Doping the holographic Mott insulator.

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Mott insulators form because of strong electron repulsions, being at the heart of strongly correlated electron physics. Conventionally these are understood as classical “traffic jams” of electrons described by a short-ranged entangled product ground state. Exploiting the holographic duality, which maps the physics of densely entangled matter onto gravitational black hole physics, we show how Mott-insulators can be constructed departing from entangled non-Fermi liquid metallic states, such as the strange metals found in cuprate superconductors. These “entangled Mott insulators” have traits in common with the “classical” Mott insulators, such as the formation of Mott gap in the optical conductivity, super-exchange-like interactions, and form “stripes” when doped. They also exhibit new properties: the ordering wave vectors are detached from the number of electrons in the unit cell, and the DC resistivity diverges algebraically instead of exponentially as function of temperature.
These results may shed light on the mysterious ordering phenomena observed in underdoped cuprates.

The “hard” Mott insulators (MI) realised in stoichiometric transition metals salts are regarded as one of the few entities that are well understood in the arena of strongly correlated electron systems [1]. The principles are given away by Hubbard-type models: given an integer number of electrons per unit cell, any charge fluctuation gives rise to an excess local Coulomb energy “$U$” and when this becomes much larger than the bandwidth, quite literally a traffic jam of electrons is formed. This state can be adiabatically continued to the weak interaction limit using conventional (Hartree-Fock) mean-field theory, where it turns into a “BCS-like” commensurate spin density wave [2]. The language of quantum information reveals the key element: Hartree-Fock rests on the assumption that the ground state is a “classical” short ranged entangled product state [3]. At strong coupling the quantized single electron charges are just localized inside the unit cell. At weak coupling one has to accommodate Fermi-statistics, but the case can be made precise that even the Fermi gas is a product state in momentum space [4]. The perfectly nested density wave (weak coupling MI) then “inherits” its lack of macroscopic entanglement from the underlying Fermi-liquid.

However, matter may also be “truly quantum” in the sense of quantum information: the vacuum state may be an irreducible coherent superposition involving an extensive part of the exponentially large many body Hilbert space. Little is known with certainty given the quantum complexity: a quantum computer is needed to address it with confidence. Indications are accumulating that the strange metals realised in the cuprate high Tc superconductors may be of this kind [5]. Upon lowering temperature in the under-doped regime, this strange metal becomes unstable towards a myriad of “intertwined” ordering phenomena that do depend critically on the ionic lattice potential [6, 7]. It has become increasingly clear that this pseudo-gap order does not seem explainable in terms of conventional mean-field language [6, 8]. Could it be that these ordering phenomena inherit the many-body entanglement of the strange metal? If so, do these submit to general emergence principles of a new kind that can be identified in experiment?

A new mathematical machinery has become available which can address this question at least to a degree. There is strong evidence that the holographic duality [9] (or AdS/CFT correspondence) discovered in string theory describes generic properties of certain classes of such densely entangled quantum matter [5]. In particular, holographic strange metals
are emergent quantum critical phases that behave in key regards suggestively similar to
the laboratory strange metals (local quantum criticality [10, 11], Planckian dissipation
[12, 13]). Here we will explore what holography has to say about the emergence of
“entangled Mott insulators”.

The results reveal generalities which are intriguing and suggestive towards experiment. On the one hand, the holographic realisation of the Mott insulator shows properties similar to the conventional variety. The optical conductivity has the similar characteristics as the inter Hubbard band transitions found in hard Mott insulators (Fig. 1e) [14, 15] and an analogue of superexchange interaction [16, 17] can be identified (Fig. 1f). Upon doping, close analogies of the “spin stripes” [18, 19, 20, 21, 22] are formed (Fig. 4b). However, they also reveal unconventional features reflecting their entangled nature. Reminiscent of the charge order in cuprates, the periodicity of the charge order that forms upon doping displays commensurate plateaux (Fig. 3b), staying constant in a range of doping levels. Most intriguingly, holography insists that charge cannot be truly localized as in a “product state” Mott insulator. Instead, a reconfigured emergent quantum critical phase emerges at low energies characterized by a DC resistivity that increases algebraically instead of exponentially for decreasing temperature (Fig. 5a). This may shine light on the longstanding puzzle of the slow (logarithmic) rise of the resistivity in striped cuprates.

Let us now discuss how we arrive at these results. Conventional Mott insulators obey
the rule that the unit cell should contain an integer number of electrons in order for them
to form. However, this implicitly rests on product state structure, and the information
regarding the graininess of the microscopic electron charge is generically washed out in
strongly entangled states including the ones described by holography. There is, however,
a truly general definition of a Mott insulator that circumvents the confines of microscopic
product states: a Mott insulator is an electron crystal that is commensurately pinned by
a periodic background potential. A crystal formed in the Galilean continuum is a perfect
metal since it can freely slide – its massless longitudinal phonon is dual to a current that
is protected by total momentum conservation. This sliding mode will acquire a pinning
energy in a commensurate background lattice and this is the general meaning of a Mott
gap.

This is not a practical way to construct a Mott insulator departing from the electron
gas at metallic densities in the Galilean continuum since this lacks a natural tendency to
crystallize. Holographic strange metals on the other hand are known to have crystalli-
sation tendencies, where the most natural form[23] intriguingly involves a most literal form of “intertwined” order similar to that observed in underdoped cuprates [7, 6, 24, 26, 27, 28, 29, 30]. The AdS/CFT correspondence shows that the properties of quantum matter can be computed in terms of a holographic gravitational “dual” in a space with one extra dimension [9, 5]. Strange metallic states appear to be in one-to-one correspondence to charged black holes in this gravitational system. It was discovered that topological terms in the gravity theory (theta- and Chern-Simons terms in even- and odd-dimensions) have the effect that the horizon of the black hole becomes unstable towards spatial modulations [31, 32] at the “expense” that the charge modulation is “intertwined” [33] with parity breaking and the emergence of spontaneous diamagnetic “particle-hole” currents.

