Symmetric Kondo Lattice States in Doped Strained Twisted Bilayer Graphene

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(Received 20 January 2023; accepted 11 September 2023; published 17 October 2023)

We use the topological heavy fermion (THF) model and its Kondo lattice (KL) formulation to study the possibility of a symmetric Kondo (SK) state in twisted bilayer graphene. Via a large-N approximation, we find a SK state in the KL model at fillings $\nu = 0, \pm 1, \pm 2$ where a KL model can be constructed. In the SK state, all symmetries are preserved and the local moments are Kondo screened by the conduction electrons. At the mean-field level of the THF model at $\nu = 0, \pm 1, \pm 2, \pm 3$ we also find a similar symmetric state that is adiabatically connected to the symmetric Kondo state. We study the stability of the symmetric state by comparing its energy with the ordered (symmetry-breaking) states found in [H. Hu *et al.*, Phys. Rev. Lett. **131**, 026502 (2023)., Z.-D. Song and B. A. Bernevig, Phys. Rev. Lett. **129**, 047601 (2022).] and find the ordered states to have lower energy at $\nu = 0, \pm 1, \pm 2$. However, moving away from integer fillings by doping the light bands, our mean-field calculations find the energy difference between the ordered state and the symmetric state to be reduced, which suggests the loss of ordering and a tendency toward Kondo screening. In order to include many-body effects beyond the mean-field approximation, we also performed dynamical mean-field theory calculations on the THF model in the nonordered phase. The spin susceptibility follows a Curie behavior at $\nu = 0, \pm 1, \pm 2$ down to ~ 2 K where the onset of screening of the local moment becomes visible. This hints to very low Kondo temperatures at these fillings, in agreement with the outcome of our mean-field calculations. At noninteger filling $\nu = \pm 0.5, \pm 0.8, \pm 1.2$ dynamical mean-field theory shows deviations from a $1/T$ susceptibility at much higher temperatures, suggesting a more effective screening of local moments with doping. Finally, we study the effect of a C_{3z}-rotational-symmetry-breaking strain via mean-field approaches and find that a symmetric phase (that only breaks C_{3z} symmetry) can be stabilized at sufficiently large strain at $\nu = 0, \pm 1, \pm 2$. Our results suggest that a symmetric Kondo phase is strongly suppressed at integer fillings, but could be stabilized either at noninteger fillings or by applying strain.

DOI: 10.1103/PhysRevLett.131.166501

Introduction.—The experiments on magic-angle ($\theta = 1.05°$) twisted bilayer graphene (MATBG) [1–3] have established the existence of a variety of interesting phases [4–25], including correlated insulating phases [26–36] and superconductivity [37–41]. Their discovery has been followed by considerable theoretical efforts [42–66] aimed at understanding their origin. An extended Hubbard model has been constructed to analyze the interacting physics [57,67–79]; however, because of the nontrivial topology of the flat bands [80–88], certain symmetries become nonlocal. Alternatively, an approach based on a momentum space model has been considered [89–97], in which correlated insulators [98–105], superconductivity [106–111], and other correlated quantum phases [112–116] have been identified and studied. Besides, various numerical calculations [117–124] have also been performed to investigate the correlated nature of the phenomena. However, the active phase diagram including the states at noninteger fillings is not well understood. The exact mapping between the MATBG and topological heavy-fermion model constructed in Ref. [125] could be used for developments in this direction. This mapping establishes a bridge between heavy fermions [126–130] and moiré systems [125,131,132]. The presence of localized moments in MATBG is supported by recent entropy measurements that have found a Pomeranchuk-type transition [15,16]. A large entropy observed at high temperatures originates from weakly interacting local moments whose fluctuations are

quenched at low temperatures [15,16]. Since a similar behavior is observed in heavy-fermion systems [126], where the fluctuating local moments are screened by conduction electrons (Kondo effect), this observation is suggestive of a Kondo state with screened local moments in MATBG.

In this Letter, we first use the Kondo lattice (KL) model [131] to describe and study the symmetric Kondo (SK) state. The SK phase preserves all symmetries; the local moments are screened. We discuss the properties of the SK state and extend the study to the symmetric state in the topological heavy-fermion (THF) model [125,127]. To address the stability of the symmetric state, we perform both mean-field and dynamical mean-field theory (DMFT) calculations of the THF model. Our calculation indicates that, at integer fillings $\nu = 0, \pm 1, \pm 2$, ordered states are energetically favored with suppressed Kondo effect. Doping away from integer fillings tends to destroy the order and enhance the Kondo effect. We also study the effect of a C_{3z}-breaking strain. Our mean-field calculations show that the ordering at $\nu = 0, \pm 1, \pm 2$ is suppressed by the strain effect and a symmetric state can be stabilized at a sufficiently large strain.

