

## Renormalization Group Study of Hidden Symmetry in Twisted Bilayer Graphene with Coulomb Interactions

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We develop a two stage renormalization group which connects the continuum Hamiltonian for twisted bilayer graphene at length scales shorter than the moire superlattice period to the Hamiltonian for the active narrow bands only which is valid at distances much longer than the moire period. In the first stage, the Coulomb interaction renormalizes the Fermi velocity and the interlayer tunnelings in such a way as to suppress the ratio of the same sublattice to opposite sublattice tunneling, hence approaching the so-called chiral limit. In the second stage, the interlayer tunneling is treated nonperturbatively. Via a progressive numerical elimination of remote bands the relative strength of the one-particle-like dispersion and the interactions within the active narrow band Hamiltonian is determined, thus quantifying the residual correlations and justifying the strong coupling approach in the final step. We also calculate exactly the exciton energy spectrum from the Coulomb interactions projected onto the renormalized narrow bands. The resulting softening of the collective modes marks the propinquity of the enlarged (“hidden”)  $U(4) \times U(4)$  symmetry in the magic angle twisted bilayer graphene.

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It has been known for some time that electron-electron Coulomb interactions cause an upward renormalization of the Fermi velocity,  $v_F$ , upon approaching the charge neutrality point (CNP) of monolayer graphene [1–7]. Such momentum dependent steepening of the Dirac cone depends on the graphene’s dielectric environment and is weaker for stronger dielectrics, but even for hexagonal boron nitride (HBN) encapsulated devices the increase can be [2]  $\sim 10\%$ – $15\%$ . Such a small change in  $v_F$  would be of limited interest if it weren’t for the recent explosion of research into the magic angle [8] twisted bilayer graphene (TBG) [9–77], where the experiments show extremely strong sensitivity of the correlated electron phenomena to the twist angle  $\theta$ . Even a  $\sim 5\%$  change of  $\theta$  away from the optimal (magic) value has been reported to produce at least a factor of 2 reduction [23,24] of the superconducting  $T_c$ , with even stronger suppression of the correlated insulator states [23].

The strong band structure sensitivity is due to the dependence on the dimensionless parameters  $w_{0,1}/v_F k_\theta$ , where  $w_0$  and  $w_1$  parameterize the interlayer tunneling energy in the AA and AB regions, respectively, and where the momentum displacement of the Dirac cones is given by  $k_\theta = 2k_D \sin \frac{\theta}{2}$ ,  $k_D = 4\pi/3a_0$ ,  $a_0 \approx 0.246$  nm (in  $\hbar = 1$  units) [8]. Therefore, at a fixed magic  $\theta$ , even a  $\sim 10\%$  difference in  $v_F$  alone would be sufficient to detune the system from the optimal flat band condition. As such, if neither of  $w_j$  renormalized due to Coulomb interactions, but only  $v_F$  did, the magic angle condition would depend

on whether the TBG was encapsulated in HBN, or only from one side, because the different dielectric environments would produce a different strength of Coulomb interactions, the former with a dielectric constant [48,78]  $\epsilon_{\text{HBN}} \approx 4.4$  and the latter with  $\epsilon \approx (1 + \epsilon_{\text{HBN}})/2 = 2.7$ . The difference in the  $v_F$ , and therefore the magic angle, would then be within the sensitivity of the correlated insulating states; no such dependence of the magic angle on the partial or complete encapsulation has been reported.

Here we develop a renormalization group (RG) approach to the Coulomb interactions in the twisted bilayer graphene and show that  $w_1$  renormalizes in precisely such a way as to compensate for the growth of  $v_F$  making the magic angle largely insensitive to the effective dielectric constant  $\epsilon$ . Interestingly, we find that  $w_0$  does not renormalize due to Coulomb interactions. Therefore, the ratio  $w_0/w_1$  shrinks and the system flows closer to the chiral limit described by Tarnopolsky, Kruchkov, and Vishvanath [47]. As illustrated in Fig. 1(c), the flow from a high energy (with the UV cutoff  $E_c$ ), where the Coulomb interaction and  $w_{0,1}$  are perturbative, to a low energy of the narrow bands where neither is, crosses over to a regime where the effects of  $w_{0,1}$  become nonperturbative, but the Coulomb interaction is still perturbative. This happens at the energy scale  $E_c^* \sim \mathcal{O}(w_1)$ , marking the beginning of the second stage of our RG; the band structure scaling collapse in Fig. 2 shows that the second stage seamlessly connects to the first stage even if  $E_c^*$  changes. In the second stage, we numerically integrate out the two most remote bands, one above