Here we study this holographic crystallisation in the presence of an external periodic potential. This demands advanced numerics to solve the gravitational problem; our “corrugated black holes” are among the most involved solutions in stationary general relativity (GR). To keep the computations manageable we focus on simple harmonic background potentials and especially a unidirectional translational symmetry breaking. We consider here specifically the minimal version of such a gravitational theory [32]. The basis is Einstein-Maxwell theory in 3+1 dimensions with a negative cosmological constant, describing the simplest holographic strange metal in 2+1 dimensions. The crucial extra ingredient is the topological parity-odd $\vartheta$-term coupling the Maxwell field $A_\mu$ with field strength $F_{\mu\nu}$ to a dynamical pseudoscalar field $\psi$, such that the action becomes,

$$S = \int d^4x \sqrt{-g} \left( R - 2\Lambda - \frac{1}{2} (\partial \psi)^2 - \frac{\tau(\psi)}{4} F^2 - W(\psi) \right) - \frac{1}{2} \int \vartheta(\psi) F \wedge F \quad (1)$$

The qualitative features we reveal depend only mildly on the precise form of the functions $\tau(\psi), W(\psi), \theta(\psi)$ (see Supplementary Material). The solution to the equations of motion will asymptote to anti-de-Sitter space (AdS), on the (conformal) boundary of which the dual theory lives. At finite density and temperature of the dual theory, a charged (Reissner-Nordstrom) black hole is present in the deep interior, which famously translates to a locally quantum critical strange metal (see Supplementary Material for the dictionary entries). As temperature is lowered, the $\vartheta$-term causes the horizon to become unstable towards a modulation of the spatial geometry that breaks translational symmetry spontaneously. Here we choose the simplest version, corresponding to a unidirectional symmetry breaking in the “x” direction (see [34, 35] for a “full” 2D crystallisation). This is driven
by the condensation of the pseudoscalar $\psi$ representing a spontaneous breaking of parity on the boundary. The structure of the $\partial$-term makes that this is accompanied by condensation of Maxwell field strength. This translates to the formation of spontaneous currents running in the $y$ direction, while a concomitant charge density wave (CDW) develops. A reliable, consistent result is only obtained if one solves the full equations of motion in the gravitational theory, and this includes the change in geometry due to back-reaction. Given the inhomogeneous nature of the bulk space time, this involves a considerable numerical GR effort since the Einstein equations represent a system of non-linear partial differential equations (see Supplementary Material). The result is represented in Fig. 1b.

One can also introduce a background periodic potential that breaks translational symmetry explicitly by representing the ion lattice in terms of a spatially modulated chemical potential in the field theory [35, 36, 37, 38, 39, 40]. It is easy to incorporate complicated forms of such “pseudo potentials” but we will focus here on the simplest choice in the form of a uni-directional single harmonic potential with wave vector $k$ and relative amplitude $A$: $\mu(x) = \mu_0(1 + A \cos(kx))$. (Fig. 1a)

Combining these two allows us to study spontaneous holographic crystallisation in the presence of a background lattice. The crystal tends to form with a preferred intrinsic wavelength $p_0$ set by the parameter $\vartheta$ and the scale of the mean chemical potential $\mu_0$. In the presence of a periodic potential characterized by wave vector $k$, one anticipates that one is considering incommensurate systems studied thoroughly in the past in classical matter [41, 42]. As already anticipated in [43], when these periodicities are sufficiently close together one expects a “commensurate lock-in” of the spontaneous crystal, gaining additional stability. These lowest order commensurate states are the holographic incarnations of Mott insulators (Fig. 1c). How literal is this “assignment”? It is instructive to consider first the optical conductivity. In the absence of the periodic potential one finds a “diamagnetic” delta function peak at zero frequency at all temperatures. The reason is that every finite density system is a perfect metal in the spatial continuum limit since total momentum is conserved. The formation of a crystal at $T_c$ spontaneously breaks translational invariance, and a longitudinal phonon emerges that is dual to a perfect current: the sliding mode. When we now switch on a sufficiently strong explicit commensurate background potential, this sliding mode will acquire a mass since the crystal gets pinned and it can no longer freely slide. This reveals itself in the optical conductivity (Fig. 1e). As the crystal forms below $T_c$, the metallic Drude peak rapidly moves off to finite frequency corresponding
Figure 1: **Formation of holographic Mott insulator** Left panel: Profiles of the spontaneous currents (arrows) and charge density (colour) in the (a) ionic lattice without spontaneous order (unbroken phase); (b) purely spontaneous intertwined CDW state, (c) commensurately locked Mott state and (d) State with aligned currents. Due to intertwinement of order this state has a different charge density than the Mott state. Note that the total current is zero in both staggered and aligned states. All solutions are at a fixed chemical potential with $T = 0.01u$, lattice potential strength $A = 2$, and $\theta$-coupling $c_1 = 17$.

Right panel (e): **Evolution of optical conductivity** upon the phase transition from metallic to Mott state. A sharp Drude peak is seen in metallic state which is pinned and broadened after the phase transition. (f): **Energy scales and superexchange**: The grand thermodynamic potential difference between unbroken phase and Mott state (blue line) and for the Mott state and aligned currents state (yellow line), as a function of the strength of the lattice potential. Clearly, the energy scale of the current ordering lacks behind the one of the charge ordering when the lattice becomes strong. Note that the grand canonical ensemble is required due to the charge difference between the two current configurations. (g): **Higher harmonics**: The difference between Fourier transform of the charge density $\hat{\rho}_q$ of the aligned (d) and staggered (c) states. Both spectra are normalized with respect to the lattice periodic mode ($\hat{\rho}_k$). The enhancement of $2k$ mode is seen for the aligned state, showing that it has twice the number of CDW per unit cell. The enhancement of the homogeneous component by $\sim 10\%$ in not shown.
Figure 2: **Holographic RG pattern**: the profiles of the electric field strength $\partial_z A_t$ (see eq. 9 in the Supplementary Material) in the gravitational theory encoding the RG flow from the UV (bottom) to the IR (top) of (a) the pure lattice that is sourced in UV and decreases to irrelevancy in the IR (b) The spontaneous charge density wave that emerges in the IR, but don’t have sources in UV (c) The lock-in that forms the Mott state. The CDW, locks to the lattice at intermediate scales and introduces the relevant explicit translation symmetry breaking in IR, giving rise to the insulating state.

to the pinning of the sliding mode. The mode itself broadens first due to increased translational symmetry breaking from the crystal. The resulting optical conductivity at $T < T_c$ strongly resembles that of hard MI with a broadening due to Hubbard interband transitions.

