b)

$$K(\vec{x}) = \frac{\vec{n} \cdot \nabla \times \vec{\eta}}{\sqrt{\det(g_{ab})}}.$$  

(5c)

At thermal equilibrium, the geodesic curvature vanishes, $k_g = 0$ leading to momentum conservation in the $\vec{x}$ direction, $d^2 \vec{x}/dt^2 = 0$ which implies the Gauss-Bonnet theorem expression is devoid of boundary terms and hence simplifies to,

$$\chi(A) = 2 - 2\gamma = \frac{1}{2π} \int_{A} \frac{1}{2} \frac{d^2 r}{\sqrt{\det(g_{ab})}} K,$$

(6)

where $\gamma$ is the genus of the emergent 2D manifold, $A$. To consistently introduce the electric field, we shall require the acceleration and the friction terms respectively, in the Langevin equation, to take the forms,

$$\vec{\eta} = \frac{2π}{m} (\vec{n} \times \vec{E}),$$

(7a)

$$\vec{p} = -\nabla \Phi_{AC}(\vec{x}),$$

(7b)

where $\vec{E} = (E_x, E_y, 0)$ is the analogue electric field on $A$ responsible for the cation extraction (intercalation) and re-insertion (de-intercalation) processes in an electrode-electrolyte setup forming a cell or battery[56] and $\Phi_{AC}$ plays the role of the particle action. Intuitively, $\Phi_{AC}$ is analogous to the Aharonov-Casher phase[122], where the fictitious magnetic moment corresponds to, $\vec{\mu} = 2π\vec{n}/m$. Thus, it is intuitive to view the positively charged cations diffusing along paths, $\vec{x}(t)$ around neutral vacancies with a magnetic moment, $\vec{\mu}$.

Moreover, taking the analogue of Gauss’ law (of electromagnetism) to be given by,

$$\nabla \cdot \vec{E} = 2m \rho_{2D}(\vec{x}),$$

(8)

the Gauss-Bonnet theorem becomes,

$$\chi(A) = -\frac{1}{2π} \int_{\partial A} \vec{p} \cdot d\vec{x} - \frac{1}{2π} \int_{A} \vec{\eta} \cdot d\vec{x} + \frac{1}{m} \int_{\partial A} d\vec{x} \cdot (\vec{n} \times \vec{E}) = \frac{1}{m} \int_{A} d^2 r \nabla \cdot \vec{E} = 2 \int_{A} d^2 r \rho_{2D} = 2\nu - 2,$$

(9a)
where we have used eq. (1) in the last line. This implies that the Gaussian curvature of the 2D manifold ought to be proportional to the effective 2D charge density,

$$K(\vec{x}) + \frac{4\pi \rho_{2D}(\vec{x})}{\sqrt{\det(g_{ab})}} = 0. \quad (9b)$$

Thus, the genus of the manifold can be interpreted as the number of cationic vacancies, \( g = \nu \) as required. Moreover, when the material lacks the activation energy needed to dislodge cations from the lattice introducing vacancies, \( \rho_{2D} = 0 \), which requires the Euler characteristic to identically vanish, \( K = 0 \).

Finally, the Langevin equation in eq. (2) motivates the equilibrium Fokker-Planck equation[123] of the form,

$$\rho_{2D}(\vec{x}) = \rho_0 \exp(-\nu \Phi_{AC}(\vec{x})), \quad (10a)$$

where \( \vec{v} = d\vec{x}/dt \) is the center of mass velocity, \( D = 1/M \) plays the role of diffusion coefficient with \( M = m\nu \) the total effective mass of the cations and,

$$g(\vec{x}) = \exp(-\nu \Phi_{AC}(\vec{x})), \quad (10c)$$

is the pair correlation function appearing in eq. (1). Thus, imposing a Boltzmann distribution (which corresponds to the number density of a system of particles of total effective mass, \( M \) with dynamics governed by a gravitational 2D potential, \( \Phi_{AC} \)) at equilibrium given by,

$$\rho_{2D} \propto \exp(-\beta M \Phi_{AC}(\vec{x})), \quad (11a)$$

where \( \beta \) is the inverse temperature implies the conditions,

$$\beta M = \nu, \quad (11b)$$
$$\beta = 1/m, \quad (11c)$$
FIG. 2. Quasi-stable configurations of the cation honeycomb lattice in the ground and excited states ((de-)intercalation process) and the directions of the electric and pseudo-magnetic fields. (a) The cations arranged in a honeycomb fashion with a single reference cationic vacancy (not shown, \( g = 1 \)) topologically equivalent to the torus. This represents the ground state of the system consistent with eq. (1). (b) The extraction process of \( g \geq 2 \) cations from the honeycomb surface by applied electric fields \( E_x \) and \( E_y \) in the \( x \) and \( y \) directions respectively. The extraction process introduces Gaussian curvature, \( K \) which can be interpreted as a pseudo-magnetic field, \( B_z \) in the \( z \) direction, which vanishes in the ground state \( (g = 1) \). Thus, the vacancies created by this extraction process can be counted by tracking the change in the electric fields at the boundary, \( \partial A \) of some emergent manifold, \( \mathcal{A} \) representing the honeycomb lattice with vacancies. (C) Stokes’ theorem on the emergent manifold consistent with Chern-Simons theory. Applying Stokes’s theorem yields the Gauss-Bonnet theorem, where \( g \) is the genus of \( \mathcal{A} \).

must be satisfied.

Moreover, the peculiar relation, \( M = 1/D \) can be better understood by applying the virial theorem[124],

\[
\frac{\nu}{\beta} = \left\langle \frac{1}{2m} \sum_{j=1}^{\nu} \vec{p}_j \cdot \vec{p}_j \right\rangle = \frac{1}{2} \left\langle \sum_{j=1}^{\nu} \vec{r}_j \cdot \frac{\partial V(\vec{r}_j)}{\partial \vec{r}_j} \right\rangle,
\]

(12a)

where the averages are evaluated at equilibrium using,

\[
\langle \cdots \rangle = \frac{\int (\cdots) \exp (-\beta H(\vec{p}, \vec{r})) \prod_{j=1}^{\nu} d^2 p_j d^2 r_j}{\int \exp (-\beta H(\vec{p}, \vec{r})) \prod_{j=1}^{\nu} d^2 p_j d^2 r_j},
\]

(12b)

and we have introduced individual particle coordinates, \( \vec{x}_j = (\vec{r}_j, 0) \) with \( \vec{r}_j = (x_j, y_j) \) the 2D coordinates. Proceeding, we shall consider the particular Hamiltonian for the cations,

\[
H(\vec{p}_j, \vec{r}_j) = \frac{\vec{p}_j \cdot \vec{p}_j}{2m} + V(\vec{r}_j),
\]

(13a)

with momenta, \( \vec{p}_j \), displacement vectors, \( \vec{r}_j \) and \( m = 1/\beta \) a mass per cation parameter defined as the inverse of the mean time/path between collisions,

\[
V(\vec{r}_j) = \frac{m}{4\mu} \sum_{k=1}^{\nu} \vec{r}_k \cdot \vec{r}_j + \cdots
\]

\[
= U(\vec{r}_j) + \frac{m}{4\mu} \sum_{k \neq j}^{\nu} \vec{r}_k \cdot \vec{r}_j + \cdots,
\]

(13b)

displaying the leading interaction term in the potential energy defined inversely proportional to \( \mu \), the self-mobility of the cations and,

\[
U(\vec{r}_j) = \frac{m}{4\mu} \vec{r}_j \cdot \vec{r}_j.
\]

(14)

Typically, other terms such as the Vashishta-Rahman potential[125], which capture interactions of the cations
with the slabs atoms especially oxygen, contribute higher order terms (represented by \( \cdots \)) potentially neglected herein. This requires that the diffusion coefficient, including cation-cation correlation terms[126], satisfy,

\[
D = \frac{1}{4\beta} \left\langle \sum_{j=1}^{\nu_k} \sum_{k=1}^{\nu} \vec{r}_j \cdot \vec{r}_k \right\rangle \approx \frac{\mu}{\nu} \left\langle \sum_{j=1}^{\nu} U(r_j) \right\rangle
\]

\[
= \frac{\mu}{\nu} \left\langle \sum_{j=1}^{\nu} \left( \vec{r}_j \cdot \frac{\partial V(r_j)}{\partial \vec{r}_j} - U(\vec{r}_j) \right) \right\rangle + \cdots
\]

\[
= \frac{2\mu}{\nu} \left\langle \sum_{j=1}^{\nu} \vec{p}_j \cdot \vec{r}_j \right\rangle - \frac{\mu}{\nu} \left\langle \sum_{j=1}^{\nu} U(r_j) \right\rangle + \cdots
\]

\[
= 2\mu/\beta - \frac{\mu}{\nu} \left\langle \sum_{j=1}^{\nu} U(r_j) \right\rangle + \cdots, \quad (15a)
\]

as \( \beta \to \infty \), where we have used the result in eq. (13b) and the virial theorem in eq. (12). Observe that, when cation-cation correlation \( (j \neq k) \) terms vanish, \( V(\vec{r}_j) \approx U(\vec{r}_j) \), whereas \( 1/\sqrt{2\mu} \) plays the role of the frequency of \( \nu \) harmonic oscillators and the diffusion coefficient becomes the self-diffusion coefficient,

\[
D \approx D_{\text{self}} = \frac{1}{4\beta} \left\langle \sum_{j=1}^{\nu} \vec{r}_j \right\rangle \approx \frac{\mu}{\nu} \left\langle \sum_{j=1}^{\nu} U(r_j) \right\rangle
\]

\[
= \frac{\mu}{2\nu} \left\langle \sum_{j=1}^{\nu} \frac{\partial U(r_j)}{\partial r_j} \right\rangle = \mu/\beta, \quad (15b)
\]

which is the Einstein-Smoluchowski relation, consistent with eq. (15a). Thus, defining the total mass as the average potential energy,

\[
\left\langle \sum_{j=1}^{\nu} U(r_j) \right\rangle \equiv M, \quad (16a)
\]

\( D = 1/M \) requires the Einstein-Smoluchowski relation be equivalent to \( \mu = \beta/M \). Consequently, since the mobility is considered a constant, we can re-define it as \( \mu = 8\pi G \), where \( G \sim \ell_P^2 \) and \( \ell_P \) is taken to be the lattice constant with dimensions of length. Finally, we obtain,

\[
\beta = \mu/D = \mu M = 8\pi GM, \quad (16b)
\]

\[
\nu = M/m = \beta M = 8\pi GM^2 = A/2G \propto S, \quad (16c)
\]

where \( G \) is a ‘gravitational’ constant, in obvious comparison with Schwarzschild black hole thermodynamics with \( A \) the black hole area and \( S \) the entropy.[127]

C. A gravitation description

A crucial observation is that the analogue electric field, \( \vec{E} \) in eq. (8) is sourced by \( 2m\rho_{2D} \), which has dimensions of mass density (instead of charge density). Introducing a dual potential[27, 62],

\[
\Phi = \int d\vec{x} \cdot \vec{n} \times \vec{\nabla} \Phi_{AC}, \quad (17)
\]

we can re-write Gauss’ law in eq. (8) using,

\[
\vec{\nabla} \Phi = \frac{2\pi}{m} \vec{E}, \quad (18)
\]

and eq. (3) as,

\[
\nabla^2 \Phi(\vec{x}) = 4\pi \rho_{2D}(\vec{x}) = -K(\vec{x}) \sqrt{\det(g_{ab})}, \quad (19a)
\]

thus fixing the 2D metric in eq. (3) to be conformal,

\[
dt^2 = \exp(2\Phi)(dx^2 + dy^2) = g_{ab}u^a v^b. \quad (19b)
\]

Thus, a 2D gravitational description for the idealized dynamics of the cations exists, where eq. (6) and eq. (9) reveal that the energy needed to create cationic vacancies in the vacuum must always balance the energy due to motion, since \( \tilde{\nu} \neq 0 \) when \( \nu \neq 1 \). Moreover, since we must always have a single reference particle as per the definition of the pair correlation function, the vacuum is a torus corresponding to \( g = \nu = 1 \). Thus, the vacuum is two-fold degenerate with respect to the Gaussian curvature, where \( K = 0 \) corresponds to the flat-torus and \( K \neq 0 \) the Riemann surface without boundary of genus \( g = 1 \).