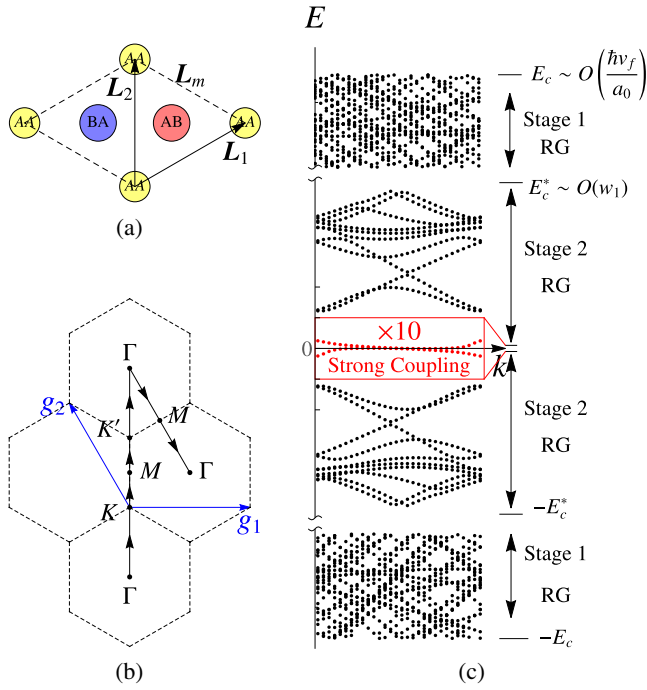


FIG. 1. (a) Moire lattice with lattice spacing  $L_m$ . (b) Moire Brillouin zone. (c) Schematic illustration of the two stage RG procedure for arriving at the strong coupling limit. In the stage 1, both the Coulomb interaction and the moire potential are perturbative, in the stage 2 only the Coulomb interaction is. In the final step, when only the narrow bands (red) remain, the interaction is the largest scale.

and one below the CNP, rotate the remaining states to diagonalize the renormalized kinetic energy, and reexpress the interaction in terms of the rotated states, iterating the procedure until we reach the narrow bands. If the resulting narrow bands' bandwidth (or, more precisely the root mean square of the renormalized kinetic energy dispersion) is much smaller than the interaction (or more precisely, the particle-hole charge gap), as we find it is near the magic angle, the final step is treated nonperturbatively in the Coulomb interaction, i.e., by solving the interaction-only problem (strong coupling limit) and then treating the renormalized kinetic energy terms as a perturbation.

The condition  $w_0 = 0$ , and thus the chiral limit [47,79,80], was previously thought to be unrealistic and the value  $w_0/w_1 \sim 0.8$  was taken from density functional theory-like calculations [28,50,81]. Our results [Eqs. (17) and (18)] show that for the Coulomb interacting system, the chiral limit becomes exact near the CNP in the limit  $E_c/w_1 \rightarrow \infty$ , albeit approaching logarithmically. This has important consequences for the effective residual interaction in the narrow band, because of the increased sublattice polarization of the narrow band wave functions [67]. We find additional enhancement of the sublattice polarization after the second stage, as well as steepening of the Wilson loop eigenvalues [42], indicating an additional approach to the chiral limit during the second stage RG.