From Fig. 1c one infers that the background lattice enhances the spontaneous order. This can be further quantified by computing the energy difference between the crystallised and uncrystallised phase of the strange metal which increases steeply as function of the lattice amplitude (Fig. 1f). Visually one notices that the currents are generically enhanced in the regions where the spontaneous charge density wave has a maximum and the current density is effectively localized in these regions. This charge localization together with the alternating pattern of these currents immediately calls to mind the hard antiferromagnetic Mott insulator with staggered spins.

This suggests that other current patterns also exist. As we shall show, bulk saddle points (local minima in the grand thermodynamic potential $\Omega$) exist where the currents are aligned. As function of the lattice potential, the energy difference between these two configurations is much smaller than the energy difference between the CDW ordered and the uncrystallized state. This implies that in the presence of a large lattice potential,
current-current dynamics is governed by a different scale than charge dynamics. This is in analogy with the spin-charge separation in conventional Mott insulators, where below the Mott transition one is dealing with a spin only system, with the spin (dis)order governed by effective “super exchange” interactions which are much smaller than the scale associated with the Mott-insulator itself. The ramification is that the dynamics we visualize in the holographic model is not what actually would happen in the true physical system. For strong lattice potentials, one first encounters the onset of the charge density wave order at the transition temperature. Only at lower temperature will the additional staggered current symmetry breaking occur, since the latter will remain thermally disordered at temperatures larger than the current-current exchange parameter. A full computation in the holographic model with no saddlepoint approximation, will exhibit this physics. The solutions here focus on a single saddlepoint only, which is of the Mott insulator type when the wave-vectors of the spontaneous and ionic crystals are close to each other.

A highlight of holography is that the extra dimension of the gravitational theory can be interpreted as the “scaling direction” of the renormalisation group of the dual field theory with the UV fixed point located on the boundary of AdS. This yields a vivid renormalisation group view on the way that the Mott-insulator is formed. The irrelevancy of the explicit potential is illustrated in Fig. 2a: the electric field sourced by the external potential falls off moving from the boundary to the deep interior. The spontaneous crystal displays however precisely the opposite flow: it is relevant in the IR without having any sources in the UV (Fig. 2b). One can now read off the commensurate pinning mechanism from the “scaling diagram”, Fig. 2c: this pinning occurs at intermediate energy scales. One sees that “halfway” the radial direction the (decreasing) external potential starts to overlap with the (increasing) “hair” coding for the spontaneous crystal.

The important question with reference to the cuprates is: what happens when these holographic Mott insulators are doped? Above we tuned the wavevectors of the explicit lattice and spontaneous crystal to be the same. Adding charge the crystal will want to form at a different intrinsic wave vector $p_0$ but the external lattice potential may force it to acquire an altered one ($p$). Driving $p$ away from $p_0$ will, however, cost potential energy due to the elastic response of the crystal, so the resulting value of $p$ is determined dynamically by these two competing mechanisms. This is a motive familiar from the study of classical incommensurate systems [42, 44] and one anticipates that generically this will promote values of $\frac{p}{k}$, which are the rationals of small coprime integers: these are
the higher order commensurate points. The states labeled by the different fractions $\frac{p}{k}$ form a set of the local minima in the thermodynamic potential $\Omega$ and the true ground state corresponds to the one with minimal $\Omega$. We performed extensive numerical computations spanning a large parameter space to identify these saddle points.

The lowest order commensurate state $p/k = 1/1$ is obviously the Mott insulator we just discussed in detail. In analogy with the conventional picture of adding microscopic charges per unit cell, we prescribe the doping level as the excess charge per lattice period compared to the Mott insulating state. We normalize by assigning doping level 100% to the $p/k = 2/1$ state, which has exactly one additional period of spontaneous CDW per unit cell (see Supplementary Material). In practice, adding excess charge to the system is accomplished by adjusting the chemical potential, while keeping the lattice wave vector fixed. The result is summarized in Fig. 3a. The noteworthy aspect is that, due to the lock-in, some commensurate points stay stable for a range of dopings, displaying a “Devil staircase” like behavior familiar from classical incommensurate systems. We shall return to this shortly.

Let us first discuss the structure of these higher order commensurate states as formed at low temperatures in sufficiently strong background potentials. The periodicity mismatch (the deviation of $p/k$ from $1/1$) is concentrated in localised solitonic textures, see Fig. 4b – the discommensurations familiar from classical incommensurate systems (see also Supplementary Material). This is not completely surprising since discommensurations are rather ubiquitous when dealing with incommensurate systems. It is entertaining to observe how the discommensurations follow the renormalization group in the extra dimension of the gravity system (Fig. 4a). The UV lattice almost everywhere locks-in the IR charge density wave, except at the discommensuration core where a curious dislocation is formed in the electrical flux in the radial direction of the gravitational theory.