It can be shown that the aforementioned idealized model is consistent with the following tensor field equations in \( d = 1 + 3 \) dimensional space-time[27],

\[
\nabla_{\mu} K_{\nu}^{\mu} = \beta \Psi^* \partial_{\nu} \Psi, \quad (20)
\]

where \( K_{\mu\nu} = R_{\mu\nu} + iF_{\mu\nu} \) is a complex-Hermitian tensor, \( R_{\mu\nu} = R^a_{\mu\nu} \) is the Ricci tensor, \( R^a_{\mu\nu} \) the Riemann tensor, \( F_{\mu\nu} = \partial_{\mu} A_{\nu} - \partial_{\nu} A_{\mu} \) is the (analogue) electromagnetic tensor, \( A_{\mu} \) is the analogue gauge potential, \( \Psi = \sqrt{\beta} \exp(im \int d\tau) \) is a complex-valued function playing the role of the quantum mechanical wave-function of the cations and,

\[
\rho(\vec{x}) = 2\rho_{2D}(\vec{x})\xi^\mu u_\mu/\beta, \quad (21)
\]

is the 3D number density, \( x^\mu = (t, \vec{r}, z) = (t, x, y, z) \) are the coordinates with \( t \) and \( z \) assumed to have the same integration cut-off, \( \beta = 1/m \), and \( u^\mu = dx^\mu/d\tau \) the four-velocity satisfying the space-time metric,

\[
d\tau^2 = -g_{\mu\nu} dx^\mu dx^\nu, \quad (22)
\]

with \( \tau \) the proper time. To see this, we require translation invariance along the \( t \) and \( z \) coordinates where,

\[
\xi^\mu = (1, \vec{0}), \quad (23a)
\]

is a time-like Killing vector requiring energy conservation, and,

\[
n^\mu = (0, \vec{n}), \quad (23b)
\]
and using eq. (9) and eq. (21), we obtain the normaliza-
tion limit, which, for a diagonalized metric tensor, implies that we must have 
∂ρ0, we must have 
\[
\partial_\mu R = \beta \partial_\mu \rho, 
\]
\[
\nabla_\mu F^{\mu\nu} = J^\nu = -\rho u^\nu, 
\]
where we have used the Bianchi identity, \( \nabla^\mu R_{\mu\nu} = \frac{1}{2} \partial^\mu R \). Since the Lie derivative of the Ricci scalar along the direction of a Killing vector must vanish, \( \xi^\mu \partial_\mu R = n^\mu \partial_\mu R = 0 \), we must have \( \partial_\rho (\vec{x})/\partial t = \partial_\rho (\vec{x})/\partial z = 0 \) as expected.

Moreover, we shall introduce the Newtonian potential, \( \Phi \), satisfying,
\[
u^\mu = \exp(\Phi)\xi^\mu = (\exp(\Phi)\vec{0}),
\]
which, for a diagonalized metric tensor, implies that \( g_{00} = \xi^\mu \xi_\mu = u^\mu u_\mu \exp(-2\Phi) = -\exp(2\Phi) \). In the Newtonian limit,
\[
g_{\mu\nu} \approx \begin{pmatrix} -\exp(-2\Phi) & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}
\]
and using eq. (9) and eq. (21), we obtain the normalization,
\[
\int_\mathcal{V} d^3x \sqrt{-\det(g_{\mu\nu})} T^{00} = \int_\mathcal{V} d^3x \sqrt{-\det(g_{\mu\nu})} \rho u^0 u^0 = \int_\mathcal{V} d^3x \rho_0^0 = -2 \int_\mathcal{A} d^2r \rho_{2D} = \frac{1}{2\pi} \int_\mathcal{A} d^2r \sqrt{\det(g_{ab})} K = \chi(\mathcal{A}),
\]
where \( \mathcal{V} = \ell \times \mathcal{A} \) is a 3D manifold built up by slices of the 2D manifold, \( \mathcal{A} \) stacked along the \( z \) coordinate, with a cut-off distance along \( \ell \) given by \( \beta \) and we have introduced the tensor, \( T^{\mu\nu} = \rho u^\mu u^\nu \). Thus, the imaginary part in eq. (24) corresponds to eq. (8) with \( \vec{E} = (F_{01}, F_{02}, F_{03}) \). Meanwhile, since the space-time metric is given by,
\[
d\tau^2 \approx -g_{\mu\nu}dx^\mu dx^\nu = \exp(-2\Phi)dt^2 - dx^2 - dy^2 - dz^2,
\]
we can recover the conformal metric in eq. (19) by considering trajectories of mass-less particles, \( dt = 0 \) restricted to the plane perpendicular to the \( z \) direction, \( dz = 0 \) with unit normal vector \( \vec{n} = (0,0,1) \). For trajectories of massive particles, \( dt \neq 0 \), and we have \( -1 = \frac{dx^2/dt^2}{dt^2} = (dx^2/dt^2)(dt^2/dx^2) = v_z^2 \exp(2\Phi) \), where \( v_z = dz/dt \) is the velocity along the \( z \) direction. Thus, since cationic motion is restricted to 2D, we must have, \( v_z = \sqrt{g_{00}} \to 0 \), which implies the limit,
\[
\lim_{v_z \to 0} g_{00}(v_z) = 0,
\]
and corresponds to \( \Phi \to \infty \).

In addition, introducing the bra-ket notation,
\[
\langle \Psi|\mathcal{O}|\Psi \rangle = \int_\mathcal{V} d^3x \Psi^\ast \mathcal{O}\Psi,
\]
where \( \mathcal{O} \) is an arbitrary Hermitian operator acting on \( \Psi \), the Euler characteristic can be re-written using eq. (20) as,
\[
\chi(A) = \int_\mathcal{V} d^3x \sqrt{-\det(g_{\mu\nu})} \rho_0 u^0 u^0 = \int_\mathcal{V} d^3x \rho_0^0 = \int_0^{-i\beta} dt \langle \Psi(\vec{x})|\exp(\Phi(\vec{x})) \frac{\partial}{\partial t} \exp(\Phi(\vec{x}))|\Psi(\vec{x}) \rangle
\]
\[
= \frac{1}{2\pi} \int_{\partial\mathcal{A}} \vec{n} \cdot d\vec{x} = \frac{1}{2\pi} \int_{\mathcal{A}} d^2r \vec{n} \cdot (\nabla \times \vec{n}),
\]
given in eq. (7), to be interpreted as a Berry connection, 2\( \rho_{2D} \) as the Berry curvature[128, 129] and the Euler characteristic of the 2D manifold, \( \mathcal{A} \) given by \( \chi(\mathcal{A}) \) to correspond to the first Chern number.[130]

In addition, the real part of eq. (20) given in eq. (24) can be integrated to yield,
\[
R = \beta \rho + 4\Lambda,
\]
where we have introduced the integration constant, 4\( \Lambda = 0 \) that can be considered to vanish. This corresponds to the trace of Einstein Field Equations,
\[
R^{\mu\nu} = \beta \left( T^{\mu\nu} - \frac{1}{2} (T^{\mu\beta} g_{\alpha\beta}) g^{\mu\nu} \right),
\]
where we have used \( T^{\mu\nu} = \rho u^\mu u^\nu \), \( u^\mu u_\mu = -1 \) and \( \beta \) is the coupling. It is worth noting that, considering emergent gravity within crystals to describe defects is not entirely a novel idea, since it has been considered in great detail for disclinations and dislocations within the context of classical geometries with torsion.[63–68] In the case here, notice that the energy-momentum \( T^{\mu\nu} \) was appropriately defined to be dimensionless, and in fact corresponds to the Euler characteristic of the 2D manifold, \( \mathcal{A} \) with the vacuum given by \( g = 0 \), as earlier remarked. Moreover, eq. (31a) is invariant under the transformation, \( T_{\mu\nu} \to T_{\mu\nu} + T_{\mu\nu} \), where \( T_{\mu\nu} \) is the trace-less energy-momentum tensor of a scale invariant/conformal field
theory with $T_{\mu\nu}g^{\mu\nu} = 0$. Finally, focusing on $T^{\mu\nu}$, the theory is scale invariant whenever the particle are massless $d\tau^2 = 0$, or the geometry is a flat-torus, $K \propto \rho = 0$, corresponding to the vacuum. Moreover, using eq. (17), eq. (21) and eq. (25), we can check that eq. (10) and thus the current density, $J^\mu = -pu^\mu$ satisfies the conservation law, $\nabla_\mu F^{\mu\nu} = \nabla_\mu J^\mu = 0$ from eq. (24).

A potential problem with the idealised model is that the cations are charged while the emergent gravitational field, $\Phi$ is not. However, this poses no problem since both descriptions are equivalent when the cations are intercalated/de-intercalated in the layered material. Thus, using eq. (31b) into eq. (32) yields,

$$\nabla_\mu u_\nu + \nabla_\nu u_\mu, \quad \text{in order for},$$

$$\nabla_\mu \nabla^\nu u_\nu = R^{\mu\nu}u_\mu. \quad (32)$$

Thus, plugging in eq. (31b) into eq. (32) yields,

$$\nabla_\mu \nabla^\nu u_\nu = \beta \left( T^{\mu\nu} - \frac{1}{2} (T^{\alpha\beta} g_{\alpha\beta}) g^{\mu\nu} \right) u_\mu. \quad (33a)$$

Thus, using $T^{\mu\nu} = \rho u^\mu u^\nu$ we find,

$$\nabla_\mu \nabla^\nu u_\nu = -\frac{1}{2} \beta \rho u_\nu, \quad (34)$$

which corresponds to the imaginary part of eq. (20) given in eq. (24).

### D. Weighted pair correlation function

The pair correlation function is given by the Boltzmann factor in eq. (11), equivalent to,

$$g(r^a) = \exp \left( M \int dt \right) = \exp \left( \frac{\nu}{2} \int d^2r \sqrt{\det(g_{ab})} R^{2D} \right), \quad (35a)$$

where we have used eq. (3), $\nu = \beta M = M/m$,

$$\Phi_{AC} = -M \int dt = -\nu \int p_a dr^a = \frac{\nu}{2} \int d^2r \sqrt{\det(g_{ab})} R^{2D}, \quad (35b)$$

and the 2D Ricci scalar, $R^{2D} = R^{abcd}g_{abcd} = 2K$ with $p_a = mV_a$ the 2D momentum, $R_{abcd} = K (g_{ac}g_{bd} - g_{ad}g_{bc})$ the 2D Riemann tensor and $R_{bd} = R_{abcd}g^{ac} = K g_{bd}$ the 2D Ricci tensor.

