Supporting Information: Doped Twisted Bilayer Graphene near Magic Angles: Proximity to Wigner Crystallization not Mott Insulation

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1. Effects of Screening

The calculation presented in the main text assumes the presence of a long-range Coulomb interaction. However, this might be a bit stringent assumption especially for a system consisting of graphene layers. In order to understand the corrections originating from screening we evaluate the dielectric function under the random phase approximation (RPA). In particular, in this Appendix we compute the RPA corrected dielectric function under the static limit ($\omega = 0$),

$$\epsilon_{\text{RPA}}(\boldsymbol{q}) = \epsilon \left[1 - v_q \Pi(\boldsymbol{q})\right] . \tag{S1}$$

Here $v_q = 2\pi e^2/\epsilon q$ is the unscreened 2D Coulomb interaction, and $\Pi(\boldsymbol{q})$ is the single-particle bubble. Since we will be limiting our discussion to $T \to 0$, we express $\Pi(\boldsymbol{q})$ only in terms of the

inter-band scattering term,

$$\Pi(\boldsymbol{q}) = -g \int \frac{d^2k}{(2\pi)^2} \frac{2}{\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}'}} \left| \psi_+^\dagger(\boldsymbol{k}) \psi_-(\boldsymbol{k}') \right|^2 . \tag{S2}$$

Here, 2 appears since we work with a 2-band system and $\varepsilon_{\boldsymbol{k}}$ is the eigenvalue of the low-energy Hamiltonian in Eq. (3) [or see Eq. (4)] and the eigenvectors of this Hamiltonian are

$$\psi_+(\boldsymbol{k}) = \frac{1}{\sqrt{2}\varepsilon_{\boldsymbol{k}}} \begin{pmatrix} v_F \boldsymbol{k} + \frac{1}{2m} (\boldsymbol{k}^\dagger)^2 \\ \varepsilon_{\boldsymbol{k}} \end{pmatrix} \quad , \quad \psi_-(\boldsymbol{k}) = \frac{1}{\sqrt{2}\varepsilon_{\boldsymbol{k}}} \begin{pmatrix} -\varepsilon_{\boldsymbol{k}} \\ v_F \boldsymbol{k} + \frac{1}{2m} \boldsymbol{k}^2 \end{pmatrix} . \tag{S3}$$

Our notation here is, $\boldsymbol{k} = k_x + ik_y$, $\bar{\boldsymbol{k}} = k_x - ik_y$, $\boldsymbol{k}' = \boldsymbol{k} - \boldsymbol{q}$, and $\vec{k} = k(\cos\theta_{\boldsymbol{k}}, \sin\theta_{\boldsymbol{k}})$. The inter-band scattering cross-section can be simplified to

$$\begin{aligned} 2\varepsilon_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}'} \left| \psi_+^\dagger(\boldsymbol{k}) \psi_-(\boldsymbol{k}') \right|^2 &= \varepsilon_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}'} - v_F^2 \vec{k} \cdot \vec{k}' + \frac{k^2 k'^2}{4m^2} \left[1 - \frac{2}{k^2 k'^2} \left(\vec{k} \cdot \vec{k}' \right)^2 \right] \\ &+ \frac{3k^2 v_F}{2m} \left[q_x \cos(2\theta_{\boldsymbol{k}}) - q_y \sin(2\theta_{\boldsymbol{k}}) \right] . \end{aligned} \tag{S4}$$

The first term is simply the vacuum term, the second one is for SLG and the third one arises for bi-layer graphene. The last term, an intermediate term in powers of momenta, is present purely due to the twist angle. In obtaining the above form of this term, we have in fact dropped several other terms since they do not contribute to the bubble due to being odd-powered in momenta.

Instead of considering the full integration, which anyway is daunting task to perform analytically, we consider only the relevant limits. In fact, for $r_s \gtrsim 1$ the validity of such a perturbative expression in Eq. (S1) is questionable. In other words, for twist angles close to magic angle ($\theta - \theta_{\text{magic}} \lesssim 0.5^\circ$) such a calculation breaks down. We thus limit our discussion on screening-effects only to twist angles away from the magic angle, in other words when the dispersion is predominantly linear. In this case, only the first two terms in Eq. (S4) could contribute,

$$\text{SLG Limit :} \qquad E_U = \frac{1}{\epsilon_{\text{RPA}}} \frac{e^2}{r} \quad , \quad \epsilon_{\text{RPA}} = \epsilon \left(1 + \frac{\pi}{8} g\, r_s^{(1)} \right) = \epsilon + \pi\alpha\, \tilde{v}(\theta) . \tag{S5}$$

Here $\epsilon = 3 - 4$ is the dielectric constant of the hBN substrate[1] used for the TBLG sample and recall $g = 8$. This result can be understood by the following argument, since $\varepsilon_{\boldsymbol{k}} \sim k$ amounts to the high-energy limit, the electrons of the two layers are almost decoupled, leading to a long-range and sing-layer like behavior, as obtained in Ref.[2] for SLG. This corrects the value of $r_s^{(1)}$ to

$$r_s^{(1,\,\mathrm{RPA})} = \frac{r_s^{(1)}}{1 + \pi r_s^{(1)}} \lesssim \frac{1}{\pi}\,. \tag{S6}$$