The noteworthy aspect is that there is additional structure: these discommensurations are at the same time domain walls in the staggered current order (Fig. 4b). Considering the current order as being analogous to the antiferromagnetic spin systems found in the standard (doped) Mott-insulators, these are just like the famous “stripes” observed in the $La_2CuO_4$ (214) family of high Tc superconductors [19] and in other doped Mott-insulators [20]: in the cuprate stripes the doped charge accumulates at the spin-pattern domain walls and the same is happening here (Fig. 4b). These stripes were actually discovered theoretically on basis of Hartree-Fock calculations well before the experimental
Figure 3: (a) The commensurate/incommensurate phase diagram. Colour shows the thermodynamically preferred commensurate fraction as a function of doping and temperature. The regions of stability of the leading 1/1, 2/1, and, as temperature is lowered, higher 3/2, 4/3, 5/3 commensurate points are seen. The shaded line on top shows the result of perturbative analysis of instabilities (see Supplementary Material). Data is taken for $A = 0.7, c_1 = 17$ (b) The commensurate plateaux as seen on the fixed temperature cut ($T \approx 0.01 \sqrt{\rho}$) of the phase diagram. Importantly, the commensurate states stay stable for a range of the charge density values. Higher commensurate points 3/2 and 4/3 correspond to 2$a$ and 3$a$ discommensuration lattices, respectively ($a$ – the lattice constant). $p_0/k$ shows the relation between spontaneous momentum of the free CDW versus the momentum of the lattice. Blue points represent the result in absence of commensurate lock in: when the amplitude of the lattice potential vanishes the preferred momentum of the structure equals the spontaneous one. The gridlines show the mesh of numerical study, where different saddle points were obtained. (c) Charge of a discommensuration as a function of doping (red line), measured in units of CDW charge density integrated over a unit cell (see (20)). The charge is obtained by considering an isolated discommensuration (one over 19 unit cells) and subtracting the contribution of the parent Mott state. The charge changes continuously as the doping is increased. Shading shows the preferred commensurate fraction as on (a), no signs of plateaux are seen in the charge of discommensuration.
Figure 4: (a) **RG structure of an isolated discommensuration** (same notation as on Fig. 2) The UV lattice lock in the IR structure everywhere outside the core of a discommensuration. In the core the “dislocation” is seen in the electric field, accounting for an excess period of the spontaneous structure in IR. **Profiles of the discommensurations.** Currents (arrows) and charge density (color) are shown for (b) **an isolated discommensuration.** The domain wall in the staggered current (defined using A and B sublattices) is clearly seen as well as excess charge in the core of a discommensuration. (c) **Higher commensurate state** with $p/k = 4/3$. The state displays superstructure with a period of 3 unit cells – 3a discommensuration lattice. The charge profile is normalized with respect to the corresponding Mott state with $A = 0.7, T = 0.01\mu$. (d) **Spectrum of discommensuration lattice.** The difference between the Fourier modes of the lattice and the parent Mott insulator. Both spectra are normalized with respect to the lattice periodic mode $q_k$. The fractional Fourier modes are clearly enhanced in the disc. lattice state. The homogeneous mode reaches $\approx 11\%$ and is not shown.
observation [18]. It is therefore clear that Hartree-Fock form of “intertwinement” of spin and charge order originates in the quantum mechanics of localized electrons. The product state nature of these mean-field stripes is revealed by the rule that the stripes have a preferred density (typically, one hole per domain wall unit cell). This is crucially different here: the “holographic stripes” have no preferred charge density.

In Fig. 3b we highlight that the higher order commensurate plateaux are in fact stable across a range of dopings. This has the implication that the charge density inside the “stripes” continuously varies over a considerable range (Fig. 3c). This is a natural outcome of the absence of localized quantized charge in this entangled matter.

This observation is directly relevant to experiment. It has proven difficult to explain the dependence of the charge order wave vector on doping as observed in the various cuprates in terms of conventional “product state” charge density waves. In most cuprates it appears that the periodicity locks locally at 4 lattice constants in the whole doping range [4, 7, 6, 8] (the exception are 214 stripes which do show a sense of preferred charge density in a limited doping range). Product state, localized electron-based Mott insulator models cannot do this. This is supported by a puzzling result obtained recently in the context of numerical approaches to the doped Hubbard model [21, 22]. This revealed that stripes are ubiquitous, with a similar surprise that these lack a preferred charge density. These heavy numerical methods wire in entanglement, the same generic motive that is hard wired in holography. The locked-in periodicity of stripes can therefore be seen as another compelling indication that strong entanglement underlies cuprate strange metals. We present it as a challenge to both theorists and experimenters to see whether explicit signatures can be found demonstrating that this behaviour is indeed caused by many-body entanglement as suggested by holography.

Last but not least we should clarify how the “insulating” nature of the Mott state and striped phases shows up in the DC resistivity. In Fig. 5a we show the results for a variety of cases including the 1/1 “Mott insulator”. The surprise is that in all cases at temperatures well below $T_c$ the resistivity diverges algebraically instead of exponentially, approximately as $r_{DC} \sim T^{-1.8}$. This is suggestively similar to the slow increase of the resistivity observed in the spin-stripe ordered cuprates [46, 47]. It represents a long standing experimental puzzle, but it could well be just a version of the algebraic behaviour we obtain from holography.

Theoretically, it is a consequence of one of holography’s big mysteries. Closer inspec-
Figure 5: DC resistivity of the holographic Mott insulator. Left panel: Different commensurate states share similar behavior, revealing power law scaling at low temperature. This signals the presence of quantum critical degrees of freedom, which remain ungapped. Right panel: At the critical point no abrupt change of resistivity is seen, suggesting a metal-insulator crossover. The dashed lines show resistivity in the unbroken state without CDW, which is metallic. Temperature is scaled with respect to the corresponding critical temperature of a given state (see e.g. Fig. 3a).

Summarizing, we have identified the holographic analogue of Mott insulators having crucial properties in common with the conventional variety, such as a Mott gap and the mechanism of super exchange interactions. By construction this analogue displays intertwinements of charge order with spontaneous currents and parity breaking of the continuum. Doping this state results in textures that have striking similarities with the stripe phases found in cuprates.

The distinct novel ingredient is that holographic matter should be strongly entangled. This new principle is reflected in specific predictions for unconventional properties due to the “unparticle” nature of this matter that beg to be further investigated in the laboratory.
Firstly, when electron matter is strongly entangled the quantisation of the electrical charge will be washed out, with the ramification that there should be no “quantised” relationship between ordering wave vectors and the number of electrons, either in momentum or real space. This may explain the doping-independence of the charge order in underdoped cuprates. Secondly, we find a restructuring of the quantum critical infrared scaling in the ordered states, reflected in a low temperature algebraic behavior in transport. This is not at all understood theoretically. One interpretation is that spontaneous symmetry breaking from the highly entangled strange metal states does not result in a purely “classical” product state, so it does not gap out all of the degrees of freedom. Instead, there is now a sector of strongly entangled quantum critical states with modified properties. This is what holography predicts. However, holography originates critically in a matrix large $N$ nature of the microscopic degrees of freedom in the field theory $[5]$, lacking any relation with the electrons of condensed matter physics. One relies on the universality of the RG that the IR physics has a larger applicability than matrix large $N$ field theories, and captures strongly entangled physics that may apply here. Is this at work in underdoped cuprates? Our suggestive findings here together with other experimental indications, are a clear call to nail this down by a focused experimental effort.