Finally, we expect the pair correlations to be calculated for varied vacancies as cations are intercalated/de-intercalated in the layered material. Thus, using eq. (16b) and introducing the number of microstates of the system, $N$ and entropy $S$ respectively by,

$$N = \exp (2\pi \nu), \quad (36a)$$

$$S = \ln N = 2\pi \nu, \quad (36b)$$

the weighted sum over the vacancy numbers corresponding to distinct topologies of $A$ yields,

$$\langle g(r^a) \rangle_A = \sum_{\nu=0}^\infty f_{\nu}(\lambda) g(r^a), \quad (36c)$$

where $f_{\nu}(\lambda)$ is the probability for the topology $\nu = g$ to occur in a given thermal (de-)intercalation process, which is assumed to depend on additional variables, indicated as $\lambda$, to be later defined and we have used $\chi(A) = 2 - 2g$,

$$g(r^a) \mid_A = \exp \left( \frac{\nu}{2} \int_A d^2r \sqrt{\det(g_{ab})} R^{2D} \right), \quad (37a)$$

and,

$$\frac{1}{4\pi} \int_A d^2r \sqrt{\det(g_{ab})} R^{2D} = \chi(A). \quad (37b)$$

### III. CONFORMAL FIELD THEORY

#### A. Minimal models as exemplars

For illustration purposes, we introduce the minimal models[11], characterized by the Virasoro algebra[131],

$$[L_n, L_m] = (n - m)L_{n+m} + \frac{c}{12}(n^3 - n)\delta_{(n+m),0}, \quad (38a)$$

$$[\bar{L}_n, \bar{L}_m] = (n - m)\bar{L}_{n+m} + \frac{\bar{c}}{12}(n^3 - n)\delta_{(n+m),0}, \quad (38b)$$

spanned by two copies of commuting generators, $L_n = L^L_n$ and $\bar{L}_n = L^{\bar{L}}_n$ for all integers $n \in \mathbb{Z}$, where $[L_n, L_m] = 0$, $c, \bar{c}$ is a real-valued constant (the central charge), satisfying $L_n, \bar{c} = [L_n, \bar{c}] = [L_n, \bar{c}] = 0$ and $\delta_{m,n}$ is the Kronecker delta. Meanwhile, the representations are characterized by a highest weight primary state, $|h\rangle, |\bar{h}\rangle$ satisfying, $L_0|h\rangle = h|h\rangle$, $\langle h|L_0 = \langle h|h\rangle$, $L_0|\bar{h}\rangle = \bar{h}|\bar{h}\rangle$, $\langle \bar{h}|L_0 = \langle \bar{h}|\bar{h}\rangle$, $L_{[n] \neq 0}|h\rangle = 0$, $\langle h|L_{[n] \neq 0}|h\rangle = 0$, $\langle \bar{h}|L_{[n] \neq 0}|\bar{h}\rangle = 0$, $\langle \bar{h}|L_{[n] \neq 0}|\bar{h}\rangle = 0$. The rest, $L_{[n] \neq 0}|h\rangle \neq 0$, $L_{[n] \neq 0}|\bar{h}\rangle \neq 0$ and $\langle h|L_{[n] \neq 0} = 0$, $\langle \bar{h}|L_{[n] \neq 0} = 0$ can be computed by applying the Virasoro algebra in eq. (38). The basis vectors of the representation form a Verma module,

$$N = 0 : |h\rangle$$

$$N = 1 : L_{-1}|h\rangle$$

$$N = 2 : L_{-2}|h\rangle, \quad L_{-1}^2|h\rangle$$

\[ N = 3 : L_{-3}[h], L_{-2}L_{-1}[h], L_{-1}L_{-2}[h], L^2_{-1}[h] \]

\[ \vdots \]

\[ N \in \mathbb{N} : \mathcal{V}_N \]

where \( \mathcal{V}_N \) contains \( p(N) \) number of elements equal to the partition function of the positive number, \( N \).\[131\]

However, the Verma module, including the linear combination of its elements is not irreducible, since it includes elements with vanishing norms called null states. Nonetheless, the quotient of the Verma module by the null states is irreducible. Finally, ensuring all elements of the quotient are positive definite (unitarity) determines the allowed values of \( h, \bar{h} \), \( c, \bar{c} \) in the models, which completely fixes the critical exponents near the point of occurrence of phase transitions known as the critical point.\[10\] On the other hand, a finite central charge \( c \neq 0, \bar{c} \neq 0 \) in eq. (38) governs the commutation relations of local conformal transformations, which requires that the entire infinite dimensional conformal symmetry to be broken. Nonetheless, the global conformal transformations of the ground state are generated by a linear combination of the generators in eq. (38) which satisfy, \( [L_n, L_{-n}]=2nL_0, [\bar{L}_n, \bar{L}_{-n}]=2n\bar{L}_0 \) with \( c, \bar{c} \neq 0 \). This singles out the condition, \( n^2-n=0 \), which requires that \( n=0, \pm 1 \), corresponding to the unbroken global conformal transformations.

### B. Liouville’s equation

Given a 2D flat pseudo-Riemannian manifold with the a flat metric,

\[ dt^2 = dy^2 - dX^2, \]

as depicted in Figure 3 (a), where \( y, X \) are the coordinates and \( dt \) is the proper distance, a Wick rotation \( X = iy \) transforms the flat pseudo-Riemannian manifold into a cylinder with the Riemannian metric,

\[ dt^2 = dy^2 + dx^2, \]

since, \( x' = x + \beta \) is periodic\[132\] in the inverse temperature, \( \beta \) as depicted in Figure 3 (b). This means that, under translations along the circumference of the cylinder, \( x \rightarrow x + \beta \), new coordinates, \( q = \exp(-2\pi wU(w, \bar{w})) \), \( \bar{q} = \exp(-2\pi \bar{w}U(w, \bar{w})) \) (where \( w = y + X = y + ix, \bar{w} = y - X = y - ix \) and \( U(w, \bar{w}) \) is a (potential energy) function of \( w, \bar{w} \)) transform as \( q' = \exp(-w'U(w', \bar{w}')) = q \) and \( \bar{q}' = \exp(-\bar{w}'U(w', \bar{w}')) = \bar{q} \) when,

\[ \beta U(w, \bar{w}) = \nu \in \mathbb{N}, \]

and,

\[ U(w, \bar{w}) = U(w', \bar{w}) = U(w, \bar{w}') = U(w', \bar{w}'), \]

where \( \nu \in \mathbb{N} \) is the winding number.

Moreover, the cylinder can be transformed into a two-torus, \( T^2 \) as shown in Figure 3 (c), by making the identification, \( |q| = 1/|\bar{q}| \) at \( |q| = 0, \infty \) corresponding to \( |\bar{q}| = \infty \). Thus, as \( |q| \rightarrow \infty \) corresponding to the edges of the cylinder, we are allowed to choose new coordinates, \( q \rightarrow 1/q \) and \( \bar{q} \rightarrow 1/\bar{q} \). This can be implemented by the transformations, \( w \rightarrow 1/w \) and \( \bar{w} \rightarrow 1/\bar{w} \), while ensuring the potential energy satisfies,

\[ U(w, \bar{w}) = -w^{-2}U(1/w, \bar{w}) = -\bar{w}^{-2}U(w, 1/\bar{w}). \]

Consequently, on the two-torus, the potential energy of the form \( U(w, \bar{w}) = U(k, \bar{k}) \), with \( k = iw, \bar{k} = -iw \), can be considered a modular form of weight 2\[133\],

\[ U(Q \cdot k, \bar{k}) = (\gamma k + \delta)^2 U(k, \bar{k}), \]

\[ U(k, Q \cdot \bar{k}) = (\gamma k + \delta)^2 U(k, \bar{k}), \]

\[ Q \cdot k = \frac{\alpha}{\gamma} \frac{\beta}{\delta} \cdot k = \frac{\alpha k + \beta}{\gamma k + \delta}, \]

\[ Q \cdot \bar{k} = \frac{\alpha}{\gamma} \frac{\beta}{\delta} \cdot \bar{k} = \frac{\alpha \bar{k} + \beta}{\gamma \bar{k} + \delta}, \]

where \( Q \in SL_2(\mathbb{Z})/\mathbb{Z}_2 = PSL_2(\mathbb{Z}) \) is an element of the quotient of the special linear group by the sign group, \( \mathbb{Z}_2 \). This requires that the translations along \( x \) displayed in eq. (41) be generated by, implemented by,

\[ Q_1 = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \in Q, \]

in order for,

\[ Q_1^\beta = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^\beta = \begin{pmatrix} 1 & \beta \\ 0 & 1 \end{pmatrix} \notin Q, \]

to correspond to a complete winding along \( x \). Meanwhile,

\[ Q_2 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \in Q, \]

corresponds to translations along \( y \) given in eq. (42).

However, since \( \beta \) is not necessarily an integer, \( Q_1^\beta \notin Q \) is not an element of \( PSL_2(\mathbb{Z}) \). This can be corrected by re-scaling the coordinates, \( (x, y) \rightarrow U^{-1}(w, \bar{w})(x, y) \), in order for the circumference of cylinder to be periodic in \( \beta U(w, \bar{w}) = \nu \in \mathbb{Z} \) instead, where,

\[ Q_1^\nu = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^\nu = \begin{pmatrix} 1 & \nu \\ 0 & 1 \end{pmatrix} \in Q. \]

This also redefines the aforementioned coordinates, \( \tilde{q}, q \) to,

\[ q(k) = \exp(i2\pi k), \tilde{q}(\tilde{k}) = \exp(-i2\pi \tilde{k}), \]

where winding around the circumference of the cylinder is given by \( k' = k + \nu \) and \( \tilde{k}' = \tilde{k} - \nu \). Moreover, setting \( G = \beta^{-1}U^{-1} \), the re-scaling requires that, \( dx' = d(Gx) = \]

\[ dx' = d(Gx) = \]
\[
\begin{align*}
xdG + Gdx &\quad = \quad ydG + Gdy, \quad \text{Thus, we obtain,} \\
dt^2 &\quad = \quad dx'^2 + dy'^2 \quad = \quad G^2(dx^2 + dy^2) \\
&\quad + \quad (x'^2 + y'^2)dG^2 \quad + \quad \frac{1}{2}(d(x^2) + d(y^2))d(G^2). 
\end{align*}
\]

Indeed, since the modular group implies the conformal group in 2D, these transformations require the metric in eq. (39) to be defined up to a conformal factor, 
\[
dt^2 = g_{ab}dx'^a dr'^b = \exp(2\Phi(x,y))(dx^2 + dy^2), \quad (49a)
\]
corresponding to eq. (19b), which satisfies Liouville’s equation, 
\[
\nabla^2_{2D} \Phi(x,y) = - K(x,y) \exp(2\Phi(x,y)), \quad (49b)
\]
given in eq. (19), requiring the last line in eq. (48) to vanish, 
\[
(x^2 + y^2)dG^2 + \frac{1}{2}(d(x^2) + d(y^2))d(G^2) = 0. \quad (50a)
\]

Here, \(g_{ab}\) is the metric tensor, \(r^a = (x,y)\) are the 2D coordinates, \(\nabla^2_{2D} = \partial^2/\partial x^2 + \partial^2/\partial y^2\) is the 2D Euclidean Laplace operator, \(K(x,y)\) is the Gaussian curvature and 
\[
\mathcal{G}(x,y) = \exp(2\Phi(x,y)), \quad (50b)
\]
is the conformal factor.

We can solve eq. (50) by first rearranging it to yield, 
\[
d\ln(G(x,y)) = \frac{\partial \ln \mathcal{G}(x,y)}{\partial x} dx + \frac{\partial \ln \mathcal{G}(x,y)}{\partial y} dy \\
= -2 \left( \frac{x dx}{x^2 + y^2} + \frac{y dy}{x^2 + y^2} \right). \quad (50c)
\]
Thus, using eq. (50b), \(\partial \Phi(x,y)/\partial x = -x/(x^2 + y^2)\) and \(\partial \Phi(x,y)/\partial y = -y/(x^2 + y^2)\), we find, 
\[
\Phi(\vec{r}) = -\frac{1}{2} \ln \left( \frac{K_0}{2} \vec{r} \cdot \vec{r} \right), \quad (51a)
\]
where \(K_0\) is a constant with dimensions of Gaussian curvature. Since \(\vec{w}w = kk = \vec{r} \cdot \vec{r} = x^2 + y^2\), we obtain, 
\[
\mathcal{G} = \exp(2\Phi) = \frac{2G}{\vec{w}w} = \frac{2G}{kk} = \frac{2G}{\vec{r} \cdot \vec{r}} \quad (51b)
\]
with \(G = 1/K_0\). Since \(\mathcal{G}^{-1} = \beta U = \nu \in \mathbb{Z}\), the allowed areas, \(A(\vec{r}) = \vec{r} \cdot \vec{r}\) on the manifold \(\mathcal{A}\) must take on integer
values, \( \nu \in \mathbb{Z} \) proportional to \( G \),
\[
\nu = \frac{A(\vec{r})}{2G} = \beta U(\vec{r}).
\]  
(52)

Thus, for consistency with eq. (16b), we ought to consider the average \( \nu \rightarrow \langle \nu \rangle \) instead, where \( \vec{r} \) is the center of mass coordinate with,
\[
\langle U(\vec{r}) \rangle \equiv M,
\]
(53a)
\[
U(\vec{r}) = \frac{M}{4\mu} \vec{r} \cdot \vec{r},
\]
(53b)
and \( \mu = 8\pi G \). Equivalently, the self-diffusion coefficient can also be calculated from the center of mass coordinate as,
\[
D \simeq D_{\text{self.}} = \frac{1}{4\beta} \langle \vec{r} \cdot \vec{r} \rangle = \frac{\mu}{\beta M} \langle U(\vec{r}) \rangle = \mu/\beta ,
\]
(54)
which is consistent with the center of mass virial theorem,
\[
\nu/\beta = \frac{1}{2} \langle \vec{r} \cdot \partial U(\vec{r})/\partial \vec{r} \rangle = \langle U(\vec{r}) \rangle = M, \quad (55a)
\]
where,
\[
\langle \cdots \rangle = \int \cdots \frac{\exp(-\beta H(\vec{p}, \vec{r})) d^2 p d^2 r}{\int \exp(-\beta H(\vec{p}, \vec{r})) d^2 p d^2 r},
\]
(55b)
and,
\[
H(\vec{p}, \vec{r}) \simeq \frac{1}{\nu} \left( \frac{p^2}{2M} + U(\vec{r}) \right),
\]
(55c)
is the Hamiltonian.