THF model and KL model.—The THF model [125] contains two types of electrons: topological conduction c electrons ($c_{\boldsymbol{k},a\eta s}$) and localized f electrons ($f_{\boldsymbol{R},a\eta s}$). The operator $c_{\boldsymbol{k},a\eta s}$ annihilates conduction c electron with momentum $\boldsymbol{k}$, orbital $a \in \{1,2,3,4\}$, valley $\eta \in \{+,-\}$, and spin $s \in \{\uparrow,\downarrow\}$. We call the c electrons with $a = 1,2$ ($a = 3, 4$) as Γ_3 ($\Gamma_1 \oplus \Gamma_2$) c electrons [125]. $f_{\boldsymbol{R},a\eta s}$ is the annihilation operator of the f electron at the moiré unit cell $\boldsymbol{R}$ with orbital $\alpha \in \{1,2\}$, valley η and spin s [125]. The Hamiltonian of the THF model [125,133] is $\hat{H}_{\mathrm{THF}} = \hat{H}_c + \hat{H}_{fc} + \hat{H}_U + \hat{H}_W + \hat{H}_V + \hat{H}_J$ with the values of parameters taken from Ref. [125]. $\hat{H}_c$ describes the kinetic term of conduction electrons and $\hat{H}_{fc}$ describes the hybridization between f-c electrons [125,133]. The interactions include an on-site Hubbard interaction of f electrons ($\hat{H}_U$), a repulsion between f and c electrons ($\hat{H}_W$), a Coulomb interaction between c electrons ($\hat{H}_V$), and a ferromagnetic exchange coupling between f and c electrons ($\hat{H}_J$) [125,133]. Based on the THF model [125], a KL model of MATBG has been constructed via the Schrieffer-Wolff transformation [131]. The KL model is described by $\hat{H}_{\mathrm{Kondo}} = \hat{H}_c + \hat{H}_{cc} + \hat{H}_K + \hat{H}_J$, where $\hat{H}_{cc}, \hat{H}_K$ emerge from the SW transformation. $\hat{H}_{cc}$ is the one-body scattering term of Γ_3 c electrons with the form of

$$\hat{H}_{cc} = \sum_{|\boldsymbol{k}|<\Lambda_c} \sum_{\substack{a,a' \in \{1,2\} \\ \eta,s}} e^{-|\boldsymbol{k}|^2\lambda^2} : c^\dagger_{\boldsymbol{k},a\eta s} c_{\boldsymbol{k},a'\eta s} : \left(\frac{-1}{D_{\nu_c,\nu_f}} + \frac{-1}{D_{\nu_c,\nu_f}} \right) \times \begin{bmatrix} \gamma^2/2 & \gamma v'_\star(\eta k_x - i k_y) \\ \gamma v'_\star(\eta k_x + i k_y) & \gamma^2/2 \end{bmatrix}_{a,a'}. \quad (1)$$

λ is the damping factor of the f-c hybridization in the THF model. γ, $v'_\star$ characterize f-c hybridization [125,133]. D_{1,ν_c,ν_f} and D_{2,ν_c,ν_f} are two parameters given in Supplemental Material (SM) [133]. $\hat{H}_K$ is the Kondo interaction between f and Γ_3 c electrons given in Sec. II, SM [133]. We also note that, ground states at filling ν and $-\nu$ are connected by a charge-conjugation transformation [125]. This can be broken by other one-body terms that are expected to be small. In what follows, we only focus on $\nu \leq 0$.

Symmetric Kondo state.—We perform a mean-field (large-N) study of the KL model [127], where the Kondo interaction is treated via a Hartree-Fock decoupling (see SM [133]) by introducing the hybridization fields

$$V_1^* = \sum_{\boldsymbol{R},|\boldsymbol{k}|<\Lambda_c} \sum_{\alpha\eta s} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{R} - |\boldsymbol{k}|^2\lambda^2/2}}{\sqrt{N_M} N_M} \langle \Psi | f^\dagger_{\boldsymbol{R},\alpha\eta s} c_{\boldsymbol{k},\alpha\eta s} | \Psi \rangle$$

