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Disorder-tuned selection of order in bilayer graphene

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The nature of the interaction driven spontaneously broken-symmetry state in charge neutral bilayer graphene (BLG) has attracted a lot of interest. Theoretical studies predict various ordered states as the candidates for the ground state of BLG, in the absence of external fields. Several experiments have been performed by different groups to identify the nature of the collective ground state in BLG. However, so far, there is no consensus: some experiments show evidence that suggests the establishment of a nematic gapless state, while others present results that are more consistent with the establishment of a fully gapped state. Moreover, even among the experiments that appear to see a bulk gap, some of the samples are found to be conducting (suggesting existence of gapless edge states), while others are insulating. Here we explore the hypothesis that disorder might explain the discrepancy between experiments. We find that the pair-breaking effect due to non-magnetic short-range disorder varies among the candidate ground states, giving rise to different amounts of suppression of their mean-field transition temperatures. Our results indicate that BLG can undergo a transition between different ordered states as a function of the disorder strength providing a simple and natural scenario to resolve the discrepancy between experimental observations.

AB-stacked bilayer graphene (BLG) [1–4] is formed by two graphene [5] layers rotated by 60^o with respect to each other and is the simplest multilayer graphene system. Its low-energy band structure is characterized by parabolic conduction and valence bands that touch at the corners, the K and K' points, of the Brillouin zone. BLG has become a model material to study the possible instabilities driven by interactions. A number of theoretical works have predicted various spontaneously-broken-symmetry states as the candidates for the ground state of BLG near the charge neutrality point in the absence of external fields [6–16]. The multiple degrees of freedom in BLG – layer, spin, and valley – give rise to the diversity of the candidate orders. In general, the proposed ordered states can be classified in two groups: (i) gapped states characterized by the opening of a full gap in the quasiparticle spectrum, and (ii) nematic states in which the quadratic band crossing points at which the conduction and valence bands touch are split into two Dirac points leaving the quasiparticle spectrum gapless. These two groups have a different structure with respect to the layer index: gapped states are layer-polarized while nematic states are not. Depending on the valley and spin structure different collective states can be identified in each general group. Gapped states with different spin-valley structures include the quantum valley Hall (QVH), quantum anomalous hall (QAH) and quantum spin hall (QSH) states, as well as a layer antiferromagnet (LAF). For a further discussion of gapped and nematic states with different spin-valley structures, see [15]. Within mean field theory, in the clean limit, the states in each group have the same transition temperature, $T^G_{c,0}$ for the gapped states, and $T^N_{c,0}$ for the nematic states.

Several experimental groups have made efforts to ascertain the nature of the ground state using high-quality suspended BLG [17–24]. They all find evidence of spontaneous symmetry breaking at low temperatures, confirming that electron-electron interactions have a strong effect in this system. However, they reach different conclusions on the identity of the ordered state: First, some experiments show evidence that supports the establishment of a nematic state [19], while others either present results that are more consistent with the establishment of a gapped state [20–24] or are consistent with both type of states [17, 18]; Second, among the experiments supporting the establishment of a gapped state, some indicate that the gapped state comes with conducting edge states [17, 18, 20, 24] and others indicate that the state is fully insulating [20–24] e.g. the LAF state. One explanation that has been proposed for this multitude of conflicting experimental results is that BLG is highly multi critical [25], and that different experimental samples fall in the basin of attraction of different correlated fixed points.

One important and unavoidable factor present in all materials that has the potential to strongly affect the formation of a broken symmetry state is disorder, due, for instance, to charge impurities, adatoms, vacancies, and ripples. For example, it is well known that the presence of magnetic impurities in BCS superconductors can strongly decrease the transition temperature (T_c) [26, 27]. The pair-breaking effect of magnetic impurities in BCS superconductors can be attributed to the different scattering off the impurities of the time-reversed fermionic states forming the Cooper pairs. Another example is the pair-breaking effect of normal impurities on exciton condensates [28, 29]. Since the broken-symmetry states in BLG involve particle hole pairing with different layer-spin-valley structures, we expect that different pairing structures could be affected differently by disorder. We consider only non-magnetic disorder, and do not take into account any spin flip scattering.