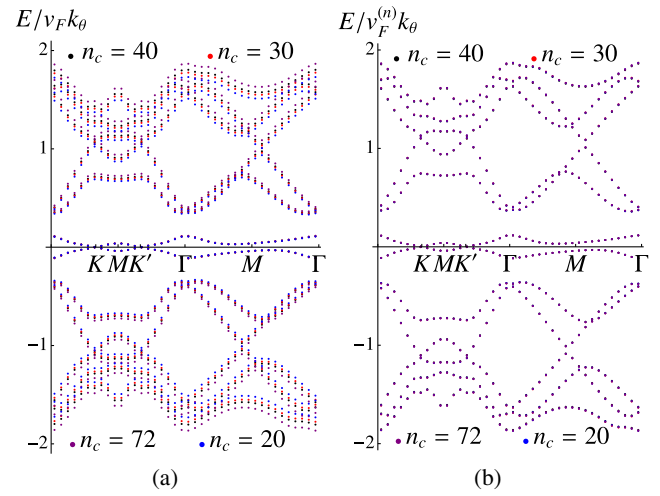


FIG. 2. (a) Low energy spectra after  $n_c - 5$  steps of the stage 2 RG for  $n_c = 72$  (purple), 40 (black), 30 (red), 20 (blue). At  $n_c$ , each starts with the same Fermi velocity,  $v_F$ , in the BM model at  $w_1/v_F k_\theta = 0.5$ , but with  $w_0/w_1 = 0.83$  (purple), 0.805 (black), 0.787 (red), and 0.768 (blue). The values are chosen based on the dielectric constant  $\epsilon = 4.4$  and scaling in Eq. (18) and the cutoff energies set by the  $n$ th band maxima at  $n_c = 72$ . (b) Results of the panel (a) rescaled by  $v_F^{(n)} = v_F/[1 + (e^2/4\epsilon v_F) \ln(E_c/E_c^*)]$  for  $E_c$  set by the band maximum at  $n_c = 72$ , demonstrating the scaling collapse and thus independence of the results of stage 2 RG on  $E_c^*$ .

The dominant part of the Coulomb interaction Hamiltonian projected onto perfectly sublattice polarized chiral limit narrow bands is invariant under a larger symmetry,  $U(4) \times U(4)$ , than for  $w_0/w_1 \neq 0$ ,  $U(4)$ , when particle-hole (p-h) symmetry [42] is exact [67]. This symmetry enhancement enlarges the manifold of nearly degenerate correlated states [67]. Our exact calculation of the collective mode spectrum in the strong coupling limit indeed shows not only four Goldstone bosons associated with the  $U(4)$  spin-valley ferromagnetism [48,67], but also a softening of four additional collective modes, indicating the approach to the  $U(4) \times U(4)$  ferromagnet [67] with its eight Goldstone bosons (see Fig. 3).

We begin with the Hamiltonian  $H = H_{\text{kin}} + V_{\text{int}}$  where

$$H_{\text{kin}} = \int d^2\mathbf{r} \chi_\sigma^\dagger(\mathbf{r}) \begin{pmatrix} \hat{H}_{\text{BM}} & 0 \\ 0 & \hat{H}_{\text{BM}}^* \end{pmatrix} \chi_\sigma(\mathbf{r}) \quad (1)$$

$$V_{\text{int}} = \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r} - \mathbf{r}') \chi_\sigma^\dagger(\mathbf{r}) \chi_{\sigma'}^\dagger(\mathbf{r}') \chi_{\sigma'}(\mathbf{r}') \chi_\sigma(\mathbf{r}) \quad (2)$$

where  $\chi_\sigma^\dagger = (\psi_\sigma^\dagger, \phi_\sigma^\dagger)$  creates an electron in valley  $\mathbf{K}$  ( $\mathbf{K}'$ ) for its upper (lower) component, and the repeated spin- $\frac{1}{2}$  indices  $\sigma$  are summed. The Bistritzer-MacDonald [8] (BM) continuum Hamiltonian [28,29,40,42,47] for twist angle  $\theta$  is

