Exciton Proliferation and Fate of the Topological Mott Insulator in a Twisted Bilayer Graphene Lattice Model

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Topological Mott insulator (TMI) with spontaneous time-reversal symmetry breaking and nonzero Chern number has been discovered in a real-space effective model for twisted bilayer graphene (TBG) at 3/4 filling in the strong coupling limit [1]. However, the finite temperature properties of such a TMI state remain illusive. In this work, employing the state-of-the-art thermal tensor network and the perturbative field-theoretical approaches, we obtain the finite-$T$ phase diagram and the dynamical properties of the TBG model. The phase diagram includes the quantum anomalous Hall and charge density wave phases at low $T$, and a Ising transition separating them from the high-$T$ symmetric phases. Due to the proliferation of excitons – particle-hole bound states – the transitions take place at a significantly reduced temperature than the mean-field estimation. The exciton phase is accompanied with distinctive experimental signatures in such as charge compressibilities and optical conductivities close to the transition. Our work explains the smearing of the many-electron state topology by proliferating excitons and opens the avenue for controlled many-body investigations on finite-temperature states in the TBG and other quantum moiré systems.

Introduction.— Since the discovery of correlated insulators and superconducting states in the magic-angle twisted bilayer graphene (TBG) [2, 3], the quantum moiré systems [4–6] become an active playground for experimental and theoretical investigations on exotic phenomena [7–36]. The intriguing quantum effects in TBG and transition metal dichacogenide (TMD), besides the superconductivity, encompass a wide range including the orbital ferromagnetism [9, 15], (emergent) quantum anomalous Hall (QAH) effect [15, 16, 34, 37, 38], large (iso)spin entropy and Pomeranchuk effect [19, 20], etc. Such a plethora of quantum states is believed to originate from the interplay of strong electron correlation and fragile band topology [39–53]. Many theoretical models have been put forward to address these interesting phenomena, and among the positive semidefinite Hamiltonians that are proposed [46, 50, 54, 55], a real-space effective model by Kang and Vafek (KV) is able to integrate both key ingredients [54, 56]. The KV model and its variants have been investigated via quantum Monte Carlo simulations, which showed certain correlated insulating states such as the inter-valley coherent and quantum valley Hall states, etc, are natural ground states at integer fillings and particularly the charge neutral point (CNP) of the TBG systems [57–60].

Away from CNP, density matrix renormalization group (DMRG) simulations upon the KV model revealed that a QAH state can emerge purely from interactions at 3/4 filling [1], which constitutes the long-sought-after topological Mott insulator (TMI) [61]. Along with other scenarios [47, 51, 62] that give rise to the Chern insulators at odd fillings, such a bona fide TMI state provides a strong coupling explanation of the observed quantized Hall conductance in experiments [15, 16]. Although the ground state with non-trivial topology in the TBG model is known, the low-energy collective excitations and the experimentally relevant finite-$T$ phase diagram are still absent. As the QAH state spontaneously breaks time reversal symmetry (TRS), a thermal phase transition is expected to take place between the topological QAH and high-$T$ symmetric phase. However, a naive estimate of the transition temperature $T_c$ according to the band gap [1] — based on the mean field theory — leads to a value of the order of 100 K, higher than the experimental value ($\lesssim 10$ K) by an...
order of magnitude [9, 15]. The difference is believed to stem from the intertwinement of electronic interaction and thermal fluctuations.

To elucidate the thermal melting of the topological phase and the associated phase diagram, we perform accurate finite-T many-body calculations with the exponential tensor renormalization group (XTRG) method [63, 64]. XTRG calculations uncover an Ising-type thermal phase transition between the low-T QAH phase and the symmetric phase, and a critical temperature reduced by one order of magnitude compared to the mean-field estimation. These observations are further explained by a field-theoretical approach, which unveiled the emergence of a collective mode of a bounded particle-hole pair—exciton. The excitons are found to have a rather flat and low-lying dispersion and proliferate as the temperature elevates, playing an essential role in the melting of the low-T phase. The proliferation of excitons leads to a modulation of electron-hole correlations in real space. The entire finite-T phase diagram including the low-T QAH and CDW phases and the intermediate exciton proliferation phase, is accurately mapped out via both XTRG and field-theoretical approaches.

These results extend the understanding of the zero-temperature phase diagram to finite-temperature and dynamical effects of collective excitations [32, 65], beyond the exactly solvable limits [51, 52, 54, 65–67]. Distinct signatures of the exciton proliferation phase are also revealed to bridge the experimentally accessible observables with theoretical understanding.

**Real-space TBG model, thermal tensor networks, and field-theoretical approach.** — The KV model considered here is described by the interaction-only Hamiltonian

$$H = U_0 \sum_O (Q_O + \alpha T_O - 1)^2,$$

where $U_0 = 1$ sets the energy unit ($\sim 40$ meV in realistic system [1]), the cluster charge term $Q_O \equiv \frac{1}{4} \sum_{\langle iO \rangle} c_i^\dagger c_{i+1}$ counts the numbers of electrons in each hexagon [c.f., Fig. 1(a)], and $T_O = \sum_{\langle iO \rangle} [(-1)^1 c_i^\dagger c_{i+1} \pm \text{h.c.}]$ represents the assisted hopping term with alternating sign [c.f. Fig. 1(b)]. The results of the present work are mainly based on the YC4 × L geometry with $L = 12$, where the lattice is under periodic/open boundary condition along vertical/horizontal direction [c.f. Fig. 1(d) for a typical YC4 geometry]. We focus on the 3/4 filling of the TBG flat bands with projected Coulomb interaction and correspondingly in Eq. (1) this means the electron number $\langle n_i(\equiv c_i^\dagger c_i) \rangle = 1/2$ with the valley and spin degrees of freedom polarized. Ref. [1] identified a CDW insulator and a topologically nontrivial QAH insulator in the ground state of the model, separated by a first-order transition at $\alpha \simeq 0.12$.

Here, we explore the finite-T properties of the TBG model with the XTRG method [63, 64], which constitutes an accurate many-body method at finite temperature, previously applied to simulate frustrated quantum magnets [71–73] as well as correlated fermions at both half filling and finite doping [74]. We retain up to $D = 1000$ states, which renders the truncation errors $\delta < 10^{-4}$ down to low-T regime.

We also employ the Gaussian state theory and field-theoretical approach to obtain both thermal and dynamical properties. The thermal state is approximated by a Gaussian ansatz, i.e., the optimal mean-field state, where the order parameters (i.e., all the single particle correlation functions) minimizing the free energy can be obtained efficiently via a set of flow equations [75, 76]. The particle-hole excitation spectrum can be obtained via the fluctuation analysis [77], or alternatively the analytic structure of the scattering $T$-matrix, i.e., the renormalized electronic interaction [c.f. the ladder diagram in Fig. 1(e)]. As the temperature increases, the interaction is strongly renormalized, which drastically modifies the self-energy [c.f. the Hartree-Fock-like contribution in Fig. 1(f)] of the single particle Green function. More details on methodologies are presented in the Supplemental Materials (SM) [85].

**Finite-temperature phase diagram.** — Fig. 2(a) summarizes our finite-T phase diagram, where the low-T phases include the CDW and QAH states, and the symmetric phase can be divided into two regimes, with the orange intermediate-T one acquiring pronounced collective (exciton) excitations and the red high-T state being trivial. As we will show below, there is a crossover between the intermediate-T and high-T regimes, while the intermediate-T and low-T phases are separated by a second-order phase transition of Ising universality. Moreover, the two low-T phases, i.e., the CDW and QAH ones, are separated by a first-order transition extending from the transition point $\alpha \simeq 0.12$ found in previous DMRG study [1].

In Fig. 3(a), the specific heat $c_V$ shows pronounced peaks around $T_c \simeq 0.041$ for $\alpha = 0.2$, indicating the existence of
Melting of the QAH and CDW states.— To detect the QAH phase, we calculate the current correlation, \( C_f(d) = \langle J_0 J_d \rangle \), where \( J_0 \equiv \frac{1}{2} \sum_{i \in \Omega_0} (c_i^\dagger c_{i+2} - \text{H.c.})/2 \) is the average of all the next-nearest-neighbor (NNN) currents [cf. purple dashed arrows in the inset of Fig. 3(b)] inside the selected hexagon \( \Omega_0 \) in the \( L/4 \)-th column of the cylinder, and \( \Omega_d \) is the \( d \)-th hexagon to the right of \( \Omega_0 \). We find \( C_f(d) \) is nearly a constant in \( d \) inside the QAH state [85], indicating the existence of a long-range order. For \( T > T_c \), \( C_f(d) \) decays exponentially with \( d \). In Fig. 3(b) we show the current correlation at a sufficiently long distance in the QAH state, i.e., \( C_f(d = 6) \) versus \( T \), which quickly drops and indicates the vanishing of QAH order above the \( cV \) peak \( T_c \simeq 0.041 \). Notably, the mean-field results [depicted as the grey dots] overestimate the vanishing of QAH order above the \( cV \) peak \( T_c \simeq 0.041 \). In Fig. 3(c), we plotted the \( C_f L^{2\beta/\nu} \) versus \( T \) and identify the critical temperature \( T_c \simeq 0.034 \) as the crossing points between curves of different system sizes. This is the \( T_c \) at the thermodynamic limit and slightly different from the peak in the specific peak in Fig. 3(a) for one system size. Then we rescale the \( x \)-axes as \( tL^{1/\nu} \) and thus see perfect data collapses within the critical regimes in the main panels of Fig. 3(c).