In this work, we study the effect of disorder on the broken-symmetry states in BLG near the charge neutrality point in the absence of external fields. Within mean field theory, in the clean limit, the transition temperature of the gapped states is higher than that of nematic states. However, we find that this scenario can be modified when the presence of disorder is taken into account. Considering non-magnetic short-range disorder, we find that in the presence of disorder that causes intravalley scattering only, the transition temperature of gapped states is suppressed more than the transition temperature of nematic states. Thus, within mean field theory, our result indicates that below a critical strength of disorder the system is prone to be in a gapped phase while above the critical disorder strength the nematic phase is favored, Fig. 1. In addition, we find that non-magnetic disorder producing inter valley scattering also contributes to the suppression of T_c for the valley unpolarized gapped states but does not affect T_c for the valley polarized gapped states. Since valley polarized gapped states have co-propagating edge modes in the two valleys (which cannot be gapped out in the absence of magnetic disorder), while valley unpolarized gapped states have counter propagating edge modes (which can be gapped out in the presence of inter valley scattering), our results on the effect of inter valley disorder could also be part of the explanation of why some experiments see conducting states with a bulk gap while others see insulating gapped states.

The mean-field Hamiltonian ($\hat{H}$) that describes a broken-symmetry state of BLG can be written as: $\hat{H} = \hat{H}_0 + \hat{\Delta} + \hat{V}$ where

$$\hat{H}_0(\mathbf{k}) = \begin{bmatrix} \hat{h}(\mathbf{k}) & 0 \\ 0 & \hat{h}^*(-\mathbf{k}) \end{bmatrix}; \, \hat{h}(\mathbf{k}) = \begin{bmatrix} 0 & \varepsilon_k e^{-i2\theta_{\mathbf{k}}} \\ \varepsilon_k e^{i2\theta_{\mathbf{k}}} & 0 \end{bmatrix}, \tag{1}$$

$\hat{V}$ is the non-magnetic disorder potential, $\mathbf{k} = (k_x, k_y)$, $\theta_{\mathbf{k}} = \arctan(k_y/k_x)$, and $\varepsilon_k \equiv \frac{\hbar^2 k^2}{2m^*}$ with $m^* \approx 0.03 m_e$. $\hat{H}_0$ is degenerate in spin space, and $\hat{h}$ is a 2×2 matrix in layer space. The two groups of candidate orders are distinguished by the structure in layer-space of the order parameter: $\hat{\Delta} = \Delta_G \hat{\sigma}_z$ for the gapped states and $\hat{\Delta} = \Delta_N \hat{\sigma}_x$ for the nematic states (without loss of generality we have chosen the complex nematic order parameter Δ_N to be real), where $\hat{\sigma}$'s are Pauli matrices acting on the layer space. Taking into account the valley degree of freedom, we have $\hat{\Delta} = \Delta_G \hat{\sigma}_z \hat{\tau}_0$ ($\Delta_N \hat{\sigma}_x \hat{\tau}_0$) for the gapped (nematic) valley-independent states, and $\hat{\Delta} = \Delta_G \hat{\sigma}_z \hat{\tau}_z$ ($\Delta_N \hat{\sigma}_x \hat{\tau}_z$) for the gapped (nematic) valley-polarized states, where $\hat{\tau}$'s are Pauli matrices acting on the valley space. The disorder potential can be written in the general form $\hat{V} = \hat{U} + \hat{W}$, with $\hat{U} \sim U_\sigma \delta_{\sigma\sigma'} \hat{\tau}_0$ and $\hat{W} \sim W_\sigma \delta_{\sigma\sigma'} (\hat{\tau}_x + i\hat{\tau}_y)/2 + h.c.$, where U_σ (W_σ, W_σ^*) is the intravalley (intervalley) disorder potential in layer σ. The influence of disorder is taken into account using the self-consistent Born approximation. After averaging over disorder realizations, the effect of disorder is captured by the self-energy matrix $\hat{\Sigma}$ that renormalizes the quasiparticle wave function and the pairing vertex of the condensate.