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A Supplementary material

A.1 The holographic setup

We consider the model of [32] which consists of 3+1 dimensional Einstein-Maxwell theory coupled to a neutral pseudo scalar. Following the conventions of [50, 51], we write the action as

\[
S = \int d^4x \sqrt{-g} \left( R - \frac{1}{2} (\partial \psi)^2 - \frac{\tau(\psi)}{4} F^2 - V(\psi) \right) - \frac{1}{2} \int \vartheta(\psi) F \wedge F + S_{\text{bndy}} \tag{2}
\]

where

\[
S_{\text{bndy}} = -\int d^3x \sqrt{-h} (K - 4 + \psi^2) \tag{3}
\]

Here \( F = dA \) is the field strength associated to the Maxwell field \( A \), while \( h \) is the metric induced at the boundary with extrinsic curvature \( K \). We have checked that the boundary term (3) obtained in [51] suffices to properly renormalize the action [52]. The AdS/CFT dictionary [53, 54, 55] relates the boundary asymptotics of the fields in (2) to the sources and responses of the energy-momentum tensor, electromagnetic currents and parity-odd order parameter in the dual 2+1 dimensional field theory. Following [32, 50, 51, 56], we choose the couplings as

\[
V(\psi) \equiv 2\Lambda + W(\psi) = -6 \cosh(\psi/\sqrt{3}), \quad \tau(\psi) = \frac{1}{\cosh(\sqrt{3}\psi)}, \quad \vartheta(\psi) = \frac{c_1}{6\sqrt{2}} \tanh(\sqrt{3}\psi),
\]

This model is bottom-up, but similar couplings can be obtained from dimensional reduction of supergravity [57]. Note that in these conventions the cosmological constant is \( \Lambda = -3 \) and the mass of the scalar is \( m^2 = -2 \). The equations of motion admit the translational invariant Reissner-Nordström (RN) charged black hole solution which can be written as

\[
ds^2 = \frac{1}{z^2} \left( -f(z) dt^2 + \frac{dz^2}{f(z)} + dx^2 + dy^2 \right), \quad A = \bar{\mu}(1 - z) dt, \quad \psi = 0 \tag{5}
\]

where

\[
f = (1 - z) \left( 1 + z + z^2 - \bar{\mu}^2 z^3 / 4 \right) \tag{6}
\]

In these coordinates the boundary is located at \( z = 0 \) while the horizon is at \( z = 1 \). The chemical potential in the dual theory is given by the constant \( \bar{\mu} \). The Hawking
temperature of this black hole reads

\[ T = \frac{12 - \bar{\mu}^2}{16\pi}. \quad (7) \]

We will be interested in stationary time-independent configurations of the form

\[ ds^2 = \frac{1}{z^2} \left( -Q_{tt} f(z) dt^2 + Q_{zz} \frac{dz^2}{f(z)} + Q_{xx} (dx + Q_{zx} dz)^2 + Q_{yy} (dy + Q_{ty} dt)^2 \right), \quad (8) \]

\[ \mathcal{A} = A_t dt + A_y dy \quad (9) \]

Here, all unknowns are functions of the holographic coordinate \( z \) and the boundary coordinate \( x \). We search for black holes with a uniform spatially constant temperature, which means that in the near horizon all functions must be regular except \( f(z) \). With this assumption, the equations of motion require \( Q_{tt}(1,x) = Q_{zz}(1,x) \), which in turn implies that the surface gravity is constant and given by \( (7) \), see e.g. [37]. Since we are interested in a dual field theory living in flat space, we require the metric to be asymptotically AdS as \( z \to 0 \). The UV boundary conditions on the gauge field will be dictated by our choice of explicit or spontaneous breaking of translations. Following the standard AdS/CFT prescription, we relate the boundary data to the dual field theory one-point functions. In particular, from the UV expansions

\[ Q_{tt} = 1 + z^2 Q_{tt}^{(2)}(x) + z^3 Q_{tt}^{(3)}(x) + O(z^4) \quad (10) \]

\[ A_t = \mu(x) - z\rho(x) + O(z^2) \quad (11) \]

\[ A_y = z J_y(x) + O(z^2) \quad (12) \]

\[ \psi = z^2 \psi^{(2)}(x) + O(z^3) \quad (13) \]

we obtain that the coefficients \( \mu(x) \), \( \rho(x) \), \( J_y(x) \) and \( \psi^{(2)}(x) \) determine the chemical potential, charge density, current density and pseudoscalar parity breaking order parameter of the dual theory, \( Q_{tt}^{(2)} \) is a function of the sources only and the energy density is given by

\[ \epsilon(x) = 2 + \frac{\bar{\mu}^2}{2} - 3Q_{tt}^{(3)}(x) \quad (14) \]

In order to break translations explicitly, we follow [35, 38] and introduce a spatially modulated chemical potential, fixing \( A_t(z = 0, x) = \mu(x) \) with

\[ \mu(x) = \mu_0 (1 + A \cos(kx)) \quad (15) \]
Without loss of generality, we set $\mu_0 = \bar{\mu}$ \cite{58}. Unless otherwise stated, we express the dimensionful parameters of the model, denoted up until now in bold script, in units of $\bar{\mu}$ by making the replacements

$$T = T\bar{\mu}, \quad k = k\bar{\mu}, \quad p = p\bar{\mu}$$ \hspace{1cm} (16)

When $\psi = Q_{ty} = A_y = 0$, all profiles acquire modulation along $x$ solely due to the $x$-dependent boundary conditions, so these solutions represent states which break translations explicitly only. They were termed “ionic lattices” in \cite{38}. As shown there, for small $\omega$, the optical conductivity can be approximated by a Drude peak with finite DC value. Moreover, these lattices are irrelevant in the IR, in the sense that the near-horizon geometry approaches the translationally invariant charged black hole solution as we lower the temperature \cite{39}. Because of this, one can think of the lattice as an UV-based structure (see Fig. 2).