$$V_2^* = \sum_{\boldsymbol{R},|\boldsymbol{k}|<\Lambda_c} \sum_{\alpha\alpha\eta s} \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{R} - |\boldsymbol{k}|^2\lambda^2/2}}{\sqrt{N_M} N_M} (\eta k_x \sigma_x + k_y \sigma_y)_{\alpha a} \times \langle \Psi | f^\dagger_{\boldsymbol{R},\alpha\eta s} c_{\boldsymbol{k},\alpha\eta s} | \Psi \rangle \quad (2)$$

with $|\Psi\rangle$ the mean-field ground state. This mean-field approach suppresses the Ruderman-Kittel-Kasuya-Yosida interaction and essentially restores the hybridization term $\hat{H}_{fc}$ of the original periodic Anderson model but in a renormalized form [127,139]. It becomes exact in the $N \to \infty$ limit [we have $N = 4$, which corresponds to the approximate flat $U(4)$ symmetry]. By solving the mean-field equations at $\nu = 0, -1, -2$, we identify a SK state that preserves all the symmetries with $V_1 \neq 0$, $V_2 \neq 0$ [133].

We describe the properties of the SK state. In Fig. 1, we plot the band structure of the SK state and compare it with the noninteracting band structure of THF model. We find the f-c hybridization in the SK state to be enhanced. Consequently, the gap of the Γ_3 states at the Γ point [125] is increased from its noninteracting value 24.75 meV at $\nu = 0$, to 168 meV, 190 meV, 213 meV at $\nu = 0, -1, -2$ respectively. Furthermore, the flat bands in SK state are mostly formed by $\Gamma_1 \oplus \Gamma_2$ c electrons with weights larger than 70%. The bandwidths of the flat bands at $\nu = -1, -2$ become 16 meV, 53 meV, which are (much) larger than the noninteracting bandwidth (7.4 meV).

The flat bands in the SK state form the same representations as the flat bands in the noninteracting THF model [125]. The flat bands in SK state then belong to a fragile topology [125] at $\nu = -1, -2$. At $\nu = 0$, due to the additional particle-hole symmetry, flat bands have a stable topology and symmetry-protected nodes at Fermi energy [82,88,125] (see Sec. IV, SM [133]). We also mention that the interplay between the Kondo effect and the topological bands has also been studied in various other systems [140–145].

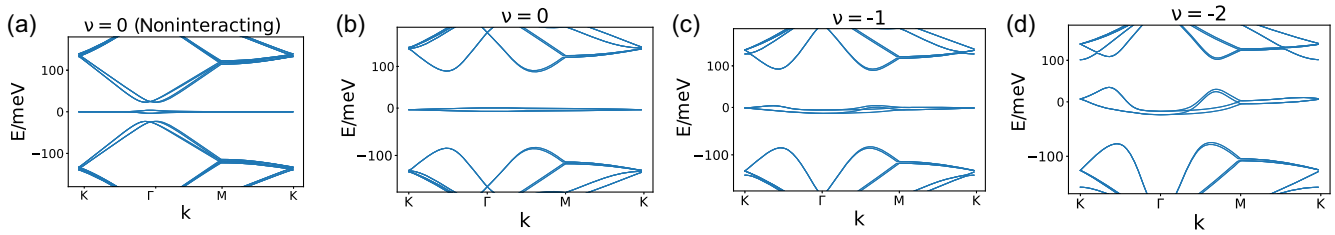

FIG. 1. (a) Band structure of the noninteracting THF model at $\nu = 0$. (b),(c),(d) Band structure of the SK phase at $\nu = 0, -1, -2$ respectively.

Symmetric state in the THF model and the effect of doping.—We next investigate the symmetric state in the THF model. We first focus on integer fillings $\nu = 0, -1, -2, -3$ and perform the mean-field calculations of the THF model (see Sec. V, SM [133]). We identify a symmetric state that preserves all the symmetries and is adiabatically connected to the SK state. To observe the stability of the symmetric state, we compare its energy (E_{sym}) with the energy (E_{order}) of the ordered (symmetry-breaking) ground states derived in Ref. [125]. The ordered ground states are a Kramers inter-valley-coherent (KIVC) state at $\nu = 0$, a KIVC + valley polarized (VP) state at $\nu = -1$, a KIVC state at $\nu = -2$, and a VP state at $\nu = -3$. However, we point out that at $\nu = -3$ translational-symmetry-broken states with lower energy exist [146]. In our calculations, $\Delta E = E_{\mathrm{sym}} - E_{\mathrm{order}} > 0$ at integer fillings indicate the ground states are ordered states instead of SK states at these fillings. However, introducing the Gutzwiller projector to our wave function may further reduce the energy of the symmetric state by including the many-body effect.