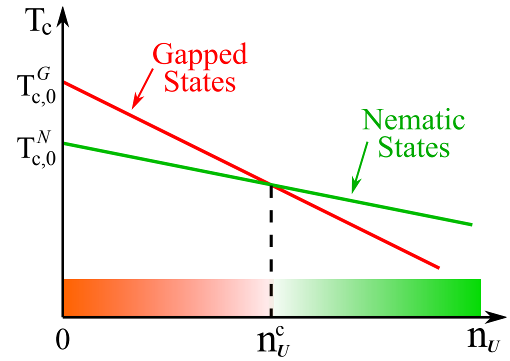

Figure 1: (Color online) Schematic illustration of the transition between the gapped phase and the nematic phase tuned by the strength of the intravalley disorder n_U. Below a critical strength, n_U^c, the gapped phase is favored, but above it the nematic phase becomes dominant.

We first consider the case in which disorder-induced valley-flip scattering processes are negligible, i.e., $\hat{W} = 0$. In this case, our discussion can be simplified to the 2×2 layer space since intravalley scattering does not lift the degeneracy between ground states that differ in valley structure. The key information is contained in the Green's function, $\hat{\mathcal{G}}$, determined by

$$\hat{\mathcal{G}}(\mathbf{k}, i\omega_n) = \left[i\omega_n \hat{\sigma}_0 - \hat{h}(\mathbf{k}) - \hat{\Delta} - \hat{\Sigma}(\mathbf{k}, i\omega_n) \right]^{-1}, \tag{2}$$

where $\omega_n = (2n+1)\pi T$ are the Matsubara frequencies, T is the temperature, and

$$\Sigma_{\sigma\sigma'}(\mathbf{k}, i\omega_n) = n_U \int \frac{d^2\mathbf{p}}{(2\pi)^2} U_{\sigma,\mathbf{k}-\mathbf{p}} \mathcal{G}_{\sigma\sigma'}(\mathbf{p}, i\omega_n) U_{\sigma',\mathbf{p}-\mathbf{k}} \tag{3}$$

is the disorder-averaged self-energy. Here n_U is the concentration of the randomly-distributed intravalley scattering centers. It is reasonable to assume n_U to be the same in the two layers.

For the gapped states, the self-consistency equation for the order parameter takes the form

$$\Delta_G = -\frac{1}{2} \Gamma_S T \sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2} \mathrm{Tr}\left[\hat{\sigma}_z \hat{\mathcal{G}}(\mathbf{k}, i\omega_n) \right], \tag{4}$$

where Γ_S is the effective coupling and $\mathrm{Tr}[\dots]$ takes the trace. The disorder renormalized Green's function can be written as

$$\hat{\mathcal{G}}_G(\mathbf{k}, i\omega_n) = \begin{bmatrix} i\tilde{\omega}_n - \tilde{\Delta}_G & -\varepsilon_k e^{-i2\theta_{\mathbf{k}}} \\ -\varepsilon_k e^{i2\theta_{\mathbf{k}}} & i\tilde{\omega}_n + \tilde{\Delta}_G \end{bmatrix}^{-1}, \tag{5}$$

where

$$\tilde{\omega}_n = \omega_n + n_U \int \frac{d^2\mathbf{p}}{(2\pi)^2} |U_{\mathbf{k}-\mathbf{p}}|^2 \frac{\tilde{\omega}_n}{\tilde{\omega}_n^2 + \varepsilon_p^2 + \tilde{\Delta}_G^2},$$
$$\tilde{\Delta}_G = \Delta_G - n_U \int \frac{d^2\mathbf{p}}{(2\pi)^2} |U_{\mathbf{k}-\mathbf{p}}|^2 \frac{\tilde{\Delta}_G}{\tilde{\omega}_n^2 + \varepsilon_p^2 + \tilde{\Delta}_G^2}. \quad (6)$$