Electron-hole correlation and exciton proliferation.— As temperature rises above \( T_c \), the excitons proliferate and result in nontrivial features on the charge correlations. As shown in Fig. 1(d) with \( T = 0.244 \) and \( \alpha = 0.2 \), we place a hole at the very center of the lattice, and find electrons exhibit bunching and anti-bunching modulation behaviors as moving away from the hole, evidencing the existence of particle-hole bound states — excitons — in the system. Such peculiar charge correlations can be quantitatively reflected in the electron-hole correlation \( g_2^{nh}(d) = \langle \hat{n}_i \hat{n}_{i+d} \rangle / \langle \hat{n}_i \rangle^2 \), with \( \hat{n}_i = 1 - \hat{n}_i \), and measured between two sites (“0” and “2”) separated by distances \( r = d(\delta_1 - \delta_2) \) [cf. Fig. 3(d)], which show increasing correlation whose “sign” changes for different distance in the regime \( T > T_c \), and shows extremum values at an intermediate temperature \( T_{ex} \simeq 0.3 \) (around the mean-field transition temperature), at which the excitons can be easily excited since the single-particle gap now roughly equals the thermal energy scale. The electrons and holes at nearest sites belonging to the same sublattice [i.e., connected via \( (\delta_1 - \delta_2) \) as shown in Fig. 1(d)] attract each other, while at further distance like \( d = 2 \) they repeal, reflecting the strong influence of excitons in the thermal states. As distance further enhances, e.g., \( d = 3 \), the electron-hole correlations become rather weak, showing that the excitons are indeed quite local. We note that, the charge correlation decays exponentially with distance, and thus the oscillation behavior is not attributed to Friedel oscillations. When the temperature further elevates and goes beyond
$T_{\text{ex}}$, even the short-range charge correlations get smeared by strong thermal fluctuations, all correlations decay ($g_{2h}^{\text{ex}} \to 1$) at about $T_{\text{c}} \sim 1$. Above this crossover temperature, i.e., in the high-$T$ regime, specific heat $c_V$ exhibit $\sim 1/T^2$ scaling as illustrated in Fig. 3(a) [85].

We also study the compressibility $\partial n/\partial \mu$ by adding a chemical potential term to the KV model [85]. In Fig. 3(d), the compressibility exhibits a steep jump above $T_{\text{c}}$ and keeps an enhanced value inside the exciton regime. This is a direct result of the exciton proliferation above $T_{\text{c}}$, where the formation of excitons (bosonic bound state) significantly enhanced the compressibility. Such a steep enhancement can be measured in the quantum capacitance and scanning single electron transistor experiments [68–70]. In fact, the compressibility enhancement above the correlated insulators (CDW and QAH phases), is qualitatively consistent with the experimental observation at the same $3/4$ filling of TBG [70].

**Dynamical signature of excitons.**— At the mean-field level, the gap between the conductive and valence bands (white dots in Fig. 4 (a)) in the QAH phase is about $0.5U_0$ (at the $\Gamma$ point in BZ), giving rise to a transition to the disorder phase at much higher temperature $T_{\text{c}} \sim 0.2$ (of the scale of 100 K for realistic materials), at the scale of the ground state band gap [1]. However, our XTRG computation finds a much lower transition temperature $T_{\text{c}} \sim 0.04$ ($\sim 10$ K) by one order of magnitude, which agrees with the experimental results [9, 15] implying the failure of the mean-field theory at finite temperatures.

To explore the mechanism of such low transition temperature, we perform the diagrammatic calculation (see details in SM [85]) on the $T$-matrix in the particle-hole channel and its correction to the self-energy of single-particle Green functions. The poles of the $T$-matrix determine the exciton spectrum. As shown by the green diamonds in Fig. 4 (a) at a representative temperature $T = 0.08$, the exciton has a much lower energy $E_{\text{ex}} \sim 0.08$ than the mean-field gap. As a result, at the finite temperature comparable with $E_{\text{ex}}$, many excitons are proliferated by thermal fluctuations, and the scattering with excitons strongly affects single electron behaviors in conductive and valence bands. The effect of excitons to the single particle Green function can be characterized by the $T$-matrix in the Hartree-Fock correction to the self energy (Fig. 1(e) and (f)). In Fig. 4 (a), we show such renormalized spectral function $A_k^{\text{ex}}(\omega)$ for electrons in conductive and valence bands at $T = 0.08$, which displays much smaller band gap than that from the mean-field theory. In Fig. 4(b,c), the spectral functions of electrons in the valence band at different temperatures show the reduced quasi-particle weight and the broadened peak as $T$ increases. It is remarkable that at the temperature inside the exciton regime, the collective mode assists the valence electron to tunnel across the band gap and redistribute in the positive frequency region. This intriguing feature is the signature of the electron dressed by the cloud of proliferated excitons, which can be probed via spectroscopy. The absorption spectra of probe light display peaks at the exciton frequencies ($\sim 100$ GHz shown in Fig. 4). Due to the strong exciton dressing, the current correlation function is thus highly reduced, as shown by the red dots in Fig. 3 (b). Accompanied with the results in Figs. 1 (d) and 3 (d), our results provide a direct observation of proliferated excitations in the $3/4$ filling setting of TBG model. We also confirm, a small kinetic term will not qualitatively change the exciton physics observed here [85].

**Discussion.**— We extend the studies of the TBG model to the finite-temperature properties and collective excitations. In particular, the excitons formed by a pair of quasi-particle and hole proliferate at intermediate temperatures, which significantly influences the charge correlations and provide a mechanism to melt the QAH phase. We therefore reconcile the large quasi-particle band gap and small QAH transition temperature observed in experiments. The excitons, as collective excitations due to Coulomb interactions, have been investigated and discussed in bilayer graphene [78, 79], TBG [67, 80], as well as the recent observation of the QAH in TMD heterobilayers [34]. We note that, the exciton physics here is a distinct feature of flat-band system, different from the Haldane-Hubbard model (see, e.g., Ref. [83]) where the excitons comprised of band electrons and holes do not experience a prolif-
eration upon rising temperature \cite{85}. Our work here shows the emergence of excitons in the strong coupling limit in a TBG lattice model, proposing intriguing exciton physics such as the charge compressibility and the spectral fingerprint in both single-particle and collective models, waiting to be explored in future experiments of quantum moiré systems. We point out that, the valley and spin degrees of freedom, which may give rise to other neutral collective modes (e.g. magnon) and possible Pomeranchuk physics, are omitted in the present model and will be addressed in a future study.

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In Supplementary Materials Sec. I, we briefly summarized exponential tensor renormalization group method, its measurements on thermodynamic quantities, and adaption to fermion systems are introduced. Sec. II is devoted to the details of determination of crossover temperature between intermediate-T regime and the high-T regime. In Sec. III, we present the current correlation calculations. In Sec. IV, we discuss the thermodynamics of the system in the small-α regime. In Sec. V, we present more thermodynamic data for various α values. In Sec. VI, we include the electronic compressibility calculations. In Sec. VII and Sec. VIII, the Gaussian state approach and the implementation of perturbative field theoretical calculations on the single-particle and collective excitations are presented. In Sec. IX, we discuss the thermodynamics of Haldane-Hubbard model. The Supplementary Materials include references [1, 63, 64, 75, 76, 81–84].
Section I: Exponential Tensor Renormalization Group Method

As shown in Fig. S1, the main idea of exponential tensor renormalization group (XTRG) [63, 64] method is, to first construct the initial high-temperature density operator \( \hat{\rho}_0 \equiv \hat{\rho}(\tau) = e^{-\tau \hat{H}} \) with \( \tau \) being an exponentially small inverse temperature, which can be obtained with ease via Trotter-Suzuki decomposition [81] or series-expansion methods [82]. Subsequently, we evolve the thermal state exponentially by squaring the density operator iteratively, i.e., \( \hat{\rho}_n \cdot \hat{\rho}_n \equiv \hat{\rho}(2^n \tau) \cdot \hat{\rho}(2^n \tau) \rightarrow \hat{\rho}_{n+1} \). Following this exponential evolution scheme, one can significantly reduce the evolution as well as truncation steps, and thus can obtain highly accurate low-\( T \) data in greatly improved efficiency.

In XTRG simulations, we compute the internal energy per site

\[
 u(T) \equiv \frac{1}{N} \frac{\text{Tr}[H \cdot \rho(T)]}{\text{Tr}[\rho(T)]},
\]  

(S1)

where \( H \) is the Hamiltonian [c.f. Eq. (1)] and \( \rho(T) \equiv e^{-H/T} \) is the density matrix of the system with \( N \) sites, and the specific heat via the derivative of internal energy, is

\[
 c_V(T) \equiv -\frac{\partial u(T)}{\partial T} = \frac{\partial u(\beta)}{\partial \ln \beta},
\]  

(S2)

with \( \beta \equiv 1/T \) the inverse temperature.

When adapting XTRG to fermion systems, one should take care of the fermionic sign of exchanging two electrons. In this work, we are working on the many-body basis \( |n_1 n_2 \cdots n_N \rangle \equiv (c_1 \dagger)^{n_1} \cdots (c_2 \dagger)^{n_2} \cdots (c_N \dagger)^{n_N} |\Omega \rangle \), where \( n_i (\in \{0, 1\}) \) is...
the number of electrons at the site $i$ and $|\Omega\rangle$ is the vacuum state. Generically in this basis, the one-body operator $c_i^\dagger c_j$ (assuming $j < i$) requires an sign $\Pi_{i=j+1}^{\Omega}(-1)^{n_i}$, in addition to transform the state $|n_1\cdots n_j\cdots n_i\cdots n_N\rangle$ to the state $|n_1\cdots n_j-1\cdots n_i+1\cdots n_N\rangle$. As shown in Fig. S2, such fermion-sign structure can be encoded in XTRG readily in a matrix product operator with bond dimension $D = 1$.

**Section II: Crossover between exciton proliferation regime and high-$T$ regime**

![Graph](image)

**FIG. S3.** In a YC4×12 system for (a) $\alpha = 0.1$, and (b) $\alpha = 0.2$, specific heat $c_V$ curves are shown versus temperature $T$ in a double-logarithmic scale. At high-temperature limit, $c_V$ behaves as $\sim T^{-2}$, and is fitted by the red dashed line $c^V_\alpha$. Panels (c) and (d) show the deviation $\delta c_V = |c_V - c^V_\alpha|$ as functions of temperature $T$. The crossover temperature between intermediate-$T$ regime and the high-$T$ one is determined by a threshold $\epsilon = 10^{-2}$.