In order for translations to be broken only spontaneously, the boundary conditions need to be translational invariant in the UV, so we take the chemical potential to be constant $\lambda = 0$ in (15), along with the vanishing of the sources dual to the leading terms in $A_y$ and $\psi$, as reflected by (10)-(13); see also \cite{51, 50, 56, 58}. The spontaneous breaking of translations — an IR effect — is due to near-horizon instabilities induced by the topological $\vartheta$-term in (2). Accordingly, the effect of the spontaneous breaking localizes near the horizon of the black hole (see Fig. 2). The features of the resulting spontaneous structure are strongly dependent on the chemical potential $\bar{\mu} \neq 0$ and the value of the coupling $c_1$ in (4): we observe that increasing $c_1$ rises the critical temperature and makes the spontaneous crystal more stable, leading to more pronounced commensurate effects, which we are after. For this reason we choose $c_1 = 17$, as opposed to \cite{32, 50, 51, 56}.

The arising spontaneous structure is characterized by the oscillating values of $A_y$ and $\psi$, which results in the observable staggered currents $J_y(x)$ in the dual theory. At the nonlinear level the $A_t$ component of the gauge field also becomes modulated with twice the momentum of $A_y$ or $\psi$ due to the quadratic interaction in $\vartheta$-term (1), see Fig. 8b. The modulation of $A_t$ corresponds to the formation of a charge density wave (CDW) on the boundary, which we write as

$$\rho_{CDW} = \rho_0 + \delta \rho \cos(px).$$ \hspace{1cm} (17)

\footnote{Holographic models exist where the lattice stays relevant in the IR \cite{58}. We will not consider those here.}
We use the momentum of this CDW $p$ as the defining momentum to describe the spontaneous structure, i.e. the staggered currents have momentum $p/2$. This notation is different from the previous studies [32, 50, 51, 56, 43]. In order to compare the results one has to make a redefinition $p_{\text{here}} = 2p_{\text{there}}$.

It is instructive to first consider spontaneous symmetry breaking perturbatively by taking $\psi, A_y$ and $Q_{ty}$ to be small functions in a Fourier basis of momentum $p$ and zero frequency and linearize. Linear instabilities exist for $T < T_c$ and arrange themselves in a “bell-shaped” curve in the $(T, p)$ plane [32], much as in the 5-dimensional case first discussed in [59], see Fig. 6a. The critical temperature corresponds to the maximum of the bell $T_c^{RN} = 0.147$, attained at a critical momentum $p_c^{RN} = 1.33$. Inside the bell-curve at any given temperature below $T_c$, one can construct non-linear solutions for a range of values of $p$. However, the ones that minimize the (spatially averaged) thermodynamic potential play a special role since they are the ones which dominate the thermodynamic ensemble. These thermodynamically preferred solutions for all $T$ form a line $p_0(T)$ inside the bell-curve, which in general deviates from $p_c^{RN}$.

The aim of this work is to study the interplay of the explicit and spontaneous symmetry breaking phenomena. We can do it in two ways: we can start with an ionic lattice and observe how the instabilities towards the formation of spontaneous structures develop, or begin with a configuration that breaks the translations of the RN solution spontaneously and introduce a modulated source as in (15). Following the former procedure, we need to examine the unstable modes of the pure ionic lattice solution. The study of these unstable modes was undertaken in [43], which revealed an interesting lock-in pattern of the spontaneous to the explicit structure. We reproduced the calculations of [43] for the parameters which will be used in our nonlinear study: $A = 0.7$ and $c_1 = 17$, see Fig. 6b,c.

We observe the lock-in of the spontaneous structure indicated by the plateaux at $p_c/k = 1$ and $p_c/k = 2$. Importantly, the higher order commensurate fractions, i.e. $p_c/k = 3/2$, cannot be observed in the perturbative approach. In the regime where the spontaneous structure is infinitesimal the total solution including the perturbative modes is forced by the lattice to be periodic with momentum $k$. Hence near critical temperature all possible commensurate fractions of $p_c/k$ are integers. This changes as soon as one considers finite amplitude of the spontaneous structure in fully nonlinear approach; the result is Fig. 3a in the main text.
Figure 6:  Left panel: **Perturbative analysis of spontaneous CDW formation:** (a) Blue curve: Unstable modes of the RN solution. Orange curve: the thermodynamically preferred momentum value $p_c(T)$ of the nonlinear solutions.
Right panel: **Pertubative lock-in of the spontaneous CDW with an explicit lattice:** (b): Behaviour of the critical temperature for varying lattice momentum $k$. For large $k$, we approach the translationally invariant value $T_{cRN} \sim 0.15$.
(c) Unstable modes in the presence of potential of amplitude $A = 0.7$ for varying lattice momentum $k$. We observe the plateaux at $p_c/k = 1$ and $p_c/k = 2$.

### A.2 Full backreacted solutions

We construct the fully backreacted nonlinear solutions by observing how a given purely spontaneous structure which arose from RN gets modified as we place it on top of an ionic lattice potential by tuning its amplitude from $A = 0$ to a finite value.

We wish to study the thermodynamic stability of the so constructed configurations, by finding the ones that minimize the spatially averaged thermodynamic potential

$$\Omega(x) = \epsilon(x) - T s(x) - \mu(x) \rho(x),$$  \hspace{1cm} (18)

where $\epsilon$ is the energy density, $T$ the temperature, $s$ the entropy density, $\mu$ the $x$-dependent chemical potential and $\rho$ the charge density.

There is a peculiar technical difficulty, which arises as soon as one addresses the nonlinear solutions. The problem involves two unrelated length scales: the wavelength of the spontaneous structure $\lambda_p = 2\pi/p$ and the wavelength of the background lattice...
\[ \lambda_k = 2\pi/k. \] In order to set up the numerical PDE solver procedure one has to specify only one scale, corresponding to the size of the computational domain with periodic boundary conditions. It is therefore clear that in practice we can only access the values \( \lambda_p \) which are rational multiples of \( \lambda_k \):

\[ \lambda_p = \frac{N_k}{N_p} \lambda_k, \quad N_k, N_p \in \mathbb{N}. \] (19)

In this case one can choose the computation domain of the size \( N_k \lambda_k \) equal to the integer number of lattice periods, which would simultaneously accommodate \( N_p \) periods of CDW. This situation is completely analogous to the “magnetic unit cell” phenomenon, which arises when one considers a crystal in external magnetic field. The unit cell in this case must simultaneously accommodate integer number of the crystal plaquettes and magnetic fluxes, and can become substantially large \[60\]. We see here that the accessible range of spontaneous structure wave-vectors \( k \) is now discrete and its density is limited by the maximal size of the computational domain, which we can handle in our numerical analysis. In what follows we will use computational domains including up to \( N_k = 20 \) periods of the lattice or up to \( N_p = 20 \) periods of the spontaneous CDW\[2\] which allows us to achieve reasonable resolution in our study of the corresponding thermodynamic potentials (see Fig.7).