In the above expressions we have assumed that the disorder strength is the same in the two layers, i.e., $|U_{\mathbf{k}-\mathbf{p}}| \equiv |U_{1,\mathbf{k}-\mathbf{p}}| = |U_{2,\mathbf{k}-\mathbf{p}}|$. In the case of short-range disorder potential $U_{\sigma,\mathbf{k}-\mathbf{p}} = U$, we obtain

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}\left(\frac{1}{\tau_2} + \frac{1}{\tau_1}\right)\frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_G^2}},$$
$$\tilde{\Delta}_G = \Delta_G - \frac{1}{2}\left(\frac{1}{\tau_2} - \frac{1}{\tau_1}\right)\frac{\tilde{\Delta}_G}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_G^2}}, \quad (7)$$

where $\frac{1}{\tau_2} = n_U U^2 \frac{m^*}{2\hbar^2}$ and $\frac{1}{\tau_1} = 0$. We can therefore see that for the gapped state the effect of intravalley disorder is analogous to the effect of magnetic impurities on BCS superconductivity [26]. From Eq. (4) and (7) the mean-field critical temperature T_c in the presence of disorder is given by a universal function in terms of the pair-breaking parameter δ [26],

$$\ln\left[\frac{T_{c,0}}{T_c}\right] = \psi\left(\frac{1}{2} + \frac{\delta}{2\pi T_c}\right) - \psi\left(\frac{1}{2}\right), \quad (8)$$

where $\psi(z)$ is the di-gamma function, and $T_{c,0}$ is the transition temperature in the clean limit. For the gapped phase $T_{c,0} = T_{c,0}^G$ with

$$k_B T_{c,0}^G = \frac{2}{\pi}\gamma E_c \exp\left[-\frac{4\pi\hbar^2}{\Gamma_S m^*}\right], \quad \gamma = 1.78, \quad (9)$$

and E_c a cutoff for the energy range of the interaction. The value of the pair-breaking parameter δ is $\delta_G \equiv \frac{1}{\tau_2} = n_U U^2 \frac{m^*}{2\hbar^2}$ for the gapped states. When $\delta_G/2\pi T_c \ll 1$, the transition temperature is linearly suppressed and we have $T_c^G = T_{c,0}^G - \frac{\pi}{4}\delta_G$.

For the nematic states, the self-consistency equation for the order parameter takes the form

$$\Delta_N = -\frac{1}{2}\Gamma_D T \sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2} \mathrm{Tr}\left[\hat{\sigma}_x \hat{\mathcal{G}}(\mathbf{k}, i\omega_n)\right], \quad (10)$$

where Γ_D is the effective inter-layer coupling. The renormalized Green's function after averaging over disorder can be written as

$$\hat{\mathcal{G}}_N(\mathbf{k}, i\omega_n) = \begin{bmatrix} i\tilde{\omega}_n & -\varepsilon_k e^{-i2\theta_\mathbf{k}} - \tilde{\Delta}_N \\ -\varepsilon_k e^{i2\theta_\mathbf{k}} - \tilde{\Delta}_N & i\tilde{\omega}_n \end{bmatrix}^{-1}, \quad (11)$$

where

$$\tilde{\omega}_n = \omega_n + n_U \times$$
$$\int \frac{d^2\mathbf{p}}{(2\pi)^2} |U_{\mathbf{k}-\mathbf{p}}|^2 \frac{\tilde{\omega}_n}{\tilde{\omega}_n^2 + \varepsilon_p^2 + \tilde{\Delta}_N^2 + 2\varepsilon_p \tilde{\Delta}_N \cos(2\theta_\mathbf{p})},$$
$$\tilde{\Delta}_N = \Delta_N - n_U \times$$
$$\int \frac{d^2\mathbf{p}}{(2\pi)^2} U_{1,\mathbf{k}-\mathbf{p}} U^*_{2,\mathbf{k}-\mathbf{p}} \frac{\varepsilon_p e^{-i2\theta_\mathbf{p}} + \tilde{\Delta}_N}{\tilde{\omega}_n^2 + \varepsilon_p^2 + \tilde{\Delta}_N^2 + 2\varepsilon_p \tilde{\Delta}_N \cos(2\theta_\mathbf{p})}. \quad (12)$$