In this section, we will discuss the determination of the crossover between the intermediate-$T$ exciton proliferation regime and the high-$T$ gas-like regime. In a high temperature $T = 1/\tau$ (i.e., a small inverse temperature $\tau$), the internal energy density of the system

$$u(\tau) = \frac{1}{N} \frac{\text{Tr}[H \cdot \rho(\tau)]}{\text{Tr}[\rho(\tau)]} = \frac{1}{N} \frac{\text{Tr}(H \cdot e^{-\tau H})}{\text{Tr}(e^{-\tau H})},$$

via Taylor expansion, can be expressed as

$$u(\tau) = \frac{1}{N} \left[ \frac{\text{Tr}(H)}{Z^0} - \frac{\text{Tr}(H^2)}{Z^0} \tau + \left( \frac{\text{Tr}(H)}{Z^0} \right)^2 \tau + O(\tau^2) \right].$$

Thus in the large-$T$ limit, it yields

$$c_V \equiv \partial u/\partial T = (\partial u/\partial \tau) \cdot (\partial \tau/\partial T) \sim T^{-2}$$

for specific heat.

As shown in Fig. S3, we show the specific heat $c_{V}$ of a YC4×12 system at both $\alpha = 0.1$ and $\alpha = 0.2$, which show predominant power-law decay at high-$T$ regime. As indicated by the red dashed lines in Fig. S3(a,b), we find the high-$T$ data asymptotically follow $c^h_{V,\alpha} = 0.034T^{-2.005}$ and $c^h_{V,\alpha} = 0.055T^{-2.005}$ for $\alpha = 0.1$ and $\alpha = 0.2$ respectively, which are well consistent with the large-$T$ limit. We thus determine the crossover temperature $T_h$ between the high-$T$ regime and intermediate-$T$ regime, by computing the deviation of the specific heat from the high-$T$ behavior, i.e., $\delta c_V = |c_V - c^h_{V,\alpha}|$. To be more specific, we classify those temperatures at which $\delta c_V > \epsilon = 10^{-2}$ as intermediate-$T$, and otherwise as high-$T$. 

...
Section III: Detailed current-current correlation calculation

As shown in Fig. S4, we calculate the current-current correlation function $C_J(d)$, defined in the main text. In a YC4×12 system at $\alpha = 0.2$, $C_J$ establish a plateau over distance $d$, in the quantum anomalous Hall (QAH) region, i.e., for $T < T_c \simeq 0.041$, whereas it decays exponentially for $T > T_c$. It means that, the lower-$T$ region for the large $\alpha$ cases spontaneously break the time-reversal symmetry, manifesting the QAH state. On the other hand, for the small-$\alpha$ case ($\alpha = 0.1$ here), $C_J(d)$ decays exponentially for both regions of $T < T_c \simeq 0.022$ and $T > T_c$.

Section IV: More details on the CDW data

In this section, we discuss more detailed thermodynamics results of the CDW phase for $\alpha < \alpha_c$. In Fig. S5(a), we show the specific heat $c_V$ curve vs. temperature $T$, which peaks at $T_c = 0.022$ predominantly, indicating a phase transition there. We also compute the density-density correlation function $\langle \hat{n}_i \hat{n}_0 \rangle = \text{Tr}(\hat{\rho} \hat{n}_i \hat{n}_0)$ at various temperatures, with site 0 being fixed at a center site and site $i$ running over the lattice. The charge structure factor

$$C_n(k) = \frac{1}{N} \sum_i e^{-ik \cdot r_0} \langle \hat{n}_i \hat{n}_0 \rangle - \langle \hat{n}_i \rangle \langle \hat{n}_0 \rangle,$$  

(S3)
is found to peak at $M \equiv (0, \pm \frac{\pi}{2})$ point in the Brillouin zone (BZ). Note there are three pairs of equivalent $M$ points in the BZ while only one of them is preferred by the cylindrical geometry, c.f., Ref. [1]. As shown in Fig. S5(b), for the low-$T$ CDW state, the CDW order parameter $C_n(M)$, structure factor at the $M$ point, experiences a sudden drop at the transition temperature $T_c \approx 0.022$ upon heating, the same temperature as the specific heat peak locates in Fig. S5(a). Again, the mean-field results overestimate $T_c$, which is believed to be corrected by the higher-order perturbative calculation towards the XTRG results.

To address the universality class of phase transitions between the CDW phase that breaks $Z_2$-type (discrete translational) symmetries to the symmetric phase at higher temperatures, we follow the same line as in the main text for the current-current correlation $C_f$, and perform the finite-size data collapsing of $C_n(M)$ in Fig. S5(c). As a function of $t (\equiv \frac{T - T_c}{T_c})$ and system size $L$, we denote it as $C_n(M; t, L)$. We again using the 2D Ising critical exponents $\beta = 1/8$ and $\nu = 1$ as the CDW phase breaks $Z_2$ symmetry. In the inset of Fig. S5(c), we plotted the $C_n(M; t, L) L^{2\beta/\nu}$ versus $T$ and identify the critical temperature $T_c \approx 0.024$ as the crossing points between curves of different system sizes. The so-estimated $T_c$ is again very closed to the peak of specific heat. Then we rescale the $x$-axes of Fig. S5(c) as $t L^{1/\nu}$ and see perfect data collapses within the critical regimes in the main panel of Fig. S5(c).

In Fig. S5(d), we see that the $g^{nh}_2$ correlation increases rapidly as the long-range anti-bunching correlation melts at the CDW transition temperature. Other than that, we also observe similar particle-hole correlation modulation in the exciton-proliferated intermediate-$T$ regime above the CDW phase, as in Fig. 3(d) of the main text. In Fig. S5(d), we also perform the calculation on the compressibility $\partial n_i / \partial \mu$ by adding a chemical potential term to the KV model. Similarly, the compressibility exhibits a steep jump above $T_c$ and keeps an enhanced value inside the exciton regime.

### Section V: Detailed $\alpha$-scan for phase diagram

![Graph showing phase diagram](image-url)

**FIG. S6.** In a $\text{YC4}\times12$ system for various $\alpha = 0.08, 0.12, 0.14, 0.16, 0.18$, the specific heat $c_V$ (the first row), the charge density structure factor $C_n(M)$ (the second row), and the current-current correlation $C_f(d = 6)$ (the last row), are shown versus temperature $T$.

In this section, we will show more results of specific heat $c_V$, charge structure factor $C_n(M)$, and the current-current correlation function $C_f(d = 6)$ for various $\alpha$ other than $\alpha = 0.1$ and 0.2, as complement to the main text. As shown in Fig. S6, in all these cases ($\alpha = 0.08, 0.12, 0.14, 0.16, 0.18$) the specific heat $c_V$ curves (the first row) clearly show sharp peaks, above which either $C_n(M)$ ($\alpha = 0.08$ and 0.12) and $C_f(d = 6)$ ($\alpha = 0.14, 0.16$ and 0.18) quickly vanish.

### Section VI: Electronic compressibility calculations

In this section, we add a chemical potential term to the original Kang-Vafek model [Eq. (1) in the main text], i.e.

$$H = U_0 \sum_{\sigma} (Q_\sigma + \alpha T_\sigma - 1)^2 - \mu \sum_i \hat{n}_i,$$

(S4)
Section VII: Gaussian state approach to twisted bilayer graphene

At finite temperature \( T \), the imaginary time evolution equation \([76]\) for density matrices \( \rho \) reads

\[
d_\tau \rho = -\{F(\rho) - f(\rho), \rho\},
\]

\( (S5) \)
which guarantees the monotonic decrease of the free energy \( f(\rho) = \text{tr}(\rho F(\rho)) \) with \( F(\rho) = H + T \ln \rho \) being the free energy operator.

We approximate the density matrix \( \rho \) by the Gaussian state

\[
\rho_G = \frac{1}{Z} e^{-\frac{1}{2} C^\dagger \Omega C},
\]

where \( Z = \text{tr}(e^{-\frac{1}{2} C^\dagger \Omega C}) \) is the partition function, \( \Omega = \Omega^\dagger \) is a matrix in the Nambu basis \( C^\dagger = (c_1^\dagger, \ldots, c_{N_f}^\dagger, c_1, \ldots, c_{N_f}) \), the creation and annihilation operators \( c_i^\dagger \) and \( c_i \) fulfill the anti-commutation relation \( \{c_i, c_j^\dagger\} = \delta_{ij} \), and \( N_f \) is the number of fermionic modes. The density matrix \( \rho_G \) is fully characterized by its \( 2N_f \times 2N_f \) covariance matrix

\[
\Gamma = \text{tr}(\rho_G C C^\dagger) = \frac{1}{e^{-\frac{N_f}{2}} + 1}. \tag{S7}
\]

By projecting Eq. (S5) in the tangential space of the variational manifold [75, 76], we obtain EOM

\[
\partial_t \Gamma = \{F, \Gamma\} - 2\Gamma F \Gamma, \tag{S8}
\]

where the mean-field free energy \( F = H - \Omega \) is determined by the mean-field Hamiltonian \( H_{ij} = -2\delta(H)_G/\delta \Gamma_{ij} \) and \( \langle H \rangle_G = \text{tr}(H \rho_G) \).