This is clearly much less than 1. In fact, for all practical twist angle considerations, one can assume r_s to be $1/\pi$, independent of the angle. However, we will be mostly interested in angles closer to the magic angle, for which we continue using $r_s(\theta, \nu)$ of Eq. (7). Keeping this in mind, we simply set $\tilde{v} = 1$ and work with $\epsilon_{\mathrm{RPA}} = 4 + \pi\alpha \approx 10$, that is precisely the value used in Ref. 1

Although not very meaningful, for the sake of completeness, we consider the other limit when the twist angle is very close to magic angle and thus making the (1st and) 3rd term in Eq. (S4) dominate. In this limit,[3] $\Pi(\boldsymbol{q}) = -N_0 \log 4$, where $N_0 = gm/2\pi$ is the density of states in the bi-layer graphene limit. The dielectric function becomes, $\epsilon_{\mathrm{RPA}}/\epsilon = 1 + q_{\mathrm{TF}}/q$, where $q_{\mathrm{TF}} = (\log 4) g\, me^2/\epsilon$ is the Thomas-Fermi screening vector. This screens the Coulomb interaction to

$$\text{BLG Limit :} \qquad E_U = \frac{2\pi e^2}{\epsilon\,(q + q_{\mathrm{TF}})} \xrightarrow{r \gg 1/q_{\mathrm{TF}}} \frac{1}{\epsilon q_{\mathrm{TF}}^2}\,\frac{e^2}{r^3}. \tag{S7}$$

2. r_s for Device D1

Here we apply the same method we used for M2 but for device D1. For that we extract m_* as a function of carrier density (Fig. 3b of Ref. 1) and compute the resultant r_s using Eq. (7) . Recall, D1 contains the discrepancy of $\nu = 2$ for hole-doped half-filling and $\nu = 2.2$ for electron doping. We obtain the value of r_s using Eq. (7) which is shown in Fig. S1 . We clearly see the dome-like behavior of r_s near $1/2$ and $3/4$ filling, a direct result of the dome seen in Fig. 5 near $\gamma = 1$ (see main text). As in the experimental data, there is no feature in r_s at $\nu = 1$. Also note the displacement of the peak in r_s away from $\nu = 2$. The dip in the conductance in Ref. 1 occurs also

occurs away from $\nu = 2$, however, in the opposite direction. Hence, at present no conclusion can be made.

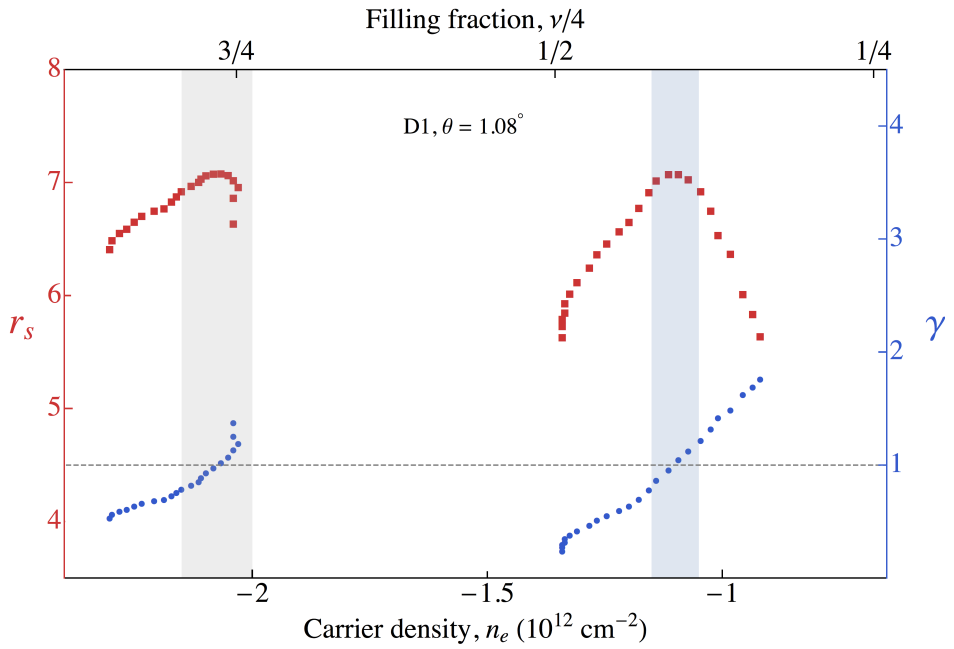

Figure S1: We redraw Fig. 4 of the main text, by using the effective mass data for sample D1. We observe maximization of r_s slightly away from $1/2$-filling but close to $3/4$-filling. The dome-like feature is a reminiscent of the one present in Fig. 3 (inset) in the main text. Since D1 is slightly away from the magic angle, it can access the small-γ region and achieve this maximization.

References

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