We next investigate the effects of doping. We stick to a narrow region $\nu \in [\nu_{\mathrm{int}} - 0.5, \nu_{\mathrm{int}} + 0.5]$ near each integer filling $\nu_{\mathrm{int}} = 0, -1, -2, -3$ and compare the energies of the ordered states E_{order} and the symmetric states E_{sym} in the THF model. The ordered solution is generated by doping the ordered state at integer filling ν_{int} and performing self-consistent calculations (see Sec. V, SM [133]). Figure 2 displays a plot of the difference of the ground state energies ΔE as a function of doping $\Delta\nu = \nu - \nu_{\mathrm{int}}$. We observe that

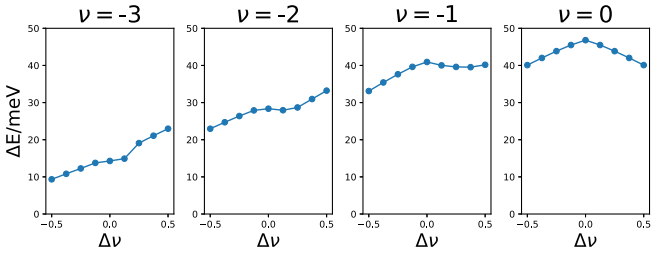

FIG. 2. Doping dependence of the ground state energy difference $\Delta E = E_{\mathrm{sym}} - E_{\mathrm{order}}$ near integer fillings $\nu = 0, -1, -2, -3$ in THF model. The ordered states we considered are KIVC ($\nu = 0$), KIVC + VP ($\nu = -1$), KIVC ($\nu = -2$), and VP ($\nu = -3$).

hole doping at $\nu = 0, -1, -2, -3$ and electron doping at $\nu = 0$ decreases the ΔE. Doping holes at $\nu = 0, -1, -2$ and doping electrons at $\nu = 0$ to the ordered states are equivalent to doping the light bands mostly formed by c electrons [125,133]. After doping, the conduction electrons stay close to the Fermi energy, and then enhance the tendency towards the Kondo effect and reduce ΔE.

However, doping electrons at $\nu = -1, -2$ is equivalent to doping heavy (flat) bands that mostly come from the f electrons. Because of the flatness of the band, the nature of the ordered states will change with doping (see Sec. V, SM [133]). From our calculations near $\nu = -1, -2$, we find that ΔE will first decrease and then increase as we increase $\Delta\nu$. The change of order moments indicates the importance of the correlation effect, which could be underestimated in the mean-field approach.

To further investigate the correlation effect, we perform DMFT calculations of the THF model in the nonordered phase at both integer and noninteger fillings. DMFT finds a qualitative difference between the strong quasiparticle renormalization at integer filling and a Fermi liquid at noninteger fillings: this can be seen from the scattering rate $\Gamma_f = -\mathrm{Im}\Sigma_f(\omega = 0)$, which is shown as a function of the total filling ν at $T = 11.6$ K in Fig. 3(a). The largest scattering rates are found close to $\nu = 0.0, -1.0$, and -2.0, progressively decreasing as one moves away from the charge neutrality point. Correspondingly, the spectral weight at the Fermi level (black and gray solid circles) is suppressed at these fillings.

Figure 3(b) illustrates the temperature-dependent screening of the local magnetic moment on the f orbitals. We determine the screening temperature $T_{\odot}$ and the effective moment μ_{eff} by fitting the z component of the local spin susceptibility to the expression $\mu_{\mathrm{eff}}^2/3(T + 2T_{\odot})$. A visualization of the deviation from Curie law can be obtained by plotting $T \times \chi_{\mathrm{spin}}^{\mathrm{loc}}(\omega = 0)$: a flat profile indicates Curie behavior and a well-defined effective local moment, while deviations signal the onset of screening and a crossover toward a Pauli-like behavior [147]. While at $\nu = 0.0, -1.0$, and -2.0 the $1/T$-like local spin susceptibility persists down to 1–2 K, the noninteger fillings deviate from Curie behavior at much higher temperatures($\sim$10 K). This deviation from Curie behavior at $\sim$10 K also marks the onset of the Kondo screening process. Our DMFT