For the Kang-Vafek (KV) model Eq. (1), the diagonal and off-diagonal blocks

\[
\begin{align*}
\epsilon &= -M^2 + 2[1 - \text{tr}(\langle cc^\dagger \rangle_G M)]M + 2M \langle cc^\dagger \rangle_G M, \\
\Delta &= -2M \langle cc \rangle_G M,
\end{align*} \tag{S9}
\]

of the mean-field Hamiltonian \( H = \begin{pmatrix} \epsilon & \Delta \\ \Delta & -\epsilon \end{pmatrix} \) in the local basis \( c_i \) of each hexagon are determined by

\[
M = \frac{1}{3} I_6 + \begin{pmatrix} 0 & t_{ab} \\ t_{ab}^\dagger & 0 \end{pmatrix}, \quad t_{ab} = \alpha \begin{pmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}. \tag{S10}
\]

where the six sites in the hexagon are labeled in Fig. S9. The energy per hexagon reads

\[
\langle H_G \rangle = \left[ \text{tr}((1 - \langle cc^\dagger \rangle_G M) - 1)^2 + \text{tr}((1 - \langle cc^\dagger \rangle_G M) \langle cc^\dagger \rangle_G M) + \text{tr}[M \langle cc^\dagger \rangle_G M \langle cc \rangle_G] \right]. \tag{S11}
\]

![FIG. S9. The labels of the six sites in the hexagon.](image)

The free energy

\[
f(\rho) = \sum G \langle H_G \rangle - \frac{1}{2} \text{tr}[(1 - \Gamma) \Omega + T \ln(e^{-\frac{\Omega}{T}} + 1)] \tag{S12}
\]

decreases monotonically in the imaginary time evolution, where the diagonal matrix \( E = \text{diag}(E_1, E_2, \ldots, E_{2N_f}) \) is constructed by the eigenvalues of \( \Omega \). In the asymptotic limit, the density matrix reaches the thermal equilibrium state, where \( H = \Omega \), and the pairing term \( \langle c_i c_j \rangle_G = \langle c_i^\dagger c_j^\dagger \rangle_G = 0 \) due to the repulsive Coulomb interaction inherited by the KV model. As a result, the off-diagonal block \( \Delta = 0 \).

In agreement with the XTRG approach, the finite-T phase diagram obtained by the optimal mean-field theory consists of the QAH states, the CDW states, and high-T trivial states. It is remarkable that the QAH and CDW states possess a lot of symmetries.
which are represented by the structure of the covariance matrix $\Gamma$. Therefore, the thermal state can be described with very little order parameters, as we will show in the following.

Let us list several typical symmetries $S$ of the Hamiltonian. The Hamiltonian has the particle hole symmetry $S_c$, the time reversal symmetry $S_T$, the translational symmetry $P_{\vec{a}_j} (j = 1, 2, 3)$, the rotational symmetry $R_3$ with respect to the center of the hexagon, the reflection symmetry $Z_{2h}$ with respect to the horizontal axis $x_1$, the symmetry $n_A Z_{2v}$ of the reflection with respect to the vertical axis $x_2$ and $c_i \rightarrow -c_i$ in one sub-lattice. The vectors and axes in the honeycomb Moiré lattice are shown in Fig. S10.

![FIG. S10. The horizontal and vertical axis $x_1$ and $x_2$. The sublattice $A$ of the honeycomb lattice are generated by linear combinations of the basis vectors $\vec{a}_1 = (-\sqrt{3}, 0)$, $\vec{a}_2 = (\sqrt{3}, \frac{\sqrt{3}}{2})$, $\vec{a}_3 = (n_1 \vec{a}_1 + n_2 \vec{a}_2$, where $n_1, n_2$ are integers. The sublattices $A$ and $B$ are connected by the vectors $\vec{b}_1 = \left(\frac{-\sqrt{3}}{2}, \frac{\sqrt{3}}{2}\right)$, $\vec{b}_2 = \left(\frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2}\right)$, $\vec{b}_3 = (0, -1)$. And here are other useful vectors $\vec{c}_1 = (0, 2)$, $\vec{c}_2 = (-\sqrt{3}, -1)$, $\vec{c}_3 = (\sqrt{3}, -1)$.

The covariance matrix $\gamma = \langle \xi^\dagger \xi \rangle_G$ in the coordinate space shows that the QAH state has symmetries $S_c$, $P_{\vec{a}_j} (j = 1, 2, 3)$, $R_3$ and the symmetry $S_T Z_{2h}$. The properties of $\gamma$ and the corresponding symmetry are listed as follows:

- The particle-hole symmetry $S_c \implies \gamma = 1 - \gamma^T \gamma = 0.5, \ \text{Re}(\gamma_{ij}(i \neq j)) = 0$.
- The translational symmetry $P_{\vec{a}_j} (j = 1, 2, 3) \implies$ The covariance matrices for all hexagons are same, e.g., $\gamma_{41} = \gamma_{53}$.
- The rotational symmetry $R_3 \implies \gamma_{41} = \gamma_{63} = \gamma_{52} = \gamma_{53} = \gamma_{42} = \gamma_{61} = \gamma_{21} = \gamma_{13} = \gamma_{32} = \gamma_{74} = \gamma_{46} = \gamma_{65} = \gamma_{43} = \gamma_{62} = \gamma_{51}$.
- The symmetry $S_T Z_{2h} \implies \gamma_{23} = \gamma_{54}^\ast$.

The symmetries play an important role since they completely determine the covariance matrix

$$\langle \xi^\dagger \xi \rangle_G = \gamma = \begin{pmatrix} \gamma_a & \gamma_{ab} \\ \gamma_{ab}^\dagger & \gamma_a \end{pmatrix}, \quad \gamma_a = \begin{pmatrix} 0.5 & \delta^\ast & \delta \\ \delta & 0.5 & \delta^\ast \\ \delta^\ast & \delta & 0.5 \end{pmatrix}, \quad \gamma_{ab} = \begin{pmatrix} \delta_{ab} & \delta_{ab2} & \delta_{ab} \\ \delta_{ab} & \delta_{ab} & \delta_{ab2} \\ \delta_{ab2} & \delta_{ab} & \delta_{ab} \end{pmatrix}$$

with only three independent order parameters

$$\delta_{ab} = \langle b^\dagger_{-A+b_j} - a^\dagger_{-A} \rangle_G,$$
$$\delta = \langle a^\dagger_{-A+b_j} - a^\dagger_{-A} \rangle_G = \langle b^\dagger_{-A+b_j} - a^\dagger_{-A+b^{-1}_j} \rangle_G,$$
$$\delta_{ab2} = \langle b^\dagger_{-A+b_j} - a^\dagger_{-A} \rangle_G, \quad j = 1, 2, 3,$$

where $a^\dagger_{-A}$ and $b_{-A}$ are the annihilation operators of electrons in sublattices $A$ and $B$.

The covariance matrix gives rise to the mean-field Hamiltonian

$$\varepsilon = \begin{pmatrix} T_a & T_{ab} \\ T_{ab}^\dagger & T_a \end{pmatrix}, \quad T_a = \begin{pmatrix} 0 & t_1 & t_2 \\ t_1^\ast & 0 & t_2^\ast \\ -t_2 & t_2^\ast & 0 \end{pmatrix}, \quad T_{ab} = \begin{pmatrix} t_1^\ast & t_3^\ast & t_1 \\ t_1 & t_3 & t_1^\ast \\ t_3^\ast & t_1 & t_1^\ast \end{pmatrix}$$
in each hexagon through Eq. (S9), with the effective hopping strengths
\[ t_1 = 2 \left( \alpha^2 + \frac{1}{9} \right) \delta_{ab} - \frac{4}{3} \alpha \delta - 2 \alpha^2 \delta_{ab2}, \]
\[ t_2 = 2 \left( -\frac{2 \alpha \delta_{ab}}{3} + \left( 3 \alpha^2 + \frac{1}{9} \right) \delta + \frac{2 \alpha \delta_{ab2}}{3} \right), \]
\[ t_3 = 2 \left( -2 \alpha^2 \delta_{ab} + 4 \alpha \delta \right) \delta_{ab2} \]
between the nearest neighbor, the second-neighbor, and the third-neighbor sites, as shown in Fig. S11.

![Image of effective hopping strengths](image)

**FIG. S11.** The effective hopping strengths of the mean field Hamiltonian in QAH phases.

In the second quantized form, the mean-field Hamiltonian of the honeycomb Moiré lattice reads
\[ H = \sum_{\vec{A}} \sum_{\vec{j}} \left[ t_1 b_{\vec{A}+\vec{a}_j}^\dagger a_{\vec{A}+\vec{a}_j} + t_2 a_{\vec{A}+\vec{a}_j}^\dagger a_{\vec{A}+\vec{a}_j} + t_3 b_{\vec{A}+\vec{a}_j}^\dagger b_{\vec{A}+\vec{a}_j} + t_4 b_{\vec{A}+\vec{a}_j}^\dagger a_{\vec{A}+\vec{a}_j} + h.c. \right], \]
where \( t_1 = 2t_1 \). The Fourier transforms \( a_k = \sum_{\vec{A}} e^{-i\vec{k} \cdot \vec{A}} a_{\vec{A}} / \sqrt{N} \) and \( b_k = \sum_{\vec{A}} e^{-i\vec{k} \cdot (\vec{A}+\vec{b}_j)} b_{\vec{A}+\vec{b}_j} / \sqrt{N} \) result in the mean-field Hamiltonian \( H = \sum_k c_k^\dagger h_{\text{QAH}}(k)c_k \) in the momentum space \( c_k = (a_k, b_k)^T \), where
\[ h_{\text{QAH}}(k) = \begin{pmatrix} h_{k,11} & h_{k,12} \\ h_{k,12}^* & -h_{k,11} \end{pmatrix} \]
is determined by
\[ h_{k,11} = t_2 \sum_j e^{-i\vec{k} \cdot \vec{a}_j} + t_2^* \sum_j e^{i\vec{k} \cdot \vec{a}_j}, \]
\[ h_{k,12} = t_3 \sum_j e^{i\vec{k} \cdot \vec{b}_j} + t_3^* \sum_j e^{i\vec{k} \cdot \vec{c}_j}. \]

The covariance matrix
\[ \langle c_k c_k^\dagger \rangle_G = \frac{1}{e^{-\beta h_{\text{QAH}}(k)} + 1} = \frac{h_{\text{QAH}}(k)}{2d_{k,c}} \left( 1 - 2f_k^2 \right) + \frac{1}{2} I_2 \]
can be obtained by the diagonalization \( U_k^\dagger h_{\text{QAH}}(k)U_k = \text{diag}(d_{k,c}, d_{k,v}) \) of the mean-field Hamiltonian \( h_{\text{QAH}}(k) \) using the unitary transformation \( U_k \), where the Fermi-Dirac distribution \( f_k^2 = 1/(e^{d_{k,c}/T} + 1) \) is determined by the dispersion relations \( d_{k,(c,v)} = \pm \sqrt{h_{k,11}^2 + |h_{k,12}|^2} \) in the conduction (c) and valence (v) bands at the temperature \( T \).