In practice, in order to construct the solution with \( N_p \) CDW periods on top of the \( N_k \) lattice cells with period \( \lambda_k \) and amplitude \( A \) we first find the spontaneous stripe solution with specific period \( \lambda_p \) from (19) on top of the translationally symmetric background. Then we concatenate \( N_p \) copies of these stripes fitting them in the enlarged calculation domain. At this point we turn on \( N_k \) periods of the background lattice by slowly changing the boundary condition for the chemical potential, eventually achieving the desired value of \( A \) in (15). This adiabatic process preserves the initial number of the CDW periods what we check numerically at every stage by counting the number of zeros of the oscillating \( A_y \) field at the horizon (see Figs.8c,d).

We explore the phase diagram at given temperature by first choosing the period and the amplitude of the explicit ionic lattice. Then we construct a set of nonlinear solutions, corresponding to the spontaneous structures with different wave-vectors \( p \) on top of this lattice. We calculate the thermodynamic potential (18) for these solutions and we find

\[ \text{Note once again, that this corresponds to 10 periods in the spontaneous currents} \]
Figure 7: **The thermodynamic potential of the striped solutions on top of the lattice:** Values shown are for lattice momentum $k = 1.06 \mu$ and various amplitude $A$ at $T = 0.01 \mu$. The minima (shown with red diamonds) are shifted from the spontaneous value to the commensurate value as the lattice amplitude is increased. Dashed line shows the energy profile of the spontaneous solution in translationally symmetric background.

A good check of our calculation is that, at $A = 0$ our solutions follow the curve, which one would obtain in the study of the spontaneous striped solutions on the homogeneous RN background [51, 50, 56]. We have checked that for $c_1 = 9.9$ our results coincide with Fig. 2 in [50]. Even though we have access only to the discrete set of values, they lie on the smooth curves which have a well defined minima.

One can see that as the amplitude rises, the minimum smoothly shifts from the incommensurate to commensurate point. Thus by increasing the amplitude we observe the smooth, at least second order phase transition. The different commensurate points, which are thermodynamically stable at different temperatures and charge density are shown on Fig. 3a in the main text.
A.3 Commensurate state

Let us first focus on two integer value commensurate states: the leading 1/1 Mott insulator and the higher 2/1 commensurate state. The features of the 1/1 state (Fig. 8a) are mostly similar to those of the pure spontaneous crystal with an important difference: now the periodicity of the overall structure is anchored by the ionic lattice wavelength $\lambda_k$. The staggered currents are seen, but they are now enhanced near the maxima of $\rho(x)$ and suppressed at the minima. This leads to the effective localization of the currents. On the other hand, the spontaneous structure brings an excess of total charge density as compared to the pure lattice (shaded region on Fig. 8a, color on Fig. 1a-d). This allows us to define a “unit of CDW charge”, $q_{CDW}$, as the integrated excess charge density in the unit cell

$$q_{CDW} \equiv \frac{k}{2\pi} \int_0^{2\pi/k} (\rho_{Mott}(x) - \rho_{lattice}(x))$$

An important feature is that in holography $q_{CDW}$ assumes continuous range of values depending on the external conditions, while in the hard Mott insulator it would be quantized in units of the electron charge.

Now we address to the higher commensurate state 2/1 (see Fig. 8b). Note that the localized peaks of the $J_y$ current are all aligned. The reason is that the 2/1 commensurate state has twice the number of CDW periods as compared to the 1/1 state (see near horizon profile on Figs. 8c & d). Every odd positive current peak is thus enhanced by the charge density, but the negative currents are dispersed and do not show well defined peaks. Nonetheless, the total current remains zero. Figure 8b shows that the total charge density of this “aligned” state is larger than that of the staggered one. This is due to the fact that it possess twice the number of spontaneous CDWs per unit cell, each bringing contributions of order $q_{CDW}$ to the total charge density. This feature allows us to denote this state as 100% doped and define the doping rate as in the main text.

A.4 Incommensurate state

As we mentioned earlier, the numerical computation in the incommensurate state is technically more involved, as the numbers of periods in (19) can become large. The isolated discommensuration is found as a solution which is closest to commensurate $\frac{N_p}{N_k} = \frac{1}{1}$ value. Given that

$$\left| \frac{N_p}{N_k} - \frac{1}{1} \right| = \frac{|N_p - N_k|}{N_k},$$

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Figure 8: Charge and current profiles of various states: (a) The explicit lattice. (b) The spontaneous CDW. The modulation of the charge density is strong in the explicit lattice, since it is directly sourced and relatively weak in the pure CDW since it is subleading to the currents order, which drives the instability.
(c) The 1/1 commensurate locked state: the Mott insulator, (d) The 2/1 commensurate locked state: the 100% doped Mott insulator. Note the staggered current pattern in the former case and aligned in the latter. The total current is zero in both cases. The charge density of the lattice in absence of CDW is shown by the green line. The shaded region shows the excess charge due to CDW, which is manifestly positive in both cases.
(e) The horizon profile in the gravitational theory of the 1/1 state. (f) The horizon profile in the gravitational theory of the 2/1 state. Show is the horizon value of $E_{hor}$ of the electric field strength, whose value near UV boundary defines the charge density, and $y$-component of the gauge field $A_y$, related to the current $J_y$ in UV. Near horizon the effect of the lattice is weak and the structure of the locked in CDW (number of its periods) is clearly seen.
we will choose $N_k = N_p - 1$ and maximal $N_p$ reachable by our numerics $N_p \leq 20$. The incommensurate solution with 20 CDW’s per 19 lattice periods would have exactly one excess CDW period per 19 unit cells as compared to the commensurate state. By inspecting this solution (Fig. 2) we see, that the solution profile coincides with the commensurate state almost everywhere except from the finite size region in the core, where this excess of one period of CDW is accounted for. We can also study the TD potential and charge density of such solution as compared to the pure commensurate state, Fig. 9, which shows clearly that this incommensurate solution can be seen as a commensurate state with one localized soliton on top of it. This soliton is a direct analogue of discommensuration studied in the context of charge density waves in \[61, 41\].