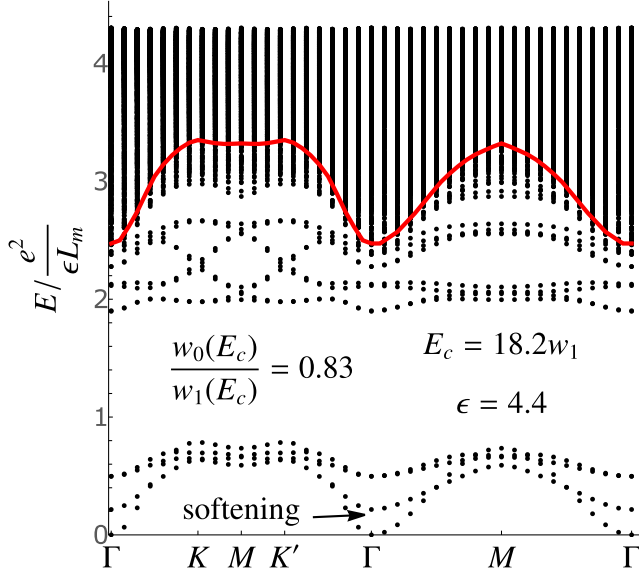


FIG. 3. The strong coupling exciton spectrum after stage 1 and 2 RG, starting the stage 1 with  $E_c = 18.2w_1$  corresponding to 2 eV for  $w_1 = 110$  meV,  $w_1/(v_F k_\theta) = 0.586$  (magic angle), and the initial  $w_0/w_1 = 0.83$ . The branch that becomes gapless at  $\Gamma$  corresponds to four Goldstone modes of the  $U(4)$  spin-valley ferromagnet with quadratic dispersion. Another branch, emphasized by the arrow, softens during the RG, eventually also becoming gapless in the chiral limit, with a total of eight Goldstone modes of the  $U(4) \times U(4)$  ferromagnet. The red curve is the onset of the particle-hole continuum.

$$\hat{H}_{\text{BM}} = \begin{pmatrix} v_F \sigma_{\frac{3}{2}} \cdot \mathbf{p} & T(\mathbf{r}) \\ T^\dagger(\mathbf{r}) & v_F \sigma_{-\frac{3}{2}} \cdot \mathbf{p} \end{pmatrix}, \quad (3)$$

where the twisted Pauli matrices acting on the sublattice indices are  $\sigma_{\frac{3}{2}} = e^{-i\frac{4}{3}\theta\sigma_z}(\sigma_x, \sigma_y)e^{i\frac{4}{3}\theta\sigma_z}$ ,  $\mathbf{q}_1 = k_\theta(0, -1)$ ,  $\mathbf{q}_{2,3} = k_\theta[(\pm\sqrt{3}/2), (1/2)]$ . The interlayer hopping  $T(\mathbf{r}) = \sum_{j=1}^3 T_j e^{-i\mathbf{q}_j \cdot \mathbf{r}}$  is controlled by two parameters  $w_{0,1}$  via

$$T_{j+1} = w_0 \mathbf{1}_n + w_1 \left[ \cos\left(\frac{2\pi}{3}j\right) \sigma_x + \sin\left(\frac{2\pi}{3}j\right) \sigma_y \right], \quad (4)$$

where  $\mathbf{1}_n$  is an  $n \times n$  unit matrix.  $\hat{H}_{\text{BM}}$  acts on its eigenfunctions

$$\Psi_{n,\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{g}} \begin{pmatrix} a_{n,\mathbf{g}}(\mathbf{k}) \\ b_{n,\mathbf{g}}(\mathbf{k}) e^{i\mathbf{q}_1 \cdot \mathbf{r}} \end{pmatrix} e^{i\mathbf{k} \cdot \mathbf{r}} e^{i\mathbf{g} \cdot \mathbf{r}}, \quad (5)$$

where  $\mathbf{g} = m_1 \mathbf{g}_1 + m_2 \mathbf{g}_2$  for integer  $m_{1,2}$  and  $\mathbf{g}_{1,2} = \mathbf{q}_{2,3} - \mathbf{q}_1$ . The slow fields at the two valleys  $\mathbf{K}/\mathbf{K}'$  are expanded in the ‘‘band’’ basis fermion annihilation operators  $d_{\sigma,\mathbf{K}/\mathbf{K}',n,\mathbf{k}}$  with crystal momentum  $\mathbf{k}$  in the first moiré Brillouin zone, and the band index  $n$  as