C. Partition function

Meanwhile, the Euler characteristic of the manifold is given by the Gauss-Bonnet theorem,
\[
\chi(T^2) = \frac{1}{2\pi} \int_{T^2} K(x,y) \sqrt{\det(g_{ab})} \, dxdy
\]
\[
= \frac{1}{2\pi} \int_{T^2} K(x,y) \exp(2\Phi(x,y)) \, dxdy
\]
\[
- \frac{1}{2\pi} \int_{T^2} \nabla^2 \Phi(x,y) \, dxdy = 2 - 2g = 0, \quad (56)
\]

Turns out, the generators \( Q_1, Q_2 \) of \( \text{PSL}_2(\mathbb{Z}) \) define the topology of \( T^2 \) as aforementioned, where the first Betti number\(^{134} \) (equivalent to \( b_1 = 2g \) with the genus given by \( g = 1 \)) corresponds to the number of generators of the group, \( \text{SL}_2(\mathbb{Z}) \) and the Euler characteristic becomes,
\[
\chi(T^2) = \chi(S^2) - b_1 = 0, \quad (57)
\]
with \( \chi(S^2) = b_0 = 2 \) the Euler characteristic of the two-sphere, \( S^2 \) and \( b_p \ (p \in \mathbb{N} \leq d = 2) \) the \( p \)-th Betti number of the manifolds, \( M = S^2, T^2 \).

Of particular importance in conformal field theories, are the conformal dimension and conformal spin respectively given by,
\[
\Delta = L_0 + \bar{L}_0, \quad (58)
\]
\[
\sigma = i(L_0 - \bar{L}_0). \quad (59)
\]

Typically, the partition function of a thermodynamic system on \( T^2 \) takes the form,\(^{131} \)
\[
Z = \text{Tr}_{V/\text{full}} \left( q^{L_0 - c/12} \bar{q}^{\bar{L}_0 - \bar{c}/12} \right), \quad (60)
\]
where \( q \) and \( \bar{q} \) are given in eq. (47) and the trace is over the unitary irreducible representation, which is irreducible and unitary. Under translations along the circumference of the cylinder (generated by \( Q_1 \)), \( k \to k+1, \bar{k}' \to \bar{k} - 1 \), and the partition function picks up the phase factors,
\[
\exp(i2\pi(L_0 + \bar{L}_0)) \exp(-i2\pi(c + \bar{c})/12). \quad (61)
\]
Thus, it is prudent to consider the special case,
\[
c/12 + \bar{c}/12 - \Delta \in \mathbb{Z}, \quad (62a)
\]
which guarantees that the partition function is translation invariant along \( x \). Moreover, we shall be interested in theories where \( \bar{c} = c = 12 \) and the conformal spin vanishes (\( h = h \)). This transforms eq. (62a) into,
\[
2 - 2h \in \mathbb{Z}, \quad (62b)
\]
where we have used, \( \Delta = h + \bar{h} = 2h \).

Meanwhile, under \( Q \in \text{PSL}_2(\mathbb{Z}) \) given in eq. (43), \( dk, d\bar{k} \) transform as,
\[
dk' = \frac{dk}{(\gamma k + \delta)^2}, \quad d\bar{k}' = \frac{d\bar{k}}{(\gamma k + \delta)^2}, \quad (63a)
\]
which means that the function,
\[
g(k, \bar{k}) = U(k, \bar{k}) dk d\bar{k}, \quad (63b)
\]
where,
\[
U(Q \cdot k, \bar{k}) = (\gamma k + \delta)^{2h} U(k, \bar{k}), \quad (63c)
\]
\[
U(k, Q \cdot \bar{k}) = (\gamma \bar{k} + \delta)^{2\bar{h}} U(k, \bar{k}), \quad (63d)
\]
is clearly invariant under \( Q \in \text{PSL}_2(\mathbb{Z}) \). Thus, in eq. (43), we have \( h = 1, \bar{h} = 1 \). Consequently, \( 2 - 2h = 0 \), which corresponds to the Euler characteristic of the two-torus, \( T^2 \).

Thus, we conjecture that, \textit{all orientable 2D Riemannian surfaces without boundary can be characterized by a conformal field theory with the conformal dimension,} \( \Delta = h + \bar{h} \) \textit{equal to the first Betti number of the surface.}
This means that the trace over the unitary representations, \( V/\text{null} \) in eq. (60) corresponds to the sum over the genus, \( h = g \) of the Riemann surfaces and the potential, \( U(k, \bar{k}) \) must transform under \( Q \in \text{PSL}_2(\mathbb{Z}) \) as a modular form of weight \( 2h, 2\bar{h} \), as in eq. (63c). This avails an avenue to build up new topologies of genus \( g \neq 1 \). The resulting manifold is a connected sum of \( g \) tori, \( \mathcal{A} = T_1^2 \# T_2^2 \# \cdots \# T_g^2 \) with Euler characteristic given by,

\[
\chi(\mathcal{A}) = \frac{1}{2\pi} \int_{\mathcal{A}} K(x, y) \sqrt{\text{det}(g_{ab})} \, dx \, dy = \chi(S^2) - \sum_{j=1}^{g} b_j^2 = 2 - 2g. \tag{64}
\]

Due to the constraint in eq. (51), we can associate the Gaussian curvature with the form,

\[
K(\vec{r}) = 2\pi K_0 |\vec{r}|^2 \left( \delta^2(\vec{r}) - \sum_{j=1}^{g} \delta^2(\vec{r} - \vec{r}_j) \right), \tag{65}
\]

where \( \delta^2(\vec{r}) = \delta(x)\delta(y) \) is the 2D Dirac delta function. Moreover, we can choose the constant to be as large as possible, \( K_0 = 1/G \sim 1/\ell_\text{p}^2 \to \infty \), in order for \( \beta U(\vec{r}) = A(\vec{r})/2G = \nu \to \infty \) (in eq. (52)) which corresponds to the continuum limit of the lattice, or alternatively \( \beta \to \infty \) at fixed values of \( U(\vec{r}) \), which corresponds to the theory at zero temperature. Consequently, we can consider the Gaussian definition for the 2D delta function,

\[
\delta^2(\vec{r}) = (K_0/\pi) \exp \left( - \frac{K_0}{2} (\vec{r}, \vec{r}) \right) = (K_0/\pi) \exp(-\beta U(\vec{r})), \tag{66}
\]

which renders the Gaussian curvature, \( K(\vec{r}) \) a function of \( G(\vec{r}) \) and hence only depends on \( U(\vec{r}) \).

Finally, we recognize that the metric,

\[
dt^2 = dx^2 - dY^2, \tag{67a}
\]

is related to the metric in eq. (39b) by the the Wick rotation, \( Y = iy \), which yields,

\[
dt^2 = dx^2 + dy^2 = dt^2. \tag{67b}
\]

This corresponds to a dual cylinder with coordinates \( k = x + Y, \bar{k} = x - Y, k = iw \) and \( \bar{k} = -iw \), where the right-left edges of a flat plane are connected instead of the top-bottom ones. This corresponds to the following replacements,

\[
k, \bar{k} \rightarrow w, \bar{w}, \tag{68a}
\]

\[
w, \bar{w} \rightarrow \bar{k}, k, \tag{68b}
\]

\[
\nu \rightarrow i\nu. \tag{68c}
\]

This is useful since the distinction between the coordinates \( w \) and \( k \) in the theory becomes a matter of convention.

Following this argument, setting \( \bar{k} - k = 2i(\lambda + \nu) \) in eq. (60), where \( \lambda = -ix \) or \( \lambda = y \), and the partition function is transformed into,

\[
Z = \ln Z = \sum_{h=0}^{\infty} f_h(\lambda) N^\lambda(h), \tag{69a}
\]

where \( N = \exp(2\pi \nu), f_h(\lambda) = \exp(2\pi \lambda(h)) \) and,

\[
Z = \int D[\varphi] \exp \left( \frac{1}{g} \text{Tr}(f(\varphi)) \right), \tag{69b}
\]

\( Z \) is the partition function of an unidentified Hermitian matrix field theory, \( \varphi^\dagger = \varphi \), where \( \lambda/N = g^2 \) is the coupling of the theory and \( f(\varphi) \) is a function of \( \varphi \) invariant under \( U(N)[4, 5] \). It is thus instructive to take the weighted sum of the pair correlation function for different topologies given in eq. (36c) to correspond to the partition function, \( Z = \langle g(r^2) \rangle_{\mathcal{A}} \). Moreover, making the identification,

\[
\sum_{A \in h} f_h(\lambda) \leftrightarrow \int D[g_{ab}(A)], \tag{70a}
\]

eq eq. (69a) becomes the partition function of 2D quantum gravity in Euclidean signature[135],

\[
Z = \int D[g_{ab}] \exp \left( \frac{1}{2\kappa} \int_{\mathcal{A}} d^2x \sqrt{\text{det}(g_{ab}) \text{R}_{2D}} \right), \tag{70b}
\]

where the dimension-less coupling constant corresponds to \( \kappa = 1/\nu \).

### IV. RESULTS

#### A. The honeycomb lattice

The honeycomb lattice within crystalline geometries has been the center of frontier research ranging from graphene to other layered materials with energy storage applications.[16, 21–26] Of particular interest is the role the symmetries of the lattice play in introducing conservation laws via Noether’s theorem, which offers vital clues not only towards establishing the explicit form of the relevant Hamiltonian, but also considering valid idealized models which capture the characteristic properties of the condensed matter system. In particular, the honeycomb lattice is spanned by the unit basis, \( \omega_1 \) and \( \omega_2 \) defining a parallelogram enclosing \( \bar{k} \) pairs of cation sites as shown by the dashed lines in Figure 4. The primitive cell corresponds to the blue-shaded rhombus, where \( \omega_1/\omega_2 = k = 1 \). Thus, the unit cell is defined as \( \omega_1/\omega_2 = k, \) where \( k = 1 \) is a special case known as the primitive cell corresponding to \( k = 1 \) and the unit cell, \( k \in \mathbb{N} \). Consequently, each unit cell, \( k \) on the honeycomb lattice is related to a larger/smaller unit cell \( k' \) by \( k' = k + \nu, \) where \( \nu \in \mathbb{N} \) is a positive integer.
FIG. 4. Honeycomb lattice of cations, viewed in the [001] direction, depicting two unit cells as dashed parallelograms. The unit basis $\hat{\omega}_1, \hat{\omega}_2$ for one of the unit cells is shown where the blue rhombus corresponds to a primitive cell of the honeycomb lattice. The cations/cationic sites are depicted by grey spheres whereas the honeycomb lattice is shown in red.