The covariance matrix gives rise to the self-consistent equations
\[ \delta_{ab} = \frac{1}{2N} \sum_k e^{-i\vec{k} \cdot \vec{a}_j} -h_{12}^* \tanh \left( \frac{d_{k,c}}{2T} \right), \]
\[ \delta = \frac{1}{2N} \sum_k e^{-i\vec{k} \cdot \vec{a}_j} -h_{11} \tanh \left( \frac{d_{k,c}}{2T} \right), \]
\[ \delta_{ab2} = \frac{1}{2N} \sum_k e^{-i\vec{k} \cdot \vec{c}_j} -h_{12} \tanh \left( \frac{d_{k,c}}{2T} \right) \]
for the order parameters. Close to the phase transition, all the order parameters tend to zero, and Eq. (S21) can be linearized as

$$\begin{pmatrix} \delta_{ab} \\ \delta \\ \delta_{ab2} \end{pmatrix} = \frac{1}{4T} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} = \frac{1}{T} M_{\text{QAH}} \begin{pmatrix} \delta_{ab} \\ \delta \\ \delta_{ab2} \end{pmatrix}. \quad \text{(S22)}$$

The critical temperature $T_c$ is thus determined by the largest positive eigenvalue $\lambda_{\text{max}}$ of

$$M_{\text{QAH}} = \frac{1}{2} \begin{pmatrix} 2\alpha^2 + \frac{2}{\beta} & -\frac{4}{\beta} & -2\alpha^2 \\ -\frac{2}{\beta} & 3\alpha^2 + \frac{1}{\beta} & \frac{2}{\beta} \\ -2\alpha^2 & \frac{4}{3\alpha} & 2\alpha^2 + \frac{1}{\beta} \end{pmatrix}.$$}

Furthermore, using symmetries we can significantly reduce the degrees of freedom in the $N_l \times N_l$ covariance matrix to three order parameters, as a result, the above analysis can be applied to the system in the thermodynamic limit. To speed up the calculation, we first numerically flow equations of $\gamma$ for a small system, and achieve the three order parameters in the thermal state. Using the order parameters of the small system as the initial condition, we solve the non-linear Eq. (S21) to obtain the order parameters for the system in the thermodynamic limit, where the free energy density

$$f(\delta_{ab}, \delta, \delta_{ab2}) = \langle H_0 \rangle_G + \frac{1}{N_f} \sum_k 2T \left[ f_k^2 \ln f_k + f_k^4 \ln f_k^4 \right] \quad \text{(S23)}$$

is minimized.

In the CDW phase, the density distribution of the CDW state has three equivalent spatial structures for the system in the thermodynamic limit, which possesses the symmetries $P_{\overrightarrow{a}_1}$, $P_{\overrightarrow{a}_2}$, and $P_{\overrightarrow{a}_3}$, respectively. We analyze one of the three equivalent CDW states that maintains the symmetry $P_{\overrightarrow{a}_1}$ without loss of generality. The structure of the covariance matrices $\gamma_{\text{odd}} \equiv \lambda$ and $\gamma_{\text{even}}$ in the odd and even rows, respectively, indicates that the CDW state possesses the symmetries $S_T$, $P_{\overrightarrow{a}_2}$, $n_A Z_2$, and the combination symmetries $S_c P_{\overrightarrow{a}_3}$, $S_c Z_{2h}$. The properties of the covariance matrices and the corresponding symmetry are listed as follows.

- The time reversal symmetry $S_T \implies \lambda = \lambda^T \xrightarrow{\lambda \mapsto \lambda^T} \gamma_{\text{odd}}$ and $\gamma_{\text{even}}$ are real symmetric matrices.
- The translational symmetry $P_{\overrightarrow{a}_1} \implies$ The covariance matrices for each rows are same, e.g., $\lambda_{11} = \lambda_{22}$.
- The combination symmetry $S_c P_{\overrightarrow{a}_3} \implies \gamma_{\text{odd}} = I - \gamma_{\text{even}}^{T}, \lambda_{14} = -\lambda_{35}, \lambda_{44} = 1 - \lambda_{55}$.
- The combination symmetry $S_c Z_{2h} \implies \lambda_{11} = 1 - \lambda_{66}, \lambda_{22} = 1 - \lambda_{55}, \lambda_{14} = 1 - \lambda_{33}, \lambda_{16} = \lambda_{25} = 0, \lambda_{14} = -\lambda_{63}, \lambda_{14} = -\lambda_{53}; \lambda_{12} = -\lambda_{56}, \lambda_{13} = -\lambda_{54}; \lambda_{15} = -\lambda_{52}, \lambda_{34} = -\lambda_{43} = 0.$
- The symmetry $n_A Z_2 \implies \lambda_{13} = \lambda_{32}, \lambda_{36} = -\lambda_{35}$.

Therefore, the covariance matrix $\gamma$ only has four independent order parameters

$$\begin{align*}
n_0 &= \langle a_{A_o} a_{A_o}^\dagger \rangle_G - \frac{1}{2}, \\
n_1 &= \langle a_{A_o} a_{A_o}^\dagger a_{\overrightarrow{a}_1} \rangle_G, \\
n_2 &= \langle a_{A_o} a_{A_o}^\dagger a_{\overrightarrow{a}_2} \rangle_G, \\
\Delta_0 &= \langle a_{A_o} a_{A_o}^\dagger a_{\overrightarrow{a}_3} \rangle_G,
\end{align*} \quad \text{(S24)}$$

where $A_o = l_1 a_1 + 2l_2 a_2$ and $l_{1,2}$ are integers. The covariance matrix

$$\gamma_{\text{odd}} = \begin{pmatrix}
1 & 0 & 0 & -\Delta_0 & 0 \\
0 & 0 & 0 & 0 & \Delta_0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{pmatrix} \quad \text{(S25)}$$
results in the mean-field Hamiltonian

\[ \varepsilon^o = \begin{pmatrix} e_1 & e_3 & e_4 & e_5 & e_6 & 0 \\ e_3 & e_1 & e_4 & -e_5 & 0 & -e_6 \\ e_4 & e_4 & e_2 & 0 & e_5 & -e_5 \\ e_5 & -e_5 & 0 & -e_2 & -e_4 & -e_4 \\ e_6 & 0 & e_5 & -e_4 & -e_1 & -e_3 \\ 0 & -e_6 & -e_5 & -e_4 & -e_3 & -e_1 \end{pmatrix} \] (S26)

in odd rows with the hopping strengths

\[ e_1 = \frac{2}{9} n_0 + 4\alpha^2 n_2, \]
\[ e_2 = -\frac{2}{9} n_0 + 2\alpha^2 (-2n_0 + 2n_1), \]
\[ e_3 = \frac{2}{9} n_1 + \frac{4\alpha}{3} \Delta_0 + \alpha^2 (-2n_0 + 2n_1 - 4n_2), \]
\[ e_4 = \frac{2}{9} n_2 - \frac{2\alpha}{3} \Delta_0 - \alpha^2 (-2n_0 + 2n_1), \]
\[ e_5 = -\frac{2}{3} \alpha (2n_0 - n_1 + n_2 - 3\alpha \Delta_0), \]
\[ e_6 = \frac{2}{9} (6\alpha (n_2 - n_1) - (1 + 9\alpha^2) \Delta_0). \] (S27)

The combination symmetry \(S_c P^{-2}_\pm\) determines the relation between the mean-field Hamiltonian in odd and even rows as \(\varepsilon^o = -\varepsilon^e\).

In the second quantized form, the mean-field Hamiltonian of the honeycomb Moiré lattice reads

\[ H = \sum_{O^o} \sum_{i,j \in O^o} c_i^\dagger \varepsilon_{i,j}^o c_j + \sum_{O^e} \sum_{i,j \in O^e} c_i^\dagger \varepsilon_{i,j}^e c_j. \] (S28)

The stripe has the translational symmetry \(P_{2\pi^o}\) and \(P_{2\pi^e}\), thus, particles with the momentum \(k_h \in \{0, 2\pi_x/\sqrt{3}, 0, 2\pi_y/3\}\) hybridize with particles with the momentum \(k_h \pm 2\pi_y/3\) and the Brillouin zone shrinks to \(k_h \in \{0, 2\pi_x/\sqrt{3}, 0, 2\pi_y/3\}\), which is different from the situation in QAH phases. The Fourier transformation gives rise to the mean-field Hamiltonian \(H = \sum_{k_h} c_{k_h}^\dagger h^{\text{CDW}}(k_h) c_{k_h}\) in the momentum space \(c_{k_h} = (a_{k_h}, b_{k_h}, a_{k_h+}, b_{k_h+})\), where

\[ h^{\text{CDW}}(k_h) = \begin{pmatrix} 0 & \tilde{h}_0(k_h) \\ \tilde{h}_0(k_h) & 0 \end{pmatrix} \] (S29)

is determined by

\[ \tilde{h}_0(k_h) = \begin{pmatrix} \varepsilon_{k_h} & \varepsilon_{k_h}^* \\ -e^{-i\pi \varepsilon_{k_h}^*} & e^{-i\pi \varepsilon_{k_h}} \end{pmatrix}, \] (S30)

and

\[ \varepsilon_k = 2e_1 - e_2 + 2e_3 \cos(\sqrt{3} k_x) - 4ie_4 \cos(\sqrt{3} k_x) \sin(\frac{3}{2} k_y), \]
\[ \bar{\varepsilon}_k = 2i e^{-i\pi \varepsilon_{k_h}} \sin(\sqrt{3} k_x). \] (S31)