$$\chi_\sigma(\mathbf{r}) = \begin{pmatrix} \psi_\sigma(\mathbf{r}) \\ \phi_\sigma(\mathbf{r}) \end{pmatrix} = \sum_{n\mathbf{k}} \begin{pmatrix} \Psi_{n,\mathbf{k}}(\mathbf{r}) d_{\sigma,\mathbf{K},n,\mathbf{k}} \\ \Psi_{n,\mathbf{k}}^*(\mathbf{r}) d_{\sigma,\mathbf{K}',n,-\mathbf{k}-\mathbf{q}_1} \end{pmatrix}. \quad (6)$$

It will be helpful for us to think about  $H_{\text{kin}}$  as a lowest order gradient expansion of a continuum field theory [40], with coupling constants that can flow due to  $V_{\text{int}}$  under the first stage of the RG.

As pointed out in Ref. [42], if the small angle rotation in  $\sigma_{\theta/2}$  is ignored, then  $\hat{H}_{\text{BM}}$  enjoys a p-h symmetry for any value of  $w_0$  and  $w_1$ ,

$$-i\mu_y \sigma_x \hat{H}_{\text{BM}}^* \sigma_x i\mu_y = -\hat{H}_{\text{BM}}, \quad (7)$$

in that if  $\Psi_{n,\mathbf{k}}(\mathbf{r})$  is an eigenstate of  $\hat{H}_{\text{BM}}$  at  $\mathbf{k}$  with eigenvalue  $\epsilon_{n,\mathbf{k}}$ , then  $-i\mu_y \sigma_x \Psi_{n,\mathbf{k}}^*(\mathbf{r})$  is an eigenstate at  $-\mathbf{k} - \mathbf{q}_1$  with eigenvalue  $-\epsilon_{n,\mathbf{k}}$ . In what follows, we will neglect the small p-h asymmetric term which is 2 orders of magnitude smaller than  $w_{0,1}$  and which we analyze in Ref. [82], and perform our RG assuming this approximate symmetry is present.

Up to an overall shift of the chemical potential, we can rewrite  $V_{\text{int}}$  as

$$V_{\text{int}} = \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r} - \mathbf{r}') \delta\rho(\mathbf{r}) \delta\rho(\mathbf{r}'), \quad (8)$$

$$\delta\rho(\mathbf{r}) = \chi_\sigma^\dagger(\mathbf{r}) \chi_\sigma(\mathbf{r}) - \frac{1}{2} \{ \chi_\sigma^\dagger(\mathbf{r}), \chi_\sigma(\mathbf{r}) \}. \quad (9)$$

For a pure Coulomb interaction  $V(\mathbf{r}) = e^2/er$ . The Hamiltonian in Eqs. (1) and (2) is defined at some high energy cutoff  $\pm E_c$  which corresponds to a maximal value of the band index  $n_c$  in our expansion. The parameters  $v_F$ ,  $w_0$ , and  $w_1$  should also be thought of as being fixed by a measurement at  $E_c$ . The last term in Eq. (9) is usually ignored, but for our RG, it will be helpful to express it as  $\frac{1}{2} \{ \chi_\sigma^\dagger(\mathbf{r}), \chi_\sigma(\mathbf{r}) \} =$

$$\bar{\rho}_{E_c}(\mathbf{r}) = 2 \sum_{|\epsilon_{n\mathbf{k}}| \leq E_c} \Psi_{n,\mathbf{k}}^*(\mathbf{r}) \Psi_{n,\mathbf{k}}(\mathbf{r}). \quad (10)$$