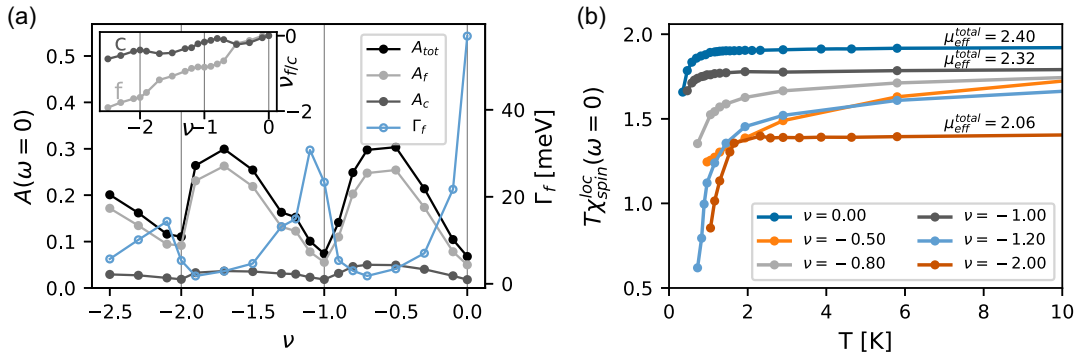

FIG. 3. DMFT solution of the THF model. (a) Doping ν dependent low-energy spectral function at the Fermi level $[A(\omega=0)]$ for the full system A_{tot}, the c (A_c) and the f electrons (A_f) at 11.6 K. Also shown is the scattering rate Γ_f as extracted from the local f electron self-energy. (b) Effective local moment $T\times\chi^{\mathrm{loc}}_{\mathrm{spin}}(\omega=0)$ as a function of temperature T for different doping levels ν. The full set of values of the screened local moments μ_{eff} and screened temperature $T_\odot$ is provided in SM, Sec. VI [133].

calculations suggest that the Kondo phase is strongly suppressed at integer fillings $\nu=0,-1,-2$, increasing the propensity toward long-range order. By doping the system, the development of Kondo screening is observed, which suggests that doping could enhance the Kondo effect. This picture is consistent with our mean-field calculations.

Effects of strain.—Since twisted bilayer graphene samples exhibit intrinsic strain [148] and the ordered states are disfavored by strain, we investigate the effect of strain in the THF model. We focus on $\nu=0,-1,-2,-3$ and introduce a C_{3z}-symmetry-breaking term [133,149–151] to qualitatively characterizes the effect of strain $\hat{H}_{\mathrm{strain}}=\alpha\sum_{\boldsymbol{R},\eta s}(f^\dagger_{\boldsymbol{R},1\eta s}f_{\boldsymbol{R},2\eta s}+\mathrm{H.c.})$ where α can reach $\sim$10 meV

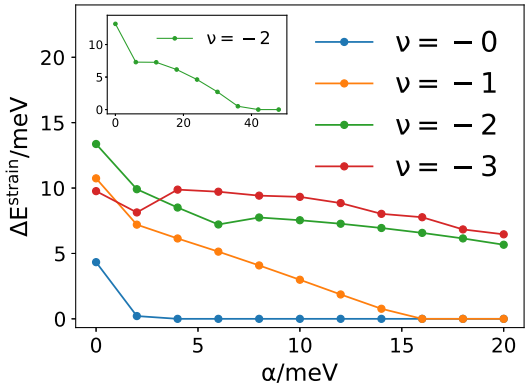

FIG. 4. Energy difference $\Delta E^{\mathrm{strain}}=E^{\mathrm{strain}}_{\mathrm{sym}}-E^{\mathrm{strain}}_{\mathrm{order}}$ between the symmetric state that only breaks C_{3z} symmetry $(E^{\mathrm{strain}}_{\mathrm{sym}})$ and the ordered state $(E^{\mathrm{strain}}_{\mathrm{order}})$ as a function of α—a parameter characterizing the strain amplitude. Inside: $\Delta E^{\mathrm{strain}}$ at $\nu=-2$ over an extended parameter region 0 meV $\leq\alpha\leq$ 45 meV. We note that even at zero strain $\alpha=0$, a symmetric state that only breaks C_{3z} symmetry has lower energy than the fully symmetric state. We also note that there are small kinks due to the transition between two ordered phases at $\alpha\sim3$ meV for $\nu=-1$, at $\alpha\sim5$ meV for $\nu=-2$, and at $\alpha\sim3$ meV for $\nu=-3$ (Sec. V, SM [133]).