Here again we assumed $|U_1| = |U_2|$. In order to discuss the influence on the phase transition temperature, we evaluate Eq. (12) in the limit $T \to T_c$, where the order parameter becomes vanishingly small, $\Delta_N \to 0$. Assuming short-range disorder, $U_{\sigma,\mathbf{k}-\mathbf{p}} = U_\sigma$, to leading order in Δ_N we obtain (for $\tilde{\omega}_n > 0$),

$$\tilde{\omega}_n = \omega_n + \frac{1}{2}\left(\frac{1}{\tau_2} + \frac{1}{\tau_1}\right)\frac{\tilde{\omega}_n}{\tilde{\omega}_n},$$
$$\tilde{\Delta}_N = \Delta_N - \frac{1}{2}\left(\frac{1}{\tau_2} - \frac{1}{\tau_1}\right)\frac{\tilde{\Delta}_N}{\tilde{\omega}_n}. \quad (13)$$

Linearizing Eq. (10) near T_c, we again find that the transition temperature satisfies Eq. (8), with the pair-breaking parameter $\delta_N = 1/\tau_2$, and that when $\frac{\delta_N}{2\pi T_c} \ll 1$, the mean-field transition temperature is linearly suppressed: $T_c^N = T_{c,0}^N - \frac{\pi}{4}\delta_N$. However, we have that both the clean limit transition temperature and the value of pair-breaking parameter are different from the ones obtained for the gapped phase. For the nematic phase, the mean-field transition temperature in the clean limit is given by

$$k_B T_{c,0}^N = \frac{2}{\pi}\gamma E_c \exp\left[-\frac{8\pi\hbar^2}{\Gamma_D m^*}\right]. \quad (14)$$

Notice that, assuming $\Gamma_D \approx \Gamma_S$, $T_{c,0}^N < T_{c,0}^G$ due to the fact that the absolute value of the argument of the exponent is a factor of 2 larger in Eq. (14) than in Eq. (9). Equation (12) shows that the renormalized quantity $\tilde{\Delta}_N$ depends on the correlation property between the disorder potentials in the two layers. When the disorder potentials in the two layers are perfectly correlated: $U_1 = U_2 \equiv U$, we have $\frac{1}{\tau_2} = n_U U^2 \frac{3m^*}{8\hbar^2}$, $\frac{1}{\tau_1} = n_U U^2 \frac{m^*}{8\hbar^2}$, so that $\delta_N = n_U U^2 \frac{3m^*}{8\hbar^2}$. In this case the relation between the pair-breaking parameter values in the two phases is $\delta_N = \frac{3}{4}\delta_G$. When the disorder potentials of the two layers are uncorrelated: $\Sigma_{12} = \Sigma_{21} = 0$, then $\frac{1}{\tau_2} - \frac{1}{\tau_1} = 0$. In the limit $T \to T_c$, $\frac{1}{\tau_2} = \frac{1}{\tau_1} = n_U U^2 \frac{m^*}{4\hbar^2}$, and the pair-breaking parameter becomes $\delta_N = n_U U^2 \frac{m^*}{4\hbar^2}$. In this case we have the relation $\delta_N = \frac{1}{2}\delta_G$. When the disorder potentials in the two layers are perfectly anti-correlated: $U_1 = -U_2$, in the limit $T \to T_c$, we have $\frac{1}{\tau_2} = n_U U^2 \frac{m^*}{8\hbar^2}$, $\frac{1}{\tau_1} = n_U U^2 \frac{3m^*}{8\hbar^2}$. Therefore the pair-breaking parameter becomes $\delta_N = n_U U^2 \frac{m^*}{8\hbar^2}$, so that

δ/δ_G	correlated	uncorrelated	anticorrelated
Gapped phase	1	1	1
Nematic phase	3/4	1/2	1/4

Table I: Comparison of the magnitudes of pair-breaking effect in the gapped and the nematic phase under different interlayer disorder correlation conditions.

	valley-polarized states (QAH, QSH)	valley-independent states (LAF, QVH)
δ/δ_G	1	$1+\frac{n_W\|W\|^2}{n_U U^2}$

Table II: Comparison of the magnitudes of pair-breaking effect between different valley-structured varieties of the gapped states.