Proceeding, since the unit basis vectors,

$$\hat{\omega}_2 + \hat{\omega}_1 = \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix},$$

(71a)

under re-scaling by $b$ becomes,

$$\hat{V}_+(k) = \hat{1} + \frac{\hat{\omega}_1}{\omega_2} = \begin{pmatrix} \omega_1/\omega_2 \\ 1 \end{pmatrix} = \begin{pmatrix} k \\ 1 \end{pmatrix},$$

(71b)

we can check that the modular transformation $Q_1^\nu \in Q$, given in eq. (46), relates the unit vectors to each other by,

$$Q_1^\nu \hat{V}_+(k) = \hat{V}_+(k) = Q_1^\nu \begin{pmatrix} k \\ 1 \end{pmatrix} = \begin{pmatrix} k + \nu \\ 1 \end{pmatrix}.$$  

(72)

Likewise, we shall introduce another valid unit basis vector,

$$\hat{\omega}_2 - \hat{\omega}_1 = \begin{pmatrix} -\omega_1 \\ \omega_2 \end{pmatrix},$$

(73a)

which under re-scaling by $\omega_1$ yields,

$$\hat{V}_-(k) = \frac{\hat{\omega}_2}{\omega_1} - \hat{1} = \begin{pmatrix} -1 \\ \omega_2/\omega_1 \end{pmatrix} = \begin{pmatrix} -1 \\ 1/k \end{pmatrix}.$$  

(73b)

We require that the two valid unit basis vectors be related by the modular transformation, $Q_2 \in Q$ given in eq. (45), as,

$$Q_2 \hat{V}_+(k) = \hat{V}_+(k) = Q_2 \begin{pmatrix} 1 \\ k \end{pmatrix} = \begin{pmatrix} -1 \\ k \end{pmatrix} \equiv \hat{V}_-(k) = \begin{pmatrix} -1 \\ 1/k \end{pmatrix},$$

(74)

corresponding to $\bar{k} = 1/k$ and hence the relation between the two dashed parallelograms. Consequently, due to the modular symmetries and scale invariance, we shall consider the partition function given in eq. (60) as describing the theory of the cations, as expected.

Moreover, we note that, $Q_2^2 = -\sigma_0$, where,

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

(75)

which implies the unit vector acquires a minus sign. Since $Q_2$ exchanges the basis $a$ with $b$, it corresponds to a discrete rotation when acting on the primitive cell. There are 4 such discrete rotations such that $Q_2^{2n} \in Q$ correspond to complete $2\pi n$ rotations of the primitive cell, where $n \in \mathbb{N}$. In addition, $Q_2^{2(2n+1)} \in Q$ exchanges one
FIG. 5. The honeycomb lattice of cations (grey spheres connected by red and green lines), as viewed in the [001] direction. The cation honeycomb lattice comprises a pair of up and down triangular sub-lattices (grey solid and dashed lines respectively), assigning opposite pseudo-spins (indicated by black up or down arrows) to each cation in the unit cell, where the green line indicates part of the honeycomb lattice within a primitive cell.

cationic site in the unit primitive cell with the other. Thus, under the exchange of two cations belonging to the same primitive cell, $V \pm$ pick up a minus sign. Consequently, $V \pm$ represent the states of the cations in a primitive cell, which gives rise to a pseudo-degree of freedom we shall refer to as pseudo-spin. Indeed, it is well-known that the 2D honeycomb structure of graphene requires an additional degree of freedom to describe the orbital wave functions sitting in two different triangular sub-lattices, known as a pseudo-spin.[78]

In the case of the cations, the two sub-lattices are shown in Figure 5 as grey solid and dashed lines, where each cationic site has a pseudo-spin up or pseudo-spin down degree of freedom to describe the orbital wave functions sitting in two different triangular sub-lattices, known as a pseudo-spin.[78]

B. Monolayer-bilayer phase transition

Trivially, in eq. (31b) on the flat-torus where $\rho \propto \rho_{2D} \propto K = 0$ and the particles are massive $u^\nu u_\nu = -1$, the theory must be scale invariant since the dilatation current, $j_\mu = x^\nu T_{\mu \nu} = \rho x^\nu u_\nu u_\mu = 0$ vanishes[7], and hence is trivially conserved. Thus, eq. (31b) becomes the vacuum condition, $R_{\mu \nu} = 0$. Non-trivially, on the two-torus, $T^2$ where $\rho \propto \rho_{2D} \propto K \neq 0$ and the particles are mass-less, $u^\nu u_\mu = 0$, the theory remains scale invariant on Minkowski space since the dilatation current, $j_\mu = x^\nu T_{\mu \nu} = \rho u^\nu u_\nu u_\mu = 0$ is conserved because $\partial_\mu j_\mu = T_{\mu \nu} g^{\mu \nu} + x^\nu \partial_\mu T_{\nu \mu} = 0$ where $\partial_\mu T_{\nu \mu} = 0$ $T_{\mu \nu} g^{\mu \nu} = \rho u^\nu u_\mu = 0$. Thus, to preserve scale invariance and hence conformal invariance, the cations either have to be considered mass-less or the Gaussian curvature must vanish, $K \propto \rho = 0$. This realization is powerful since the theory of cations requires their effective masses in the theory to be given by, $m = 1/\beta$, where we have often taken the zero temperature limit, $\beta \to \infty$, where the conformal field theory described consistent with Liouville’s equation lives. However, for finite temperature, scale invariance is maintained if and only if $\rho = 0$. Thus, a finite $\rho$ breaks scale invariance and hence conformal invariance. Ideally, scale symmetry in the honeycomb lattice manifests when all bonds between the atoms are
of equal size. This means that, introducing additional bonds that differ in length from the rest is expected to break this symmetry.

We are interested in 2D honeycomb materials whose cationic dynamics not only exploit the CFT/gravity aspects discussed above, but also other features such as phase transitions and critical phenomena to be discussed hereafter. In particular, the discussions that follow, we specifically consider the conditions that lead to the pairing of pseudo-spin states of cations in the honeycomb sub-lattices of honeycomb layered tellurates such as Ag$_2$M$_2$TeO$_6$ (where M is a transition metal (such as Co, Ni, Mg, Cu and Zn) or alkaline-earth metal (such as Mg), or a combination of multiple transition metals), layered binary and ternary oxides such as Ag$_6$O$_2$ (or equivalently as Ag$_3$O) and Ag$_2$MO$_2$ (M = Co, Cr, Ni, Cu, Fe, Mn, Rh), Ag$_3$Ni$_2$O$_4$, and layered halides such as Ag$_2$F [79–87, 89, 90], which requires conformal symmetry breaking resulting in a cation monolayer-bilayer phase transition. In this description, the relevant CFT exists at the critical point of the phase transition.[10] As an exemplar, it is prudent to focus on the case of honeycomb layered Ag$_2$Co$_2$TeO$_6$, whose crystallographic structure and scanning transmission electron microscope (STEM) images are displayed in Figure 6. Figure 6 (a) depicts a unit cell of Ag$_2$Co$_2$TeO$_6$ showing the alignment of the atoms as viewed in the [100] crystallographic axis. Ag atoms are drawn in grey, Te atoms in pink, Ni atoms in green and O atoms in red. In addition, a perspective view of the unit cell is shown in Figure 6 (b). The Ag layers form two triangular lattices (drawn as dashed grey lines (down) or solid grey lines (up)) comprising a single bilayer. Figure 6 (c) shows a high-angle annular dark-field (HAADF) STEM image of Ag$_2$Co$_2$TeO$_6$ crystallite revealing bilayer planes of Ag atoms (marked by the brighter and larger golden spots) located between the layers of Co atoms (represented by the darker amber spots) and Te atoms (denoted by the smaller golden spots). The corresponding annular bright-field (ABF) STEM imaging (shown in Figure 6 (d)), reveals also the atomic position of O atoms, affirming the atomic model shown in Figure 6 (a). The rather confounding result that the Ag cations are arranged in bilayers is understood herein to be reflective of the underlying non-commutative (non-Abelian) SU(2) algebra arising from the pseudo-spins interacting to form bosonic degrees of freedom whose order parameter $\Psi$ satisfies eq. (20) and hence $|\Psi|^2 = \rho$. This entails a description of cationic diffusion within the bilayers, which necessitates the three generators of SU(2) (Pauli matrices) to represent the various interactions of the Ag atoms within and across the layers.[87]

Consider the primitive cell of the honeycomb lattice of cations given in Figure 4 by the blue-shaded rhombus. Each primitive cell is comprised of two cationic sites as earlier discussed. We shall assign an index, $j = 1, 2, 3 \cdots k$ for each primitive cell on the honeycomb lattice. Figure 6 (a) and (b), show that such a honeycomb lattice bifurcates into bilayers as seen in the STEM images (Figure 6 (c) and (d)), with each primitive cell contributing a single cation from a specific site to form two triangular sub-lattices on top of each other, as shown in Figure 5. This implies that we can assign a wave function, $\varphi_\alpha(\vec{r}_j)$ for each Ag atom, where $\vec{r}_j = (\vec{r}_1 - \vec{r}_2)_j$ is the displacement vector of the first cationic site in the primitive cell relative to the second.

Proceeding, we shall introduce the basis vectors of the unit cell as before,

$$\hat{\omega}_1 = \omega_1 \left( \begin{array}{c} 1 \\ 0 \end{array} \right) = \omega_1 | \uparrow \rangle, \quad \hat{\omega}_2 = \omega_2 \left( \begin{array}{c} 0 \\ 1 \end{array} \right) = \omega_2 | \downarrow \rangle,$$

which requires that $\omega_1/\omega_2 = 1$. Moreover, as discussed before, there exists discrete/modular symmetry generators $Q_1 = T, Q_2 = S \in Q$ where $Q$ is an element of PSL$_2(\mathbb{Z})$, and,

$$T = \left( \begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array} \right), \quad S = \left( \begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right),$$

act on the basis, $\hat{\omega}_1 + \hat{\omega}_2$, which map unit/primitive cells by either discrete re-scaling ($T$) or rotations ($S$) as shown in Figure 7 and Figure 8 respectively. This implies that the underlying quantum field theory is conformal in nature. In particular, discrete expansions are given by,

$$T^k = \left( \begin{array}{cc} 1 & k \\ 0 & 1 \end{array} \right),

$$

where $\omega_1/\omega_2 = k = N/2 \in \mathbb{N}$ is an integer and $N$ is the number of cationic sites within the region bounded by the basis vectors defining the unit cell. Moreover, a double rotation corresponds to,

$$S^2 = -\sigma_0 = -\left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right),$$

which represents the primitive cell as viewed from below, hence explaining the negative sign.

Performing the double rotation operation twice yields the identity matrix, $S^2 = \sigma_0$, suggesting the honeycomb primitive cell can be identified by two eigenvalues, $\pm 1/2$, corresponding to two pseudo-spins defining a pair of triangular sub-lattices. Thus, it is the two cationic sites with eigenvalues $\pm 1/2$ which bifurcate into bilayers, that is responsible for breaking scale invariance of the honeycomb lattice. This is evident by realizing that re-scaling the basis, $\omega_1 \rightarrow \Omega \omega_1, \omega_2 \rightarrow \Omega \omega_2$, where $\Omega$ is the scaling factor, leaves $k = \omega_1/\omega_2 = 1/k$ invariant in the monolayer, but is ill-defined for the bilayer due to bifurcation.