In the first stage, we split  $\chi_\sigma(\mathbf{r}) = \chi_\sigma^>(\mathbf{r}) + \chi_\sigma^<(\mathbf{r})$  and integrate out the fast modes  $\chi_\sigma^>(\mathbf{r})$  with kinetic energy  $E'_c < |\epsilon_{n,\mathbf{k}}| \leq E_c$ , such that  $E'_c \gg w_{0,1}$ . In this regime, the  $V_{\text{int}}$  can be treated perturbatively. Its contribution to the slow mode Hamiltonian is then

$$V_{\text{int}} \rightarrow \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r} - \mathbf{r}') \delta\rho^<(\mathbf{r}) \delta\rho^<(\mathbf{r}') + \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r} - \mathbf{r}') \chi_\sigma^<\dagger(\mathbf{r}) \delta\mathcal{F}(\mathbf{r}, \mathbf{r}') \chi_\sigma^<(\mathbf{r}'), \quad (11)$$

where  $\delta\rho^<(\mathbf{r}) = \chi_\sigma^<\dagger(\mathbf{r}) \chi_\sigma^<(\mathbf{r}) - \bar{\rho}_{E'_c}(\mathbf{r})$  which follows from the p-h symmetry. The correction to the  $\hat{H}_{\text{BM}}$  comes from

$$\delta\mathcal{F}(\mathbf{r}, \mathbf{r}') = \sum_{E'_c < |\epsilon_{n\mathbf{k}}| \leq E_c} \text{sign}(\epsilon_{n\mathbf{k}}) \begin{pmatrix} f_{n,\mathbf{k}}(\mathbf{r}, \mathbf{r}') & 0 \\ 0 & f_{n,\mathbf{k}}^*(\mathbf{r}, \mathbf{r}') \end{pmatrix}, \quad (12)$$

where  $f_{n,\mathbf{k}}(\mathbf{r}, \mathbf{r}') = \Psi_{n,\mathbf{k}}(\mathbf{r})\Psi_{n,\mathbf{k}}^\dagger(\mathbf{r}')$ . We can now write

$$\sum_{E'_c < |\epsilon_{n\mathbf{k}}| \leq E_c} \text{sign}(\epsilon_{n\mathbf{k}}) f_{n,\mathbf{k}}(\mathbf{r}, \mathbf{r}') = \oint_{\mathcal{C}} \frac{dz}{2\pi i} \langle \mathbf{r} | \hat{G}(z) | \mathbf{r}' \rangle \quad (13)$$

where  $\hat{G}(z) = (z - \hat{H}_{\text{BM}})^{-1}$ , and the contour  $\mathcal{C}$  encloses the  $z$ -plane real line segment  $(-E_c, -E'_c)$  in the clockwise, and segment  $(E'_c, E_c)$  in the counterclockwise, sense. As long as  $E'_c \gg w_{0,1}$ , the dominant contribution to the contour integral can be found by replacing  $\hat{G}(z) \approx \hat{G}_0(z) + \hat{G}_0(z)\hat{T}\hat{G}_0(z) + \mathcal{O}(w_{0,1}^2/E_c^2)$ . For small  $E_c - E'_c$ , we thus find that in the first RG stage [82],

$$\frac{dv_F}{d \ln E_c} = -\frac{e^2}{4\epsilon}, \quad (14)$$

$$\frac{dw_0}{d \ln E_c} = 0, \quad (15)$$

$$\frac{dw_1}{d \ln E_c} = -w_1 \frac{e^2}{4\epsilon v_F}, \quad (16)$$

and  $e^2$ , being the prefactor of a nonanalytic term, does not renormalize when high energy modes are eliminated [83]. Integrating the above equations, i.e., progressively reducing the cutoff to  $E_c^*$  gives

$$\frac{w_1(E_c^*)}{v_F(E_c^*)} = \frac{w_1(E_c)}{v_F(E_c)}, \quad (17)$$

$$\frac{w_0(E_c^*)}{w_1(E_c^*)} = \frac{w_0(E_c)}{w_1(E_c)} \left/ \left( 1 + \frac{e^2}{4\epsilon v_F(E_c)} \ln \frac{E_c}{E_c^*} \right) \right. \quad (18)$$

Equation (17) implies that the magic angle condition is largely insensitive to the renormalization. Equation (18) shows that even if we start away from the chiral limit [47] at the UV scale  $E_c$ , at a lower energy scale  $E_c^*$  we approach it. Next, we combine this stage 1 RG with the nonperturbative (in moire potential) stage 2 numerical RG at  $6w_1 \gtrsim E_c^*$ , but we stress that results are insensitive to the choice of  $E_c^*$  as long as  $w_{1,0}/E_c^*$  is small so that stage 1 is under control. The scaling collapse of the band structure shown in the Fig. 2 demonstrates this insensitivity for  $w_1/v_F k_\theta = 0.5$ ,  $e^2/v_F = 2.2$ , and  $\epsilon = 4.4$  with several choices of  $n_c$ . We also find an increase of the sublattice polarization and steepening of the Wilson loops along the RG evolution [82], indicating a further approach of the chiral limit during stage 2.