$\delta_N = \frac{1}{4}\delta_G$. We summarize the magnitudes of the pair-breaking effect in the gapped and the nematic phases for different interlayer disorder correlation conditions in Table I. Irrespective of the interlayer correlations of disorder, the disorder suppression of T_c is weaker in the nematic state than in the gapped state, and thus disorder can drive a transition from a gapped state to a nematic state.

Next, we discuss the effect of intervalley disorder, i.e., $\hat{W} \neq 0$. Valley-flip processes distinguish between states with different valley structure. In the following we consider the case in which the two types of disorder potential $\hat{U}$ and $\hat{W}$ are uncorrelated, $|U_1| = |U_2| \equiv U$, $|W_1| = |W_2| \equiv |W|$, and the density of intervalley scattering centers n_W is the same in the two layers. In the gapped phase, taking into account the presence of intervalley scattering, for the valley-independent states (LAF, QVH) the scattering rates in Eq. (7) become: $\frac{1}{\tau_2} = \left(n_U U^2 + n_W |W|^2\right)\frac{m^*}{2\hbar^2}$, $\frac{1}{\tau_1} = 0$, indicating an enhancement on the pair-breaking effect characterized by $\delta_{G,v} = \left(n_U U^2 + n_W |W|^2\right)\frac{m^*}{2\hbar^2} = \delta_G\left(1+\frac{n_W|W|^2}{n_U U^2}\right)$. On the other hand, for the valley-polarized states (QAH, QSH), we obtain $\frac{1}{\tau_2} = n_U U^2\frac{m^*}{2\hbar^2}$, $\frac{1}{\tau_1} = n_W |W|^2\frac{m^*}{2\hbar^2}$, indicating that the pair-breaking effect is unaltered since the influence of the intervalley disorder only introduces a non pair-breaking component. Table II summarizes the effect of intervalley scattering on the different gapped states. Our results suggest that the valley-independent states (LAF, QVH) are more likely to appear in samples with very low disorder while the valley-polarized states (QAH, QSH) could survive at higher disorder concentrations. For the nematic phase we find that if W_1 and W_2 are uncorrelated, states with different valley structure are equally affected and therefore the intervalley disorder does not favor a specific valley-structure.

In conclusion, we find that in the presence of non-magnetic short-range intravalley disorder, the resulting pair-breaking effects have different magnitude in the gapped and the nematic phase: the transition temperature is suppressed more strongly in the gapped phase than in the nematic phase. Moreover, we find that in the nematic phase the pair-breaking effect of the disorder depends significantly on the interlayer correlation properties of the disorder: the pair-breaking effect is weaker in the uncorrelated case than in the perfectly correlated case, and it is weakest for the case of perfectly anticorrelated disorder. We also find that the presence of inter-valley disorder enhances the pair-breaking effect of disorder for the valley-independent gapped states (which have counter propagating edge modes that can be gapped out to give a fully insulating state) but that it merely contributes a non pair-breaking component to the valley-polarized gapped states (which have co-propagating edge modes). We therefore postulate that clean BLG might have a valley-independent gapped ground state (e.g. LAF or QVH), which does not have protected edge modes, but that small amounts of inter valley disorder can drive it into a valley polarized gapped state with edge modes (e.g. QAH or QSH), and that intra valley disorder can drive it into a nematic state. Therefore, our results provide a natural explanation for the discrepancies between the experiments that have recently been done to assess the nature of the BLG collective ground state in the absence of external fields.

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