The covariance matrix

\[ \left( \begin{pmatrix} c_k \\ c_{k^e} \end{pmatrix} \begin{pmatrix} c_k^\dagger \\ c_{k^e}^\dagger \end{pmatrix} \right)_G = \frac{1}{e^{-\frac{\Delta_{\text{CDW}}(k)}{2T}} + 1} \left( \frac{1}{2\pi e^{2\Delta_{\text{CDW}}(k)}} \tilde{h}_0(k) (1 - 2f_k) \right) \] (S32)

can be obtained by the diagonalization \(U_k^\dagger h^{\text{CDW}}(k) U_k = \text{diag}(E_k, E_k, -E_k, -E_k)\) of the mean-field Hamiltonian \(h^{\text{CDW}}(k)\) using the unitary transformation \(U_k\), where the Fermi-Dirac distribution in the CDW phase \(f_k = 1/(e^{E_k/T} + 1)\) is determined by the dispersion relation \(E_k = \sqrt{|\varepsilon_k|^2 + |\varepsilon_k|^2}\) at the temperature \(T\).
The covariance matrix leads to the self-consistent equations

\[
\begin{align*}
n_0 &= \frac{1}{N} \sum_k \frac{\epsilon_k}{2E_k} \tanh \left( \frac{E_k}{2T} \right), \\
n_1 &= \frac{1}{N} \sum_k e^{ik\bar{a}_1} \frac{\epsilon_k}{2E_k} \tanh \left( \frac{E_k}{2T} \right), \\
n_2 &= \frac{1}{N} \sum_k e^{-ik\bar{a}_3} \frac{\epsilon_k}{2E_k} \tanh \left( \frac{E_k}{2T} \right), \\
\delta_0 &= \frac{1}{N} \sum_k e^{-ik\bar{a}_3} - \frac{\epsilon_k}{2E_k} \tanh \left( \frac{E_k}{2T} \right),
\end{align*}
\] (S33)

for the order parameters. Close to the phase transition, all the order parameters tend to zero, and Eq. (S33) can be linearized as

\[
\begin{align*}
4Tn_0 &= 2e_1 - e_2 = \left( \frac{2}{3} + 4\alpha^2 \right) n_0 - 4\alpha^2 n_1 + 8\alpha^2 n_2, \\
4Tn_1 &= e_3 = -2\alpha^2 n_0 + \left( \frac{2}{9} + 2\alpha^2 \right) n_1 - 4\alpha^2 n_2 - \frac{4\alpha}{3} \delta_0, \\
4Tn_2 &= e_4 = 2\alpha^2 n_0 - 2\alpha^2 n_1 + \frac{2}{9} n_2 + \frac{2\alpha}{3} \delta_0, \\
4T\delta_0 &= e_6 = \frac{2}{9} \left[ -6\alpha n_1 + 6\alpha n_2 + \left( 1 + 9\alpha^2 \right) \delta_0 \right].
\end{align*}
\] (S34)

The critical temperature \( T_c = \lambda_{\text{max}}/4 \) is determined by the largest positive eigenvalue \( \lambda_{\text{max}} \) of the matrix

\[
M_{\text{CDW}} = \begin{pmatrix}
\frac{2}{3} + 4\alpha^2 & -4\alpha^2 & 8\alpha^2 & 0 \\
-2\alpha^2 & \frac{2}{9} + 2\alpha^2 & -4\alpha^2 & -\frac{4\alpha}{3} \\
2\alpha^2 & -2\alpha^2 & \frac{2}{9} & -\frac{2\alpha}{3} \\
0 & \frac{1}{3}\alpha & \frac{4}{9}\alpha & \frac{2}{9} + 2\alpha^2
\end{pmatrix}.
\] (S35)

Finally, the finite-T phase diagram S12 under the self-consistent mean-field approximation can be obtained, where the first-order transition between the QAH and CDW phases is displayed.

![Finite-T phase diagram](image)

**FIG. S12.** The finite-T phase diagram obtained by the Gaussian state theory.

**Section VIII: Exciton spectra and self-energy corrections**

At zero temperature, the single-particle Green’s function from the Gaussian state approach (the self-consistent mean-field theory) agrees excellently with the result from DMRG [1]. With respect to the Gaussian thermal state \( \rho_G \) described by three
order parameters in QAH phases, the KV Hamiltonian (S36) is decomposed into normal ordered terms via the Wick theorem as

\[ H = \langle H \rangle + \sum_{\alpha} c_{\alpha}^\dagger M_{\alpha\beta} c_{\beta} + \sum_{\alpha} c_{\alpha}^\dagger M_{\alpha\beta} c_{\beta} M_{\gamma\delta}, \]

where the Fourier transformation \( V_k = \begin{pmatrix} e^{ikr_A} & 0 \\ 0 & e^{ikr_B} \end{pmatrix} \) is determined by the relative distance \( r_A = ((0, 0), (\sqrt{3}, 0), (\sqrt{3}/2, -3/2))^T \) and \( r_B = ((\sqrt{3}/2, 1/2), (\sqrt{3}, -1), (0, -1))^T \), and we use the Einstein summation convention for the Greek alphabet.

At finite temperature, the two-particle spectrum can be obtained by the ladder diagram approximation beyond the mean-field theory, as shown in Fig. S13, and the self-energy correction, e.g., the Hartree term, becomes

\[ \Sigma_{k,\alpha\beta}^{(H)} = -\left( \frac{2}{N} \right)^2 \sum_{p\neq q} T \sum_{\omega} G_{k-q,\alpha\beta}^{(0)} (\omega_k - \omega_q) (V_k^\dagger MV_p)^{\alpha\beta} (V_{p-q}^\dagger MV_{k-q})^{\alpha\beta}, \]

\[ D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \omega_q) \equiv \frac{1}{(i\omega_k - h_{\text{QAH}}(k))}. \]

The exciton spectrum can be determined by the density-density correlation function

\[ D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \omega_q) = \int_0^\beta d\tau D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \tau) e^{i\omega_q \tau}, \]

\[ D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \tau) = -\langle T c_{p-q, \gamma_1}^\dagger (\tau) c_{p-q, \beta_1} (\tau) c_{p', \beta_2} (0) c_{p', q, \gamma_2} (0) \rangle. \]

It follows from the Heisenberg EOM that

\[ -\partial_\tau D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \tau) = \left( (c_{p-q, \gamma_1}^\dagger c_{p-q, \gamma_2}) \delta_{\beta_1, \beta_2} - (c_{p, \beta_1}^\dagger c_{p, \beta_2}) \delta_{\gamma_1, \gamma_2} \right) \delta_{p, p'} \delta (\tau) + \sum_{k'} M_{p,k'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} D_{k'p'}^{\beta_2 \gamma_2} (q, \tau), \]

where

\[ M_{p,k'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q) = \left( h_{\text{QAH}}^{\gamma_1} (p) \delta_{\beta_1, \beta_2} - \delta_{\beta_1, \beta_2} h_{\text{QAH}}^{\gamma_1} (p-q) \right) \delta_{p, p'} \]

\[ + \frac{2}{N} \left( (c_{p, \beta_1}^\dagger c_{p, \beta_2}) G (V_k^\dagger MV_k)^{\beta_1 \beta_2} (V_{k-q}^\dagger MV_{p-q})^{\gamma_1 \gamma_2} \right) \]

\[ - (V_p^\dagger MV_p)^{\beta_1 \beta_2} (c_{p-q, \gamma_2}^\dagger c_{p-q, \gamma_1} G (V_{k-q}^\dagger MV_{p-q})^{\gamma_1 \gamma_2}). \]

We define the correlation function \( D_{kp}^{\beta_1 \gamma_1, \beta_2 \gamma_2} \equiv D_{pp'}^{\beta_1 \gamma_1, \beta_2 \gamma_2} U_{p-q, \gamma_1}^\dagger U_{p', \beta_1}^\dagger U_{p', \beta_2} U_{p-q, \gamma_2}^\dagger \) in the quasi-particle basis using the transformation \( U_k \). The Fourier transform of EOM (S39) results in

\[ \tilde{D}_{kp}^{\beta_1 \gamma_1, \beta_2 \gamma_2} (q, \omega_q) = \left[ \frac{1}{[D^{(0)}(q, \omega_q)]^{-1} - V(q)} \right]_{k,p}^{\beta_1 \gamma_1, \beta_2 \gamma_2}. \]
where the bare density-density correlation function reads
\[
\tilde{D}_{kp}^{(0)\beta_1\gamma_1,\beta_2\gamma_2}(q,\omega_q) = \frac{f_{k'-q}^{\gamma_1} - f_{k}^{\beta_1}}{i\omega_q - (d_{k,\beta_1} - d_{k'-q,\gamma_1})}\delta_{\beta_1,\beta_2}\delta_{\gamma_1,\gamma_2}\delta_{kp,p'},
\]  
(S42)
and the interaction \[
\chi_{k,k'}^{\beta_1\gamma_1,\beta_2\gamma_2}(q,\omega_q) = -2t^{\beta_1\gamma_1}_k V^{\beta_2\gamma_2}_{k,k'} V_{k'-q,k'-q}/N
\]
of two quasi-particles is determined by \[
V^{\beta_1\beta_2}_{k,k'} = (U^{\dagger}_k V^\dagger_{k} MV_k U_{k'})_{\beta_1\beta_2}.
\]
The spectral decomposition results in
\[
\tilde{D}_{p,p'}^{\beta_1\gamma_1,\beta_2\gamma_2}(q,\omega_q) = \sum_{\lambda} \chi_{p,\lambda}^{\beta_1\gamma_1}(q) \frac{1}{i\omega_q - d_{2,\lambda}(q)} \chi_{p',\lambda}^{\beta_2\gamma_2*}(q),
\]  
(S43)
where the poles \(|d_{2,\lambda}(q)|\) of \[
\tilde{D}_{p,p'}^{\beta_1\gamma_1,\beta_2\gamma_2}(q,\omega_q)
\]
appear in pairs due to the particle-hole symmetry of \([D^{(0)}(q,\omega_q)]^{-1} - V(q)\).