As it is apparent on Fig. 9 a single discommensuration possess a finite net charge

\[ q_{\text{disc.}} = \frac{1}{19\lambda k} \int_0^{19\lambda k} \rho_{20/19}(x) - \rho_{1/1}(x) dx, \]

(22)

which is manifestly positive, is of order $q_{\text{CDW}}$ \[20\] and has a direct analogue in the hard Mott insulator model. Indeed, the discommensurations in the conventional Mott state are associated with one extra or missing electron in the unit cell. In this case the charge of $q_{\text{disc.}}$ would be exactly 1. The holographic model, on the contrary, allows for continuous variations in $q_{\text{disc.}}$, see Fig. 3c.

One can see that further deviation from the commensurate point 1/1, according to \[21\], is achieved by rising the density of discommensurations. At higher commensurate points they can form a super lattice with a, period of several ionic lattice constants $a$ (Fig. 4c). For instance, the discommensuration lattice with $3a$ period corresponds to the commensurate fraction $p/k = N_p/N_k = 4/3$, which is stable at low temperature in a window of doping levels as shown on the phase diagram Fig. 3a.

A.5 Optical Conductivity

In order to further investigate the properties of the above described solutions, we extract their electric conductivity as a function of frequency, $\sigma(\omega)$, along the $x$-direction, closely following \[40\]. The optical conductivity in inhomogeneous setups has also been studied in e.g. \[37, 38, 39\].

Extracting $\sigma(\omega)$ is a considerably involved numerical problem, which requires to first construct a given background to sufficient accuracy and then solve the perturbation equations on top of this solution. We found that our usage of the standard MachinePrecision
Figure 9: Profile of the contribution to thermodynamic potential and charge density of a single discommensuration. This solution has one excess period of the CDW per 19 unit cells, corresponding to the commensurate fraction $p/k = 20/19$ at $A = 0.7, T = 0.01\mu$. The positive definite total charge of the discommensuration is seen. The size of discommensuration, as obtained from the thermodynamical potential density is about 5 unit cells. All values are measured in units of $\mu$.

computations of Wolfram Mathematica [62] limits the reliability of our AC conductivity results to the region in the vicinity of the critical temperature. For the results within this region we successfully perform a set of numerical consistency checks, which includes vanishing of the constrains and gauge fixing conditions. We have also checked that our results satisfy the sum rule on the integrated spectral weight: $\lim_{\omega \to 0} S(\omega) \rightarrow 0$, where

$$S(\omega/\mu) \equiv \int_{0}^{\omega/\mu} (Re[\sigma(\omega')] - 1)d\omega'.$$

(23)

If one is interested only in the DC conductivity, $\sigma_{DC} = \sigma(\omega = 0)$, it is possible to largely simplify the calculation since we can obtain a formula for this observable solely in terms of the horizon data [39, 63, 64, 65, 66]. The relevant formula for our system was obtained in [66], which we have rederived in full agreement. Additionally, for all the cases we have studied, the limit $\omega \to 0^+$ of $\sigma(\omega)$ agrees with the computation of $\sigma_{DC}$ in terms of the horizon data, which serves as another test of our numerics.
A.6 Numerical techniques and Precision control

In the present study we rely heavily on numerical analysis of the holographic nonlinear solutions. Moreover, in order to study the phase diagram and cover the parameter space we have to obtain several thousands of solutions, with some of them requiring quite large calculation grids in the spatial direction. This situation places very strict requirements on the numerical techniques which we use, the precision and the accuracy of the results.

We have chosen a single patch pseudospectral scheme in the holographic direction and used Wolfram Mathematica\(^\text{\textregistered}\) to implement the numerical algorithm. The main limitation which we encounter is the necessity to work with MachinePrecision numbers in the compiled function, which eventually limits the precision of our results. Element-wise operations can be efficiently compiled with Compile, which brings up a spectacular acceleration. We use precompiled linear algebra solvers and sparse matrices, which delivers decent speed of calculations.

It should be noted that direct inversion (Newton-Raphson method) for the case of pseudospectral discretization is extremely demanding for large grids, so we have decided to use a relaxation scheme instead. We employ the differential operator evaluated in the low order finite difference derivative scheme as a preconditioner. The result is a nonlinear Richardson relaxation with Orszag preconditioning (See Sec. 15.14 and eq.(15.115) in \cite{67}). At the end of the day, we managed to optimize the calculation scheme to the extent that it takes about half an hour to obtain the precise solution on our largest grid of size \(\sim 330_x \times 80_z\) (pseudospectral) using a single core of a laptop CPU (Intel Core i7-5600U @ 2.60GHz ) and about 3 Gb of RAM.

As one can see from our results, the difference between the free energies of the solution with spontaneous structure and the one without is just of order of a few per cents of the free energies themselves. This means that in order to reliably study this difference, we need to evaluate the free energies with accuracy of at least \(10^{-4}\). We observe that for a single patch Chebyshev grid the maximum \(N_y\) resolution is limited by the rounding errors at \(N_y = 80\). The accuracy of the thermodynamical potential for a grid of this size is about \(10^{-7}\). We used this value as a numerical error estimate throughout the present study and it has proven to be sufficient to obtain our main results. One should keep in mind that in the numerical procedure we solve the modified DeTurk equations. Thus, it must be checked that the Einstein equations are satisfied, which we do by two independent measures: the maximal value of the trace of the Einstein equations and the maximum...
value of the norm of a DeTurck vector. For temperatures $T > 0.01$, these values are both of order $10^{-7}$, which is quite satisfactory [39].

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