Proceeding, it is prudent to consider the 2-spinor,

$$\varphi_\alpha(\vec{r}_j) = \left( \begin{array}{c} \varphi_\uparrow(\vec{r}_j) \\ \varphi_\downarrow(\vec{r}_j) \end{array} \right) \equiv \varphi_\uparrow(\vec{r}_j) | \uparrow \rangle + \varphi_\downarrow(\vec{r}_j) | \downarrow \rangle,$$

$$J^0_j \propto |\varphi_\uparrow(\vec{r}_j)|^2 = |\varphi_\downarrow(\vec{r}_j)|^2 + |\varphi_\uparrow(\vec{r}_j)|^2,$$

where $J^0_j = \rho_j(\vec{r}_j) g_j(\vec{r}_j)$ is time component of the current density, $g_j(\vec{r}_j)$ is the pair-correlation function, and $\rho_j(\vec{r}_j)$
FIG. 6. Visualization of Ag atom bilayers in honeycomb layered $\text{Ag}_2\text{Co}_2\text{TeO}_6$. (a) A unit cell of $\text{Ag}_2\text{Co}_2\text{TeO}_6$ showing the arrangement of atoms as viewed in the [100] zone axis. Ag atoms are shown in grey while Co and Te atoms are shown in green and pink, respectively. Oxygen atoms are shown in red. (b) A perspective view of the unit cell of $\text{Ag}_2\text{Co}_2\text{TeO}_6$ showing the arrangement of the atoms. The Ag layers form two triangular lattices (drawn as dashed grey lines (down) or solid grey lines (up)) comprising a single bilayer. The green double arrows show a few pairs of cations which belong in the same primitive cell, as indicated by the green solid line in Figure 5. (c) HAADF-STEM image of $\text{Ag}_2\text{Co}_2\text{TeO}_6$ taken along [100] zone axis and, (d) the corresponding ABF-STEM image. The contrast ($I$) of the high-angle annular dark-field (HAADF) STEM image is proportional to the atomic number ($Z$) of elements (where $I \propto Z^{1.7} \approx Z^2$). Bilayer planes of Ag atoms ($Z = 47$), marked by the brighter and larger golden spots, are located between the layers of Co atoms ($Z = 27$) represented by the darker amber spots, and Te atoms ($Z = 52$) denoted by the smaller golden spots. As for annular bright-field (ABF) STEM imaging, $I \propto Z^{1/3}$, which means elements such as O ($Z = 8$) can also be discerned. The Te-Co-Co-Te sequential arrangement of the Te atoms and Co atoms, typical in honeycomb frameworks, is succinctly visualised. Ag atoms bilayers (highlighted by arrows) are sandwiched between the honeycomb slabs. An atomistic model has been embedded on the STEM image as a guide.
The honeycomb lattice of cations depicting the action of the $Q_1 = T$ generator of $SL_2(\mathbb{Z})$ on the primitive vectors. (a) The primitive vectors $\hat{\omega}_1$ and $\hat{\omega}_2$ of the honeycomb lattice, where $\omega_2/\omega_1 = 1$ is the number of pairs of cations/cationic sites enclosed within the primitive cell. (b) $Q_1 = T$ transformation corresponding to the re-scaling of the primitive vector, $\omega_2$ and hence an expansion of the unit cell, $\omega_2/\omega_1 = 2$.

The electric field satisfies Gauss’ law,

$$\beta \nabla \cdot \vec{E}_j(\vec{r}_j) = \rho_j(\vec{r}_j)g(\vec{r}_j) = \vec{n} \cdot \vec{B}_j(\vec{r}_j),$$

where $\rho_j(\vec{r}_j)$ is the 2D bulk number density and $g(\vec{r}_j)$ is the pair correlation function at each primitive cell. The pair correlation function is normalized as,

$$\int d^2r_j \vec{n} \cdot \vec{B}_j = \int d^2r_j \rho_j(\vec{r}_j)g_j(\vec{r}_j) = k - 1,$$

where $k = \omega_1/\omega_2$ is the number cationic pairs in the unit cell labeled by $j$. This implies that, for the primitive cell with $k = 1$, the integral vanishes. Thus, the Euler characteristic associated with the primitive cell corresponds to the geometric phase,

$$\chi(A_j) = \frac{1}{2\pi} \int d^2r_j \sqrt{\det(g'_{ab})}K_j(\vec{r}_j)$$

$$= -\frac{1}{2\pi} \int d^2r_j \nabla^2\Phi_j(\vec{r}_j) = -\frac{1}{2\pi} \int d^2r_j \cdot (\vec{n} \times \vec{\nabla}_j \Phi_j(\vec{r}_j))$$

$$= \int d^2r_j \vec{\nabla}_j \cdot \vec{A}_j(\vec{r}_j)$$

$$= \int d^2r_j \vec{n} \cdot \vec{B}_j(\vec{r}_j)$$

$$= -2 \int d^2r_j \vec{n} \cdot \vec{E}_j(\vec{r}_j)$$

$$= 2 - 2k = 0.$$
FIG. 8. The honeycomb lattice of cations and discrete rotations (ω₂/ω₁ = 1) generated by \( Q_2 = S ∈ SL_2(\mathbb{Z}) \) acting on the primitive cell. Some pseudo-spin states of the honeycomb lattice have been included for clarity. The primitive cell is rotated as shown in (a), (b), (c) and (d) by the application of \( Q_2 = S \) transformation, such that \( Q_2^2 = S^2 = -\sigma_0 \) corresponds to inversion of (a), (b) to (d), (c) respectively, where \( \sigma_0 \) is the 2 × 2 identity matrix, requiring that \( Q_2^4 = \sigma_0 \). The inversion corresponds to the honeycomb lattice originally viewed from above to appear viewed from below, equivalent to the exchange of the two pseudo-spin states relative to the primitive basis vectors.

where \( k = \omega_1/\omega_2 = 1 \) is the genus of a 2-torus, implying that,

\[
\rho_j(\vec{r}_j)g_j(\vec{r}_j) = -\frac{K_j(\vec{r}_j)}{4\pi} \exp(2\Phi_j(\vec{r}_j)).
\] (89)
Particularly, we can define the primitive cell as a two-torus by identifying the opposite sides with each other following the illustration in Figure 3. Consequently, the entire honeycomb lattice with vacancies can be treated as a connected sum of all the tori, \( A_j = T^2_j \) at each honeycomb primitive cell with Euler characteristic, \( \chi(T^2_j) = 0 \). The Euler characteristic of the emergent manifold \( \chi(A = T^2_1 \# \cdots \# T^2_k) \) thus becomes,

\[
\chi(\mathcal{M}) = \chi(\mathcal{M}_1 \# \cdots \# \mathcal{M}_k) = \sum_{j=1}^{k} \chi(M_j) - (k-1)\chi(S^2) = 2 - 2k, \tag{90a}
\]

where we have used the property,

\[
\chi(\mathcal{M}_1 \# \cdots \# \mathcal{M}_k) = \sum_{j=1}^{k} \chi(M_j) - (k-1)\chi(S^2) = 2 - 2k, \tag{90b}
\]

of Euler characteristics of connected sums of manifolds, \( \mathcal{M}_j \) and \( S^2 \) is the two-sphere with Euler characteristic, \( \chi(S^2) = 2 \). Thus, the number of cationic sites can be succinctly linked to the genus of the emergent manifold. Moreover, making the choice,

\[
\rho_j(\vec{r}_j) = -\frac{K_j}{4\pi} \exp(\Phi_j(r_j)), \tag{91a}
\]

\[
g_j(\vec{r}_j) = \exp(\Phi_j(\vec{r}_j)) = \exp(-\beta \phi_j(\vec{r}_j)), \tag{91b}
\]

where \( \beta = 1/m \) and \( \phi_j(\vec{r}_j) = -m\Phi_j(\vec{r}_j) \) is the average work needed to bring the two pseudo-spin up and pseudo-spin down cations of effective mass, \( m \) from infinite separation to a distance \( r_j \) apart while assuming a cavity distribution function of order unity\[138\], we can set \( \rho_j(\vec{r}_j) = 0 \) to obtain the solution,

\[
\Phi_j(\vec{r}_j) = \ln \left( \frac{C_j}{\|\vec{r}_j - \vec{r}_j\|^{2\Delta}} \right), \tag{91c}
\]

in 2D with \( C_j \) and \( \Delta \) constants. This corresponds to \( K_j = 0 \), and hence \( k = 1 \), which is the primitive cell. Proceeding, we consider the Liouville action, in \( d \) dimensions\[139\],

\[
I \propto \sum_j \int \frac{d^d x_j}{2} \sqrt{\text{det}(\tilde{g}^j_{ab})} \left( \gamma^{ab} \frac{\partial \Phi_j}{\partial x^a} \frac{\partial \Phi_j}{\partial x^b} - K_j \exp(2k\Phi_j) \right)
+ \sum_j \int \frac{d^d x_j}{2} \sqrt{\text{det}(\tilde{g}^j_{ab})} Q(k) \tilde{R}_j \Phi_j, \tag{92a}
\]

where \( \tilde{g}^j_{ab} \) is a \( d \)-dimensional metric tensor at \( j \), \( \tilde{R}_j \) is the Ricci scalar associated with the metric tensor, \( Q(k) \) is a parameter dependent on \( k \), \( d = 2 \) and

\[
\vec{F}_j = (\vec{x}_1 - \vec{x}_{1,j}) = (\vec{r}_1 - \vec{r}_1, z_1 - z_{1,j}) = (\vec{r}_j, z_j). \tag{92b}
\]

Since the Ricci scalar vanishes \( (\tilde{R}_j = 0) \) when the Euclidean metric is flat, \( \tilde{g}^j_{ab} = \delta_{ab} \), the last term in eq. (92a) vanishes and the Liouville action reduces to,

\[
I \propto \sum_j \int \frac{d^d x_j}{2} \left( \nabla \Phi_j \cdot \nabla \Phi_j - K_j \exp(2\Phi_j) \right). \tag{93}
\]

Thus, for arbitrary \( Q(k) \), eq. (93) can be varied with respect to \( \Phi_j(\vec{x}) \) to yield eq. (84b) when \( d = 2 \) dimensions (corresponding to \( z_1 = z_{1,j} \) in eq. (92b)) and \( k = 1 \).

To appropriately define \( \Delta \), we make use of scale invariance,

\[
\vec{x}_j \rightarrow \Omega \vec{x}_j, \quad \Phi(\vec{x}_j) \rightarrow \Omega^{\Delta} \Phi(\vec{x}_j), \tag{94}
\]

when,

\[
K_j = 0, \quad \Delta = \frac{1}{2}(d - 2), \tag{96}
\]

where \( \Omega \) is an arbitrary scaling factor. Thus, the correlation function can be set as the pair correlation function,

\[
g_j(\vec{r}_j) = \frac{C_j}{|\vec{x}_1 - \vec{x}_{1,j}|^{2\Delta}} = (\Phi_j(\vec{x}_1)\Phi_j(\vec{x}_{1,j})). \tag{97}
\]

Moreover, by the Pauli hamiltonian in eq. (82) with \( H_j = 0 \) the ground state and \( \vec{n} \cdot \vec{B}_j(\vec{r}_j) = -K_j \exp(2\Phi_j(\vec{r}_j)) = 0 \), where the theory is scale invariant, we must have,

\[
\vec{p}_j(\vec{r}_j) = (\vec{p}_1 + \vec{p}_1)_j = \vec{A}_j(\vec{r}_j) = \frac{1}{m}(\vec{n} \times \vec{E}_j), \tag{98a}
\]

which introduces the Chern-Simons current density\[140\],

\[
\vec{J}_j \propto \vec{p}_j = \vec{A}_j(\vec{r}_j) = \frac{1}{m}(\vec{n} \times \vec{E}_j). \tag{98b}
\]

On the other hand, when,

\[
\vec{n} \cdot \vec{B}_j(\vec{r}_j) = -K_j \exp(2\Phi_j(\vec{r}_j)) \neq 0, \tag{99}
\]

and the current density takes the Chern-Simons form given in eq. (98b), scale invariance and hence conformal symmetry appears to be broken since \( K_j \propto \rho_j \neq 0 \) and the particles are massive. Nonetheless, near the critical point where the phase transition occurs, the pair correlation function must take the form given in eq. (97). However, this is not evident in \( d = 2 \) when \( K_j \neq 0 \) but is manifest in \( d = 3 \) when \( \vec{z}_1 \neq \vec{z}_{1,j} \) and,

\[
\vec{r}_j \rightarrow \vec{x}_j = (\vec{r}_j, z_j), \tag{100}
\]

where Liouville’s equation given in eq. (84b) transforms into the Emden-Chandrasekhar equation\[141\] with solution given by eq. (91c) provided,

\[
K_j = K_0 \Delta \exp(-f(\Delta)\Phi_j(\vec{x}_j)), \tag{101a}
\]

\[
f(\Delta) = \Delta^{-1} - 2 = 0, \tag{101b}
\]

and the normalization constant is given by,

\[
C_j^{-1/\Delta} = K_0^2/2. \tag{101c}
\]

We note that, the Gaussian curvature, \( K_j \) given in eq. (10) or eq. (65) differs from the form herein in eq. (101).
since the theory is in $d = 3$ dimensions. Evidently, we can retrieve eq. (10) by the transformations, $f(\Delta) \rightarrow \nu$, $\Phi_j \rightarrow \Phi_{AC}$ and $\eta_j = (\eta_j - \eta_{j,0}) = 0$, which transforms the 3D theory to the 2D conformal field theory discussed above. This suggests that, at the critical point where $z_j = 0$ and $K_j \neq 0$, we ought to consider conformal invariance of the entire parameter space of Liouville conformal field theory.[12]