It turns out that the lowest band with the dispersion relation \(d_{\alpha}(q) = \min_\lambda |d_{2,\lambda}(q)|\) corresponds to a collective mode, i.e., the exciton excitation. The bottom of the exciton band is at the \(\Gamma\)-point, and at zero temperature its energy is about 0.08 for \(\alpha = 0.2\), i.e., one order of magnitude smaller than the bare quasi-particle gap. Additionally, the exciton is robust in the presence of the kinetic energy of the bare electron as illustrated in Fig. S14. The wavefunction of the exciton state in the coordinate space, i.e., the Fourier transformation of \(\chi_{p,\lambda}^{\beta_1\gamma_1}(q)\), shows that the exciton with the center-of-mass momentum \(q\) is in the bound state of one electron in the conductive band and one electron in the valence band.

**FIG. S14.** The bare quasi-particle gap (stars) and the exciton band (circles) obtained via the Hamiltonian \(H_{\text{new}} = -t_0 \sum_{(i,j)} (\epsilon_i^c c_j^c + h.c.) + U_0 \sum_{Q}(Q_0 + \alpha T_0 - 1)^2\) at the effective kinetic strength \(t_0 = 0, 0.02, 0.04, 0.06, 0.08\) and 0.1, where \(\alpha = 0.2\), the interaction strength \(U_0 = 1\) and the temperature \(T = 0.04\). The exciton energy is always one order of magnitude smaller than the mean-field gap in the presence of the kinetic energy.

The two-particle correlation function leads to the self-energy correction \(\Sigma_k^{(H)} = U_k \tilde{\Sigma}_k^{(H)} U_k^\dagger\) via Eq. (S37), where \(\tilde{\Sigma}_k^{(H)}\) is the self-energy
\[
\tilde{\Sigma}_k^{(H)} = \frac{4}{N^2} \sum_{pp'q} 1 - \frac{f_{k'-q}^{\gamma_1}}{i\omega_k - d_{k'-q,\alpha\beta}} \chi_{p,\gamma_1}^{\beta_1\gamma_1}(q) \chi_{p',\gamma_2}^{\beta_2\gamma_2*}(q) V^{\beta_1\gamma_1}_{k,p\gamma_1} V^{\beta_2\gamma_2}_{k',p',k'-q}
\]
(S44)
of the quasi-particle, and \(n_k(d_{2,\lambda}(q)) = 1/\exp(d_{2,\lambda}(q)/T) - 1\) is the Bose-Einstein distribution.

We get the Matsubara single-particle Green function with the first-order exciton correction
\[
- \int d\tau e^{i\omega_k \tau} (T_\tau c_k(\tau) c_k^\dagger(0)) = \frac{1}{i\omega_k - \hbar QAM(k) - \Sigma_k^{(H)}},
\]
(S45)
In the quasi-particle picture, the single-particle Green function becomes
\[
G_k(\omega_k) = -U_k^\dagger(c_k^c c_k^{\dagger}(-\omega_k)) U_k = \frac{1}{i\omega_k - d_k - \tilde{\Sigma}_k^{(H)}} = \sum_s \frac{\tilde{Z}_{k,s}}{i\omega_k - \tilde{\varepsilon}_{k,s}}
\]
(S46)
where $\bar{Z}_{k,s}$ and $\bar{Z}_{k,s}$ are the poles and residues of $G_k(\omega_k)$, respectively, which satisfies sum rules $\sum_s \bar{Z}_{k,s} = I_2$ and $\sum_s \bar{Z}_{k,s} \bar{Z}_{k,s} = d_k$.

The Fock correction to the quasi-particle Green function can also be included as

$$\Sigma^{(F)}_{k,\gamma\beta} = \sum_p T^{p,k}_{p,k} \gamma\beta (q = 0, \omega_q = 0) T \sum_{\omega_p} \left[ G^{\gamma_1\beta_1}_{p} (\omega_p) - \bar{G}^{(0)\gamma_1\beta_1}_{p} (\omega_p) \right],$$

where the interaction $T$-matrix is obtained by

$$T^{p,k}_{p,k} \gamma\beta (q, \omega_q) = V^{p,k}_{p,k} \gamma\beta + \sum_{q',\nu} V^{p,k}_{p,q'} D^{q_1\nu_1}_{q_2\nu_2} (q, \omega_q) V^{q_2\nu_2}_{q',k},$$

and

$$T \sum_{\omega_p} \left[ G^{\gamma_1\beta_1}_{p} (\omega_p) - \bar{G}^{(0)\gamma_1\beta_1}_{p} (\omega_p) \right] = \sum_s \bar{Z}_{p,s} [f (\bar{\varepsilon}_{p,s}) - 1] + \delta_{\gamma_1\beta_1} (1 - f^{\gamma_1}_k)$$

determined by $G_k(\omega_k)$ and $\bar{G}^{(0)\gamma_1\beta_1}_{p} (\omega_p) = \delta_{\gamma_1\beta_1} / (i\omega - d_{p,\gamma_1})$.

Finally, the full single-particle Green function including the Hartree-Fock-like corrections becomes

$$G^{(F)}_k (\omega_k) = \frac{1}{i\omega_k - d_k - \Sigma^{(R)}_k - \Sigma^{(F)}_k} = \sum_s \frac{Z_{k,s}}{i\omega_k - \varepsilon_{k,s}},$$

where $\varepsilon_{k,s}$ and $Z_{k,s}$ are the poles and residues of the spectral function $G^{(F)}_k (\omega_k)$, respectively. The retarded Green’s function $G^{(R)}_k (\omega) = G^{(F)}_k (i\omega_k \rightarrow \omega + i\eta)$ is obtained by the analytic continuation, which determines the spectral function $A_k(\omega) = \text{Im} G^{(R)}_k (\omega)/\pi$. In our numerical calculation, we choose $\eta = 0.004$.

Due to the particle-hole symmetry, $A_k^{\dagger} (x) = A_k^{\dagger} (-x)$ and we only focus on the valence. Comparing with the spectral function of the free Green function $A^{(0)\nu}_k (x) = \delta(x - d^{\nu}_k)$, we find that when the temperature increases, not only the quasi-particle gap is reduced, but the broadened spectral function $A^{\nu}_k (x)$ even has the non-zero distribution at the positive frequency, as shown in Fig. S16. This is a strong evidence of the exciton band electron dressed by the excitons. The reduction of the quasi-particle weight and the spectral distribution in the negative frequency domain indicates the decrease of the current-current correlation. As shown in Fig. 3, with the correction of the exciton the current-current correlation decreases much faster than the mean-field result. However, the perturbative expansion fails to predict the correct critical temperature obtained by XTRG. This is because at the higher temperature, many excitons are proliferated, which strongly affect the quasi-particle spectrum as well as the particle-hole spectrum. As a result, the bare Green function in the calculation of the $T$-matrix should be replaced by the exact Green function, namely, the self-consistent calculation of the Green function is required, which will be our future work.

In the CDW phase, the calculation on the $T$-matrix and self-energy corrections can also be performed in the similar way, which also shows the low lying exciton excitation confirmed by the XTRG results.

The Fourier transformation gives rise to the interacting Hamiltonian

$$H_I = \frac{1}{N} \sum_{k_h, k_h, q_h} c^{\dagger}_{k_h - q_h, \alpha \beta} \bar{V}_{\alpha \beta} c_{k_h, \alpha \beta} - \frac{1}{N} \sum_{k_h, k_h, q_h} c^{\dagger}_{k_h - q_h, \alpha \beta} \bar{V}_{\alpha \beta} c_{k_h, \alpha \beta} + \frac{1}{N} \sum_{k_h, k_h, q_h} P_{\beta \beta_1} P_{\alpha \alpha_1} \bar{V}_{\alpha \beta} c_{k_h, \alpha \beta} c_{k_h, \alpha \beta} :$$

in the momentum space $c_{k_h} = (a_{k_h}, b_{k_h}, \bar{a}_{k_h}, \bar{b}_{k_h})$, where the $4 \times 4$ interacting matrix $\bar{V}_{k, k'; p, p'} = \begin{pmatrix} V^I_k M p & 0 \\ 0 & V^I_k M p' \end{pmatrix}$ and the permutation matrix $P = \sigma^z \otimes I_2$. 

FIG. S15. The Fock-like self energy $\Sigma^{(F)}_{k,\gamma\beta}$. 

The Fock correction to the quasi-particle Green function can also be included as
FIG. S16. The conductive and valence bands of the free single-particle Green’s function (white dots), the exciton band (green diamonds), and the spectral function $A_0(\omega)$ of the full single-particle Green’s function on the valence band at $T = 0.02, 0.04, 0.06$ and $0.08$ for $\alpha = 0.2$ (QAH phase). As temperature increases, the proliferation of excitons manifests.