in real materials (Sec. V, SM [133]). We compare the mean-field ground-state energies of the symmetric states $(E^{\mathrm{strain}}_{\mathrm{sym}})$ and the ordered states $(E^{\mathrm{strain}}_{\mathrm{order}})$ at nonzero strain. Because of the C_{3z} strain, the symmetric states here preserve all the symmetries except for the C_{3z}. In Fig. 4, we plot the energy difference $\Delta E^{\mathrm{strain}}=E^{\mathrm{strain}}_{\mathrm{sym}}-E^{\mathrm{strain}}_{\mathrm{order}}$ as a function of the effective strain amplitude α. We observe ΔE at $\nu=0,-1,-2$ vanishes at sufficiently large strain. A detailed analysis [133] of the wave function shows that the ordered state cannot be stabilized and converged to a symmetric solution at large strain. We thus conclude that a symmetric phase can be stabilized by sufficiently large strain at $\nu=0,-1,-2$. As for $\nu=-3$, we mention again that other ordered states exist [146]. We leave a systematic analysis of $\nu=-3$ for future study. Finally, we comment that even at zero strain, a symmetric state that breaks C_{3z} symmetry has lower energy than the fully symmetric state.

Discussion and summary.—We have performed a systematic study of the SK state in the MATBG by analyzing its band structure, topology, and stability. Our main result is that an ordered state, instead of a SK state, will be the ground state of the system at integer filling $\nu=0,-1,-2$. However, we find doping and C_{3z}-breaking strain can suppress the ordering and enhance the tendency toward the Kondo state. Most importantly, the possibility of the Kondo effect in the MATBG as we demonstrated leads to a natural explanation of entropy experiments [15,16]. As has been established in the heavy-fermion systems [126], the presence of Kondo ground state leads to crossover behaviors from a fluctuating local-moment phase at high temperature to a Kondo phase with screened local moment at low temperature. The fluctuating local moments, which follow a Curie behavior, produce a large entropy accumulation at high temperature. However, at low temperature, the local moments are screened by the electrons via the Kondo effect [126] and the quenched fluctuations of the local moments lead to a small entropy. Remarkably, this is exactly what has been observed in the recent entropy experiments [15,16], namely a large entropy at high temperature and a small entropy at low temperature.

Note added.—After finishing this work, we learned that related, but not identical, results have also recently been obtained by the S. Das Sarma [154], P. Coleman [155], and Z. Song groups [156]. We also mention that results from Z. Song's group are compatible with our DMFT results.

We thank Philipp Eck and Luca de' Medici for useful discussions. B. A. B.'s work was primarily supported by the DOE Grant No. DE-SC0016239, the Simons Investigator Grant No. 404513. H. H. was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant Agreement No. 101020833). J. H. A. was supported by a Hertz Fellowship. D. C. was supported by the DOE Grant No. DE-SC0016239 and the Simons Investigator Grant No. 404513. A. M. T. was supported by the Office of Basic Energy Sciences, Material Sciences and Engineering Division, U.S. Department of Energy (DOE) under Contract No. DE-SC0012704. G. R, L. K, T. W., G. S., and R. V. thank the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for funding through QUAST FOR 5249-449872909 (Projects P4 and P5). G. R. acknowledges funding from the European Commission via the Graphene Flagship Core Project 3 (Grant agreement ID: 881603). L. C. and G. S. were supported by the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter–ct.qmat Project-ID 390858490-EXC 2147, and gratefully acknowledge the Gauss Centre for Supercomputing e.V. [152] for funding this project by providing computing time on the GCS Supercomputer SuperMUC at Leibniz Supercomputing Centre [153]. L. C. gratefully acknowledge the scientific support and HPC resources provided by the Erlangen National High Performance Computing Center (NHR@FAU) of the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) under the NHR project b158cb. NHR funding is provided by federal and Bavarian state authorities. NHR@FAU hardware is partially funded by the German Research Foundation (DFG)—440719683. T. W. acknowledges support by the Cluster of Excellence "CUI: Advanced Imaging of Matter" of the Deutsche Forschungsgemeinschaft (DFG)–EXC 2056–Project ID No. 390715994. G. R. gratefully acknowledges the computing time granted by the Resource Allocation Board and provided on the supercomputer Lise and Emmy at NHR@ZIB and NHR@Göttingen as part of the NHR infrastructure (Project No. hhp00061). R. V.'s contribution was supported in part by the National Science Foundation under Grants No. NSF PHY-1748958 and No. PHY-2309135.

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