In particular, it is known that the field $V_j(k) = \exp(2k\Phi_j)$ or $V_j(k) = \exp(2k\Phi_j)$ is primary when the conformal dimension is given by,

$$\Delta = \frac{k}{2} (Q(k) - k) = \frac{\bar{k}}{2} (Q(\bar{k}) - \bar{k}), \quad (102a)$$

while the marginal condition for conformal invariance of the primary field is $\Delta = 1/2$, where $\Delta$ appears in eq. (101) and $z_j \rightarrow 0$, which is equivalent to,

$$Q(k) = Q(\bar{k}) = k + \bar{k}, \quad (102b)$$

where $N = 2k \neq 0$ is the number of cationic sites in a unit cell of the honeycomb lattice with basis vectors given in eq. (76) and $\bar{k} = 1/k$. The central charge is given by,

$$c = 1 + 6Q^2(k) = 1 + 6Q^2(\bar{k}) = \bar{c}. \quad (102c)$$

However, the theory is known to be unitary only for $c = 1$ and $c = \infty$ corresponding to $k \rightarrow \infty$ or $\bar{k} \rightarrow \infty$ ($Q(k) = Q(\bar{k}) \rightarrow \infty$) and $Q(k) = 0$, respectively. However, for $z_j \neq 0$, the theory is 3D, which breaks scale invariance due to, $K_j \neq 0$. This results in the bifurcation of the honeycomb lattice following the Pauli Hamiltonian with $\vec{B_j}(\vec{x_j}) \neq 0$ since $\vec{z}_j \neq \vec{z}_l$. Consequently, this bifurcation corresponding to a monolayer-bilayer phase transition further lowers the energy as depicted in Figure 9 (c) and Figure 9 (d), leading to deviations $\delta E$ from the ground state,

$$\frac{\delta E_j}{2} = \langle \varphi_1 | H_j(\vec{r}_j) | \varphi_1 \rangle = \frac{1}{2m} \vec{n} \cdot \vec{B}_j(\vec{x_j}) \langle \varphi_1 | \sigma_3 | \varphi_1 \rangle = \frac{1}{2m} \rho_j(\vec{x_j}) g_j(\vec{R}_j) = -\langle \varphi_\uparrow | H_j(\vec{r}_j) | \varphi_\downarrow \rangle \neq 0. \quad (103)$$

Consequently, the two layers must be separated by the energy barrier,

$$\delta E_j = \frac{\delta E_j}{2} = \frac{\vec{n} \cdot \vec{B}_j(\vec{x_j})}{2m} (|\sigma_3| \uparrow - |\sigma_3| \downarrow) = \frac{1}{m} \rho_j(\vec{x_j}) g_j(\vec{x_j}) = -\frac{K_j^2}{4\pi m} \exp(2\Phi_j(\vec{x_j})) = -\frac{\Delta/2\pi m}{(|\vec{x_j} - \vec{x_j}_i|)^2}, \quad (104a)$$

which is interpreted as the argentophilic interaction between the Ag cations responsible for stabilizing the Ag bilayer.[87] This interaction is attractive in nature, and thus loosely binds the opposite pseudo-spin Ag cations to each other, interpreted as a pseudo-boson analogous to a Cooper pair.[76]

C. Anti-de Sitter space-time

To further analyze the nature of this attractive force between like charges, recall that within the idealized model previously discussed, the inverse temperature is given by $\beta = 1/m = 8\pi GM$, where $G \sim \ell_P^2$ and $\ell_P$ is the honeycomb lattice constant and $M$ is the total effective mass of the cations. Thus, using $\Delta(d = 3) = 1/2$, the argentophilic interaction satisfies the condition for the unit cell,

$$\delta E_j \frac{\delta E_j}{M} = \frac{2G}{(|\vec{x}_j - \vec{x}_j_i|)^2} \equiv \frac{1}{\beta U_j(\vec{r}_j)} = G(\vec{r}_j), \quad (104b)$$

where $G$ is the analogue of Newton’s constant and $|\delta E_j/M| = 1/k = 1$ in the limit, $\vec{x}_j \rightarrow \vec{r}_j$. In fact, eq. (104b) is the analogue of eq. (52), where $\nu = k = 1$ corresponds to the condition for the primitive cell. Considering the gravitation theory $\Delta(d = 3) = 1/2$ given by eq. (31b), the metric in eq. (28) and the particle action correspond to the Newtonian limit,

$$\delta \tau_j^2 \simeq \exp(-2\Phi_j(\vec{x})) d\tau_j^2 - d\vec{x}_j \cdot d\vec{x}_j, \quad (106a)$$

and,

$$S_j(\vec{x}_j) = -m \int d\tau_j \left[ \sqrt{\exp(-2\Phi(\vec{x}_j))} - \frac{d\vec{x}_j}{d\tau_j} \cdot \frac{d\vec{x}_j}{d\tau_j} \right] \simeq \frac{m}{2} \int dt \left( \frac{d\vec{x}_j}{d\tau_j} \cdot \frac{d\vec{x}_j}{d\tau_j} + 1 - \exp(-2\Phi(\vec{x}_j)) \right) \simeq \frac{m}{2} \int dt \left( \frac{d\vec{x}_j}{d\tau_j} \cdot \frac{d\vec{x}_j}{d\tau_j} - \frac{\vec{x}_j \cdot \vec{\dot{x}}_j}{2G} \right), \quad (106b)$$

respectively, where we have used eq. (91c) and eq. (105).

Introducing displaced coordinates, $\vec{y}_j = \vec{x}_j - \sqrt{2\ell_P} \vec{n}$, where $d\vec{y}_j = d\vec{x}_j$, $\vec{n} \cdot \vec{n} = 1$, $\ell_P^2 = G$ and $\vec{n} = \vec{0}$, eq. (106) is transformed into,

$$\delta \tau_j^2 \simeq \left( 1 + \frac{\vec{y}_j \cdot \vec{y}_j}{2G} \right) d\tau_j^2 - d\vec{y}_j \cdot d\vec{y}_j, \quad (107a)$$

and,

$$S_j(\vec{y}_j) \simeq \frac{m}{2} \int dt \left( \frac{d\vec{y}_j}{d\tau_j} \cdot \frac{d\vec{y}_j}{d\tau_j} - \frac{\vec{y}_j \cdot \vec{\dot{y}}_j}{2G} \right). \quad (107b)$$

Thus, eq. (107) corresponds to the Newtonian limit,

$$\nabla^2 g_{00}(R_j) = -2\Delta, \quad (108a)$$

$$R_j^2 = \vec{y}_j \cdot \vec{y}_j, \quad (108b)$$
of the $1+3$ dimensional anti-de Sitter (AdS) spacetime,[91],

$$d\tau_j^2 = -g_{00}(R_j)dt_j^2 + g_{11}(R_j)dR_j^2 + R_j^2d\Omega_j^2, \quad (108c)$$

$$g_{00}(R_j) = \frac{1}{g_{11}(R_j)} = -\left(1 + \frac{R_j^2}{2G}\right), \quad (108d)$$

which satisfies the Einstein manifold $R_{\mu\nu} = \Lambda g_{\mu\nu}$ with a negative cosmological constant, $\Lambda = -3/2G = -3/2k_p^2 < 0$ and $d\Omega^2$ the metric of the two-sphere. Finally, since,

$$\Phi_j(x_j) = \ln \left(\frac{\|x_j \cdot x_j\|}{2G}\right) = \ln k = -\ln k = 0, \quad (109a)$$

corresponds to $k = 1/\bar{k} = 1$, the conformal field theory describing the primitive cell living at the origin, $R_j^2 = 0$,

$$|\hat{y}_j|^2 = |x_j - \sqrt{2}n|d^2 = 0, \quad (109b)$$

corresponding to Minkowski space time.

This duality is analogous to AdS/CFT correspondence[91] whereby a conformal field theory lives at the boundary of AdS. While such a boundary would correspond to the condition given in eq. (29) in the idealized model equivalent to restricting cationic motion to the $x-y$ plane, $(d_{zj}/dt = \sqrt{g_{00}(R_j)} = 0)$, in the case of bilayers, an exchange of cations between the triangular sub-lattices leads to $d_{zj}/dt \neq 0$. In fact, the speed in the $z$ direction becomes imaginary since,

$$d_{zj}/dt_j = \sqrt{g_{00}(R_j)} = i \exp(-\Phi_j(R_j)). \quad (110a)$$

The exchange of cations can be understood as a result of quantum tunneling with traversal time $\tau_T = \int_0^\beta dz_j/m/|p_z|j \sim 1/(p_z)|j$ measured by a Lamor’s clock, where the wavevector, $(p_z) = ndz_j/dt_j$ of the wave function, $\varphi_j(z_j, \vec{r}_j) \propto \exp(i(p_z)z_j) = \exp(-|z_j|)z_j$ is imaginary.[142] Consequently, since $\Phi_j = 0$, the wave function penetrates a depth $\beta = 1/m$, the cut-off scale along the $z$ direction. Finally, recall that the unit cells with $k \neq 1$ cannot be mapped to the primitive cell with $k = 1$ via the generator, $T^k \equiv Q$ given in eq. (78a). This corresponds to a mapping of $\Phi(R_j) = 0$ to $\Phi(R_j) \neq 0$, and hence represents mappings of the primitive cell to larger unit cells with $k \geq 1$. Consequently, the penetration depth becomes,

$$\beta \rightarrow \beta \exp(\Phi(R_j)) = \beta/\sqrt{-g_{00}(R_j)}, \quad (110b)$$

which corresponds to gravitational red-shift.

V. DISCUSSION

Layered materials demonstrating a bilayer arrangement of metal atoms exist, a vast majority being Ag-based layered oxides and halides such as $\text{Ag}_2\text{MO}_2$ ($M = \text{Co, Cr, Ni, Cu, Fe, Mn, Rh}$), $\text{Ag}_2\text{F}$, $\text{Ag}_2\text{O}_2$ (or equivalently as $\text{Ag}_3\text{O}$), $\text{Ag}_3\text{Ni}_2\text{O}_4$, and more recently $\text{Ag}_2\text{M}_2\text{Te}_6\text{O}_{16}$ (where $M = \text{Ni, Mg, Co, Cu, Zn}$).[79–90] Despite having equal positive charges, Ag atoms in these compounds form idiosyncratic structural frameworks with cluster-like agglomerates of conspicuously short $\text{Ag}^+ - \text{Ag}^+$ interatomic distances akin to those of elemental Ag metal, suggestive of unconventional weak attractive interactions between d-orbitals of monovalent Ag atoms ($d^{10}$-$d^{10}$ orbital interactions), what is referred to in literature as argentophilic interactions.[143] This postulation for the origin of weak attractive argentophilic interactions between Ag cations stems from diffuse reflectance spectroscopy measurements performed in a series of Ag-rich ternary oxides, which indicate a special electronic state of $\text{Ag}^+$ in the ultraviolet-visible regime.[144] The unique structural features are accompanied by the formation of an empty orbital band of mainly Ag-5s orbital character near the Fermi level, capable of accommodating additional electrons, which translates to a range of anomalous subvalent states in Ag cations.[80] In principle, subvalent Ag cations have been reported in Ag-rich oxide compositions such as $\text{Ag}_9\text{SiO}_4$, $\text{Ag}_5\text{GeO}_4$, $\text{Ag}_5\text{Pb}_2\text{O}_6$, $\text{Ag}_3\text{Os}_6\text{O}_9$, $\text{Ag}_3\text{O}$, $\text{Ag}_{10}\text{B}_2\text{O}_{10}$, and halides such as $\text{Ag}_2\text{F}$ and the theoretically predicted $\text{Ag}_6\text{Cl}_4$.[89, 90, 145–150] Subvalency of Ag ($\text{Ag}^{0.5}$) in $\text{Ag}_2\text{Ni}_2\text{O}_2$ was demonstrated using X-ray absorption spectroscopy, resonant photoemission spectroscopy, magnetic susceptibility measurements and quantum chemical calculations.[80, 86, 151–153] The underlying structural characteristics in such materials induces special physico-chemical properties such as good metallic conductivity, as has been noted in $\text{Ag}_2\text{Ni}_2\text{O}_2$.[86]