Note that at each step of our procedure we rediagonalize the BM-like model in the subspace of the low energy bands

corrected by  $V_{\text{int}}$ . We also reexpress the  $V_{\text{int}}$  in Eq. (8) in terms of the current (rotated) eigenstates of the BM model below the running energy cutoff, and because  $\bar{\rho}_{E'_c}(\mathbf{r})$  is invariant under the basis rotation, the p-h symmetry is explicitly preserved. After the final step, we are thus left with two renormalized narrow bands per valley, and  $V_{\text{int}}$  containing  $\rho(\mathbf{r})$  and  $\bar{\rho}_0(\mathbf{r})$  both expressed in terms of the final renormalized wave functions  $\tilde{\Psi}_{n\pm,\mathbf{k}}(\mathbf{r})$ , with the upper and lower bands denoted by  $n+$  and  $n-$ , respectively. Because the p-h symmetry is preserved during this procedure, we can choose  $\tilde{\Psi}_{n-,\mathbf{k}}(\mathbf{r}) = -i\mu_y \sigma_x \tilde{\Psi}_{n+,-\mathbf{k}-\mathbf{q}_1}^*(\mathbf{r})$ . Substitution of such field operators Eq. (6) gives  $\rho(\mathbf{r}) = \sum_{\mathbf{k}\mathbf{k}'} \sum_{\sigma=\uparrow,\downarrow} D_{\mathbf{k}\sigma}^\dagger \mathcal{P}_{\mathbf{k}\mathbf{k}'}(\mathbf{r}) D_{\mathbf{k}'\sigma}$ , where within the narrow band  $D_{\mathbf{k}\sigma}^\dagger = (d_{\mathbf{K},n+,\mathbf{k}\sigma}^\dagger, d_{\mathbf{K},n-,\mathbf{k}\sigma}^\dagger, d_{\mathbf{K}',n+,\mathbf{k}\sigma}^\dagger, d_{\mathbf{K}',n-,\mathbf{k}\sigma}^\dagger)$ . Suppressing  $\mathbf{k}\mathbf{k}'$  and  $\mathbf{r}$  dependence,  $\mathcal{P} = b_0 1_4 + b_1 \tau_3 \tilde{\sigma}_1 + b_2 1_2 \tilde{\sigma}_2 + b_3 \tau_3 \tilde{\sigma}_3$ , thus commuting with all 16 generators of spin-valley  $U(4)$  symmetry [67]  $1_4 s_\mu$ ,  $\tau_3 1_2 s_\mu$ ,  $\tau_2 \tilde{\sigma}_2 s_\mu$ ,  $\tau_1 \tilde{\sigma}_2 s_\mu$ , where  $\mu = 0, 1, 2, 3$  and  $\tau$  acts on valley,  $\tilde{\sigma}$  on band, and  $s$  on spin components ( $s_0 = 1_2$ ).

If a state  $|\Omega\rangle$  is annihilated by  $\delta\rho(\mathbf{r})$  for all  $\mathbf{r}$ , then it is a ground state at the strong coupling because  $V_{\text{int}}$  is positive definite [48,67]. Moreover, any state obtained by a global  $U(4)$  rotation is also a ground state, and, at the CNP, can be obtained from a fully filled valley polarized state [48,67]. The exact  $n$ -body excitations above any one ground state can also be obtained by solving an  $(n-1)$ -body problem because  $V_{\text{int}} X |\Omega\rangle = \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r}-\mathbf{r}') \{ \delta\rho(\mathbf{r}), [\delta\rho(\mathbf{r}'), X] \} |\Omega\rangle$  and because the center of mass momentum is conserved. Therefore, solving the operator eigen equation