The two-particle spectrum is also obtained by the ladder diagram approximation. The self-energy correction, e.g., the Hartree term, becomes

$$
\Sigma^{(0)CDW}_{k_h,\alpha\beta} = - \left( \frac{2}{N} \right)^2 \sum_{p_h,p'_h} \sum_{\omega_{q_h}} G^{(0)CDW}_{k_h-q_h,\alpha_1\alpha_2} (\omega_{q_h} - \omega_{p_h}) D_{p_h,p'_h}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h,\omega_{q_h})
$$

(S52)

where the free single-particle Green function $G^{(0)CDW}_{k_h} (\omega_{q_h}) = 1/(i\omega_{q_h} - \hbar^{CDW}(k_h))$. The exciton spectrum can be determined by the density-density correlation function

$$
D_{p_h,p'_h}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h,\tau) = \int_0^\beta d\tau' D_{\beta_1\gamma_1,\beta_2\gamma_2}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h,\tau) e^{i\omega_{q_h}\tau'},
$$

(S53)

$$
D_{p_h,p'_h}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h,\tau) = - \langle T \tau c_{p_h-q_h,\gamma_1} (\tau) c_{p_h,\gamma_1} (\tau) c_{p_h,\beta_1} (0) c_{p'_h-q_h,\gamma_2} (0) \rangle.
$$

(S54)

It follows from the Heisenberg EOM that

$$
-\partial_\tau D_{p_h,p'_h}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h,\tau) = (c_{p_h-q_h,\gamma_1} c_{p_h,\gamma_2}) G_{\beta_1,\beta_2} - (c_{p_h,\beta_2} c_{p_h,\beta_1}) G_{\gamma_1,\gamma_2}) D_{p_h,p_h} (\tau) + M_{p_h,k_h}^{\beta_1\gamma_1,\beta_2\gamma_2} (q_h) D_{k_h,p_h}^{\beta_2\gamma_2} (q_h,\tau),
$$

(S55)
of two quasi-particles is determined by $u_{\beta_1 \gamma_1} \gamma_2 (q_h, \omega_{q_h}) = 2 \left( V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_n} \right)$ of two quasi-particles is determined by $V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, k_h} = U_{k_n - q_n, \gamma_1}^{(\gamma_1 \beta_1 \gamma_1 \gamma_2)} \delta_{k_n - q_n, k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_n}$ and $V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_h} = U_{k_n - q_n, \gamma_1}^{(\gamma_1 \beta_1 \gamma_1 \gamma_2)} \delta_{k_n - q_n, k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_h} - V^{(h, h_+)_{\beta_1 \gamma_1}}_{k_n - q_n, (P)k_n}$.

The spectral decomposition results in

$$\tilde{D}_{\beta_1 \gamma_1 \beta_2 \gamma_2}^{\beta_1 \gamma_1 \beta_2 \gamma_2} (q_h, \omega_{q_h}) = \frac{1}{i \omega_{q_h} - M(q_h)} \tilde{N}_{\beta_1 \gamma_1 \beta_2 \gamma_2} (q_h, \omega_{q_h})$$

(861)

In the CDW phase, the lowest band with the dispersion relation $\delta_{ex} (q) = \min_{\lambda} |d_{2, \lambda} (q)|$ also corresponds to a collective mode, i.e., the exciton excitation. The lowest energy of the exciton is about 0.15 for $\alpha = 0.1$, which is smaller than the quasi-particle gap, similar to what happens in the QAH phase. However, the exciton band structure in the CDW phase is significantly distinct from that in the QAH phase due to the different spatial symmetries, as shown in Fig. S17.

The self-energy corrections, i.e., the Hartree-Fock corrections $\Sigma_{CDW}^{HF}$ and $\Sigma_{\alpha}^{CDW}$, can also be obtained in the similar way as Eq. (S44) and Eq. (S47). One only has to change the corresponding quasi-particle Green function and the interaction matrix to those in the CDW phase, which results in the full single-particle Green function

$$G^{CDW}_{k_h} (\omega_{k_h}) = - \langle c_{k_h \gamma_1} (\omega_{k_h}) \rangle = \frac{1}{i \omega_{k_h} - h^{CDW} (k_h) U_{k_h} - \Sigma_{k_h}^{CDW} - \Sigma_{\alpha}^{CDW}}$$

(862)

and the spectral functions $A^{\beta}_{\beta_1} (\omega)$. Due to the symmetries mentioned in the last section, there are two degenerate valence bands and two degenerate conductance bands, as a result, four single-particle spectral functions are obtained in the CDW phase. Due to the particle-hole symmetry, we only focus on the spectral function $A^{\beta}_{\beta_1} (\omega)$ for one of the degenerate valence bands. When the temperature increases, the quasi-particle gap is reduced and the exciton mode assists the valence electron to tunnel across the band gap, as shown in Fig. S18.

Via choosing the specific path in the momentum space, as illustrated in Fig. S19, the difference of the spectral function between the QAH and CDW phases are explicitly displayed. In our case, the period of the spectral function in the CDW phase is reduced by half in the $y$ direction. In the QAH phase, the translational symmetry $P_{2 \gamma} (i = 1, 2, 3)$ are preserved. However, the stripe in the CDW phase spontaneously breaks the translational symmetry $P_{2 \gamma} (i = 1, 2, 3)$ and preserves the translational symmetry $P_{2 \gamma} (i = 1, 2, 3)$, as a result, the period in the momentum space is reduced.

Section IX: Numerical results on Haldane-Hubbard model

We perform DMRG ($T = 0$) and XTRG ($T > 0$) calculations of the spinless Haldane-Hubbard model (HHM) whose Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle} (c_{i \gamma_1}^\dagger c_{j \gamma_1} + h.c.) - t' \sum_{\langle \langle ij \rangle \rangle} (e^{i \phi_{ij} / c_{i \gamma_1}^\dagger c_{j \gamma_1} + h.c.}) + V \sum_{\langle ij \rangle} (n_i - \frac{1}{2}) (n_j - \frac{1}{2})$$

(863)
FIG. S17. The quasi-particle gap \( \Delta_{qp} = 2d_{x,c}(2E_k) \) and the exciton band \( d_{ex} \) in the QAH (CDW) phase, where \( \alpha = 0.2(0.1) \). The exciton energy is one order of magnitude smaller than the quasi-particle gap. Besides, the bands in the CDW phase have the reduce period in the \( y \) direction.

FIG. S18. The conductive and valence bands (white dots), the exciton band (green diamonds), and the spectral function \( A_v(\omega) \) at \( T = 0.02, 0.04, 0.06 \) and \( 0.08 \) for \( \alpha = 0.1 \) in the CDW phase.

where \( t' = 0.2t, \phi_{ij} = \frac{\pi}{2} \) and the direction of next-nearest-neighbor (NNN) pair \( \langle \langle ij \rangle \rangle \) follows the standard Haldane model [84], and introduce the nearest-neighbor (NN) repulsion as in, e.g., Ref. [83]. The model in Eq. (S63) keeps the particle-hole symmetry and thus guarantees half filling in the finite-temperature XTRG calculations below. \( t = 1 \) is set as the energy scale below.

In Fig. S20(a), we show the DMRG results of charge density difference \( (n_A - n_B) = \sum_{i \in A} n_i - \sum_{i \in B} n_i \) between sublattice A and B, which serves as an order parameter of the charge density wave (CDW) phase with large \( V \). Around \( V_c \approx 0.01 \), we find a sudden jump from zero to finite value in \( n_A - n_B \), which suggests a first-order phase transition there. Note that, this transition \( V_c \) is half of the corresponding value in Ref. [83], due to the fact that, for the spinless fermion here, half of the Coulomb interaction terms (i.e. those \( n_i n_j \) terms) are discarded.
FIG. S19. The single-particle spectral function $A_k(\omega) = A^v_k(\omega) + A^c_k(\omega)$ for both the valence and conductive bands. (a) $\alpha = 0.2$ (QAH phase) and (b) $\alpha = 0.1$ (CDW phase). The period of the spectral function in the CDW phase is reduced by half.

FIG. S20. In a YC4×12×2 Haldane-Hubbard model, (a) sub-lattice charge density difference $n_A - n_B$ obtained from DMRG calculation are shown versus nearest neighboring Coulomb repulsion strength $V$ in the cases with $V = 0, 0.5, 1.5$ (CI) and $V = 3$ (CDW). (b) Specific heat $c_V$ obtained from XTRG calculation is shown versus temperature $T$ for different cases, i.e. $V = 0, 0.5, 1.5$ (CI) and $V = 3$ (CDW). The period of the specific heat in the CDW phase is reduced by half. Note that, with the increasing interaction strength from $V = 0$ to $V = 1.5$ in the CI phase, the position of the specific heat round peaks moves to higher temperatures. It contradicts the exciton proliferation picture, where the larger binding energy induced by interactions (the extremely lower exciton excitation mode) gives rise to the lower position of the specific round peaks as $V$ increases.

As shown in Fig. S20(c-d), the fluctuation spectra analysis confirms that the exciton bounded states are hardly occupied in the CI phase of the HHM, in stark contrast to the TBG model where exciton proliferation occurs in the QAH phase. The reason why excitons are rarely occupied in the HHM is that the exciton energy scale is always higher than the system temperature. Here are two cases: (a) When the nearest-neighbor interaction $V$ is relatively small (say, $V = 0.5$), as illustrated in Fig. S20(c), the Haldane term predominates and the exciton energy remains roughly at the same value of the energy gap 2 even if the temperature increases. (b) It is even more interesting for a larger $V$ (say, $V = 1.5$). As temperature increases, the attractive interaction between electrons and holes is screened by the individual thermal excitations, resulting in a reduced exciton binding energy and a larger spatial distribution of the exciton wavefunction. For instance, the exciton energies are $E_{ex} \simeq 0.8, 1.1$, and 1.7 for $V = 1.5$ at temperatures $T = 0, 0.5$ and 1, respectively. As shown in Fig. S20(d), the exciton energy is always higher than the corresponding temperature, therefore the exciton modes are hardly populated by thermal fluctuations. This explains why the specific heat curves in Fig. S20(b) change only slightly as $V$ increases from 0 to 1.5.

With the above numerical calculations and field-theoretical analysis on HHM, we conclude a fundamental difference in terms of distinct exciton energies and thermal properties when compared to the flat-band twisted bilayer graphene systems. The uniqueness of the latter originates from the interaction-driven, emergent, single-particle band in the strongly coupling limit.