Herein, we first reviewed the important aspects of an idealized model of cationic diffusion in specific layered materials, whereby the number of cations or their vacancies is treated as the genus of an emergent 2D manifold without boundary whose partition function can be understood within the context of large $N$ theories.[16, 27, 28] Since cationic vacancies can be interpreted as topological defects of the manifold,[27] diffusion quantities have a dual geometric description, whereby the cationic vacancies, genus, Gaussian curvature and time-like Killing vector of a 1 + 3 dimensional manifold are dual to the cations, cationic number, 2D charge density and the $\mathbb{U}(1)$ gauge potential, respectively as summarized in Table I. Moreover, the 2D diffusion dynamics of the cations can be described by the field equations given in eq. (20), which constrain the trace of the Einstein Field Equations in eq. (31b) with the inverse temperature given by $\beta = 8\pi GM$, where $M$ is the total effective mass of the cations equivalent to the average potential energy of the cations and $G$ is the mobility analogous to Newton’s constant. While eq. (20) contains a complex-Hermitian $G_{\mu\nu}$, its structure differs from complex general relativity[154, 155] since the metric tensor and affine connection are real and torsion free. The 2D diffusion dynamics of the cations is retrieved from the
FIG. 9. Energy frustration (Pauli-exclusion principle) avoided by the topology of a flat torus ($K = 0$) and two-torus ($K \neq 0$) respectively. Adjacent pseudo-spin up or down cations, indicated by black up or down arrows respectively, can be mapped onto each other along red and green lines, whereby the red honeycomb lattice lines connect adjacent opposite pseudo-spin cations which lie in adjacent primitive cells whereas the green honeycomb lattice lines connect adjacent opposite pseudo-spin cations which lie within the same primitive cell. (a) A primitive cell of the honeycomb lattice (given in Figure 5), showing a pair of pseudo-spin up and down cations. (b) The system exploiting the topology of the two-torus to avoid energy frustration. The two-torus is related to the flat torus in (a) by the transformations depicted in Figure 3. The pseudo-spin up cation sits on the inside surface of the two-torus with negative curvature ($K < 1$) whereas the pseudo-spin down cation sits on the outside surface with positive curvature ($K > 1$) and paired cations with opposite pseudo-spins sits on the zero curvature region ($K = 0$). (c) A depiction of the red and green connections of opposite pseudo-spin cations of the entire honeycomb lattice as a flat torus ($K = 0$), which avoids energy frustration by mapping like pseudo-spin cations onto each other, leaving only a single red circle and a green line to represent the entire honeycomb lattice. The Gaussian curvature, $K$ vanishes everywhere along the green line. (d) The quasi-particle/excited states and ground state of the system with energy gap, $|\delta E_j| \propto K - (-K) = 2K$ (eq. (104a)). The $K = 0$ state persists along the green line only at the cross over between $K > 0$ and $K < 0$, where $K = 0$, which corresponds to a paired pseudo-fermionic state forming a pseudo-boson. Thus, the flat torus depiction in (c) is related to the two-torus by $\delta E_j \to 0$, which corresponds to the critical point.
We considered the ground state of the theory with a single primitive cell \((k = 1)\). The idealized model requires that the emergent manifold is a torus of genus \(g = k = 1\), corresponding to two solutions given by a flat-torus with a vanishing Gaussian curvature and a two-torus with a finite Gaussian curvature. Thus, the theory lives on a torus, and is compatible with 2D Liouville conformal field theory. To see the relevance of the torus with respect to the pseudo-spins, recall that we argued that a finite Gaussian curvature breaks scale invariance and hence conformal symmetry. Within the honeycomb lattice shown in Figure 5, each pseudo-spin up (down) \(\text{Ag}^+\) cation within a primitive cell is bonded to three adjacent pseudo-spin down (up) \(\text{Ag}^+\) cations, where the two of the three pseudo-spin down (up) \(\text{Ag}^+\) cations lie on two different primitive cells adjacent to the primitive cell containing the pseudo-spin up (down) \(\text{Ag}^+\) cations. This ensures that there is no (geometric) spin frustration within the entire honeycomb lattice.[156] However, given that each primitive cell is related to the others by translations along the basis vectors, the localized cations in adjacent primitive cells must occupy the same energy state.

In particular, since the interaction energy of any two adjacent \(\text{Ag}^+\) cations depends only on their relative distance in the \(x-y\) plane (translation invariance), provided the cations are considered localized \(\text{i.e.} \overrightarrow{E} = (E_x, E_y, 0) = 0\) in Figure 2 (a), kinetic energy terms do not contribute to the energy suggesting that bonds of equal length imply that, considering only next neighbor interactions, all cation pairs occupy the same ground state. However, since the pseudo-spin of cations is assumed subject to the Pauli exclusion principle, this introduces energy frustration into the system, which precludes either translation invariance, localization or both. Nonetheless, the topology of the system and hence a finite pseudo-magnetic field where \(K \propto B_z \neq 0\) provides a recourse to treat the cations as pseudo-bosons avoiding the energy frustration. Thus, the system exploits the topology of a flat-torus (Gaussian curvature, \(K = 0\)) or the two-torus \((K \neq 0)\) shown in Figure 9, where opposite sides of the primitive cell shown in Figure 9 (a) are associated with each other, forming a flat-torus with vanishing Gaussian curvature \((K = 0)\) or a two-Torus with a finite Gaussian curvature \((K \neq 0)\) given in Figure 9 (b). This maps the three pseudo-spin down (up) \(\text{Ag}^+\) cations to each other and hence identifies them as the same cation hence avoiding energy frustration. In addition, in the case of the two-torus \((K \neq 0)\), opposite pseudo-spin pairs within a primitive cell experience an attractive interaction proportional to the finite Gaussian curvature, which acts as a pseudo-magnetic field[137] along the \(z\) coordinate, leading to the energy gap and hence a bifurcation of the honeycomb lattice into two triangular sub-lattices with opposite pseudo-spins.

This monolayer-bilayer phase transition can be understood as the pairing of opposite pseudo-spin cations (Cooper pairs[76]) within a given primitive cell as illustrated in Figure 9 (c) and (d), leading to pseudo-spin zero bosons with an order parameter given by \(|\Psi|^2 \propto K \propto \Delta = (d-2)/2\), where \(K \to 0\) or \(d \to 2\) is the critical point of the phase transition. In particular, since the pseudo-bosons are not subject to Pauli exclusion, this mechanism avoids energy frustration. As a result, the system is gapped, with the energy difference between the two layers given by \(e\) (104), corresponding to argentophilic interaction.[87] Since the pseudo-magnetic field is proportional to the Gaussian curvature, which in turn is related to the cationic vacancy number density via the Gauss-Bonnet theorem, this critical phenomenon can be interpreted to correspond to the two-torus solution \((K \neq 0)\). Alternatively, considering each triangular sub-lattice as a honeycomb lattice, after the bifurcation, each honeycomb sub-lattice consists of a vacancy and a cation such the emergent manifold is of genus 1. Thus, sufficient minimum activation energy of the order of the mass gap is needed to break the argentophilic bond, creating \(\text{Ag}\) quasi-particles and higher genus states during \(\text{Ag}\) de-intercalation processes.

We are interested in the necessary and sufficient conditions for the observation of \(\text{Ag}\) bilayers. Cross-examining the aforementioned \(\text{Ag}\)-based bilayer materials, we find that all the \(\text{Ag}\)-based bilayers are triangular sub-lattices of the honeycomb lattice, whereby the bonds take the arrangement, \(\cdots \text{Ag}^- \text{Ag}^- \text{Ag}^- \text{Ag}^- \cdots\) and \(Z = O, F\) or Cl is an anion. Thus, for a monolayer-bilayer transition to be viable in these materials, it is expected that a linear/dumbbell coordination with \(\cdots \text{Ag}^- \text{Ag}^- \text{Ag}^- \cdots\) will be formed, where two \(\text{Ag}\) triangular sub-lattices with opposite pseudo-spin merge to form a single honeycomb lattice \(\text{albeit}\) unstable, where each vertex of the triangle contributes a single cation to the primitive cell. This implies that the \(\text{Ag}\) subvalent state is a necessary condition but by no means sufficient. Our framework is consistent with the following necessary and sufficient conditions for the observation of stable bilayers of cations in layered materials[157]: 1) observation of a pair of cation triangular sub-lattices of the honeycomb lattice; whereby the bonds take the arrangement, \(\cdots \text{Ag}^- \text{Ag}^- \text{Ag}^- \text{Ag}^- \cdots\) and \(Z = O, F\) or Cl is an anion. Thus, for a monolayer-bilayer transition to be viable in these materials, it is expected that a linear/dumbbell coordination with \(\cdots \text{Ag}^- \text{Ag}^- \text{Ag}^- \cdots\) will be formed, where two \(\text{Ag}\) triangular sub-lattices with opposite pseudo-spin merge to form a single honeycomb lattice \(\text{albeit}\) unstable, where each vertex of the triangle contributes a single cation to the primitive cell. This implies that the \(\text{Ag}\) subvalent state is a necessary condition but by no means sufficient. Our framework is consistent with the following necessary and sufficient conditions for the observation of stable bilayers of cations in layered materials[157]: 1) observation of a pair of cation triangular sub-lattices of the honeycomb lattice; 2) a bond between the subvalent cation and \(Z\), where \(Z\) must be an anion and; 3) existence of weakly attractive cation-cation interactions related to allowed cation subvalent states.

Condition 1 is associated with the honeycomb lattice, which bifurcates into two triangular sub-lattices. This bifurcation is expected to further lower the free energy, producing a stable structure. The honeycomb lattice also assigns opposite pseudo-spins to the pair of cations in each primitive cell, which guarantees that the bifurcation forms a pair of triangular sub-lattices with a particular spin orientation. Condition 2 implies that the \(\text{Ag}\) honeycomb lattice ought to be in linear/dumbbell coordination with \(Z\) anions. Consequently, conditions
TABLE I. Summary of gauge (diffusion)/gravity (geometry) duality of the idealized model in layered materials.

| gauge (diffusion) | gravity (geometry) |
|-------------------|--------------------|
| cation            | vacancy            |
| Chern number      | genus of a 2D surface |
| U(1) gauge field  | Killing vector     |
| temperature, 1/β  | effective mass, m  |
| 2D number density | 2D Ricci scalar    |
| Langevin equation | Gauss-Bonnet theorem |
| Chern-Simons theory | Liouville CFT    |
| pseudo-magnetic field | Gaussian curvature |
| conformal field theory | anti-de Sitter space-time |
| Fokker-Planck equation | Liouville’s equation |

1 and 2 imply that honeycomb monolayered materials with linear/dumbbell coordination with Z anions are unstable due to energy frustration, and possibly difficult to realize experimentally. Apart from the aforementioned Ag-based compounds, subvalent compounds containing mixed atom clusters of Ag and Hg have been reported,[158] while metalophilic interactions in compounds entailing other congener coinage metal atoms such as gold and copper (aurophilic and cuprophilic interactions, respectively), have been envisaged.[159, 160] Moreover, thallophilic interactions [161] can be envisaged in thallium-based layered oxides such as Tl₂MnTeO₆,[92] which exhibits a bilayer arrangement of thallium (Tl) atoms. Since other materials such as Tl₂MnTeO₆ share the aforementioned conditions with Ag-based systems, the theoretical framework herein is consistent with their monolayer-bilayer phase transition.

In conclusion, we have described the bilayer structure of cations observed in honeycomb lattices as emergent from conformal symmetry breaking. The critical point of monolayer-bilayer phase transition is described by Liouville conformal field theory and is consistent with Anti-de Sitter space as a gravitational dual. The results and insights herein further augment the vast literature on conformal field theory in condensed matter systems[3, 7, 11], while serving as a frontier framework to explore ideas such as AdS/CFT correspondence, often employed in quantum gravity research.[91, 162, 163]

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