$$\text{EX} = \frac{1}{2} \int d^2\mathbf{r} d^2\mathbf{r}' V(\mathbf{r}-\mathbf{r}') \{ \delta\rho(\mathbf{r}), [\delta\rho(\mathbf{r}'), X] \}, \quad (19)$$

provides the exact excitation states in the strong coupling limit. Equation (19) can be readily solved for a single particle excitation and we show the result in Ref. [82]. Here we focus on the charge neutral excitations (excitons)  $X = \sum_{mm'\mathbf{k}} f_{mm'\mathbf{k}}^{\alpha\beta}(\mathbf{q}) d_{\alpha m, \mathbf{k}}^\dagger d_{\beta m', (\mathbf{k}-\mathbf{q}) \text{ mod } \mathbf{g}}$ , with spin and valley labels  $\alpha, \beta$ , by finding the eigenfunctions  $f_{mm'\mathbf{k}}^{\alpha\beta}(\mathbf{q})$ . Because of the spin-valley  $U(4)$  invariance of these equations, it is sufficient to solve for one spin and valley projection, the rest can be obtained by the symmetry. The numerically obtained exciton spectrum at the magic angle is shown in Fig. 3 for the center of mass momentum  $\mathbf{q}$  along the path shown in Fig. 1(b). The quadratically vanishing dispersion of the lowest branch corresponds to the four  $U(4)$  ferromagnetic Goldstone bosons [84]. Under the RG a second set of four modes softens. This corresponds to approaching the (“hidden”)  $U(4) \times U(4)$  invariant chiral limit [67] with its eight Goldstone bosons. Their gap is a measure of the  $U(4) \times U(4)$  anisotropy terms and for the parameters in the Fig. 3 this gap is  $\Delta_{U(4) \times U(4)} \approx 0.2e^2/\epsilon L_m \sim 5$  meV; the gap vanishes at the

chiral limit. Note that the modes disperse despite a complete absence of kinetic energy terms due to the nonlocal structure of the projected density operators [48].

The  $H_{\text{kin}}$  breaks the spin-valley  $U(4)$  symmetry down to  $U(2) \times U(2)$  and causes splitting of the degenerate ground state manifold. We can obtain an upper bound on the resulting anisotropy terms from second order perturbation in (renormalized) kinetic energy (i.e., “superexchange”) by replacing the energy of the excited states at  $\Gamma$  with the lowest energy exciton that has a nonzero overlap on the kinetic energy operator ( $E_{ph}^{\text{min}} \approx 2e^2/\epsilon L_m$  for Fig. 3). For a spin independent valley rotation, parameterized by three Euler angles,  $e^{i\frac{1}{2}\alpha\tau_3} e^{i\frac{1}{2}\omega\tau_2} e^{i\frac{1}{2}\beta\tau_3}$  we find that the energy splitting per unit cell,  $\Delta_{U(4)}$ , is bounded from above by  $-(\sin^2 \omega)4 \int d^2\mathbf{k} e_{n+\mathbf{k}}^2 / (A_{\text{BZ}} E_{ph}^{\text{min}})$ . The lowest energy state for such a rotation is the Kramers intervalley coherent state [67] at  $\omega = \frac{\pi}{2}$ . For the parameters in Fig. 3, we find that  $\Delta_{U(4)} < 6.7 \times 10^{-3} e^2/\epsilon L_m \sim 0.17$  meV, justifying the strong coupling approach.

The theory presented here can be extended to include the RPA effects and the p-h asymmetry, which will be important for any detailed quantitative comparison with experiments. Nevertheless, the Coulomb RG induced softening of the hidden symmetry collective modes, whose natural energy scale would normally be  $\sim e^2/\epsilon L_m \sim 25$  meV, suggests that they may not be frozen out even at  $\sim 50$  K. Finally, our results offer a significant shift of perspective in that the chiral limit [47]—previously considered unphysical—gains the status of an attractive mid-IR RG fixed point when  $E_c/w_1 \rightarrow \infty$ .

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