Wess-Zumino-Witten Terms in Graphene Landau Levels

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(Received 30 November 2014; published 1 June 2015)

We consider the interplay between the antiferromagnetic and Kekulé valence bond solid orderings in the zero energy Landau levels of neutral monolayer and bilayer graphene. We establish the presence of Wess-Zumino-Witten terms between these orders: this implies that their quantum fluctuations are described by the deconfined critical theories of quantum spin systems. We present implications for experiments, including the possible presence of excitonic superfluidity in bilayer graphene.

DOI: 10.1103/PhysRevLett.114.226801 PACS numbers: 73.22.Pr, 75.10.Jm, 72.80.Vp

Introduction.—A number of recent experimental [1–7] and theoretical [8–19] works have focused on the presence of antiferromagnetism in neutral monolayer and bilayer graphene in an applied magnetic field. It has also been argued that a nonmagnetic state with lattice symmetry breaking in the Kekulé valence bond solid (VBS) pattern (see Fig. 1) is proximate to the antiferromagnetic (AF) state [13,14,17,18]. Bilayer graphene offers a particularly attractive area for studying the interplay between the AF and VBS order because it may be possible to tune between them by applying a transverse electric field [1,14,18].

The presence of the competing AF and VBS orders sets up the possibility [18] of novel quantum criticality between these orders, similar to that found in insulating quantum spin models [20–30]. However, these quantum spin models apply in the limit of very large on-site Coulomb repulsion between the electrons, and this is not the appropriate parameter regime for graphene. Here we examine a complementary limit of large magnetic field and moderate interactions, so that it is permissible to project onto an effective Hamiltonian acting only on the zero energy Landau levels. Such a limit has been widely used with considerable success in describing the properties of graphene. (Note, however, that we are still in the regime where the cyclotron gap is still smaller than the tight-binding hopping parameters, with magnetic fields smaller than 10 T.) Our main new result is that the Landau level projected effective action for the AF and VBS orders has a topological Wess-Zumino-Witten (WZW) term [31–33] for both the monolayer and bilayer cases.

The WZW term has a quantized coefficient, and it computes a Berry phase linking together spatial and temporal textures in the AF and VBS orders. It can be viewed as a higher dimensional generalization of the Berry phase of a single spin S degree of freedom, which is equal to S times the area enclosed by the spin worldline on the unit sphere. Similarly, the WZW term here measures the area on the surface of the sphere in the five-dimensional AF and VBS order parameter space. The presence of this term implies [34–36] that the field theories of deconfined criticality [21,22] apply to graphene. Such theories describe the quantum phase transition not in the conventional Landau terms of fluctuating order parameters, but using fractionalized degrees of freedom coupled to emergent gauge fields. We will also discuss experimental implications of these results.

Model and results.—We begin by directly stating the Hamiltonian of the low energy graphene bands (see, e.g., Refs. [16,18] for details)

$$H = v\begin{pmatrix} 0 & a^q \\ a^{\dagger q} & 0 \end{pmatrix}, \tag{1}$$

where v is a Fermi velocity, $a = p_x - ip_y - (e/c)(A_x - iA_y)$ with (p_x, p_y) the electron momentum, (A_x, A_y) is the vector potential of the applied magnetic field, the matrix acts on the graphene sublattice index, and $q = 1$ for monolayer graphene, while $q = 2$ for the bilayer case. For bilayers, the sublattice index coincides with the layer index. For both monolayers and bilayers, there is an additional twofold valley degeneracy, along with the usual twofold spin degeneracy (in the absence of a Zeeman coupling).

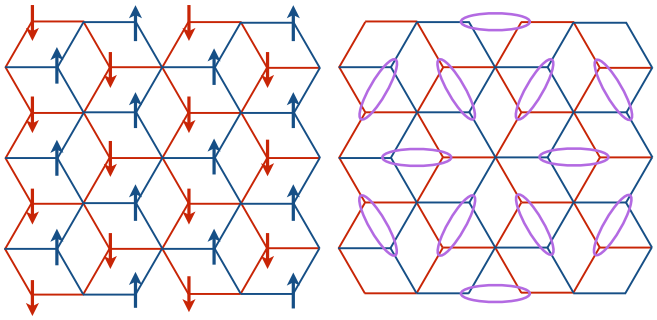

FIG. 1 (color online). AF (left) and Kekulé VBS states of bilayer graphene. The blue (red) lines indicate the honeycomb lattice of the top (bottom) layer. The ellipses in the VBS state denote the links between the top and bottom layers which are equivalently distorted with respect to the parent lattice.

The a, $a^\dagger$ obey commutation relations proportional to those of the ladder operators of a harmonic oscillator, and so it is easy to diagonalize H. In this manner we obtain q zero energy Landau levels, which are spanned by the orthonormal eigenfunctions $\psi_l(\boldsymbol{r})$, where $l = 1, \ldots, qN_\Phi$, with N_Φ the number of flux quanta. So we write the electron annihilation field operator projected to the zero energy Landau levels as

$$\Psi(\boldsymbol{r}) = \sum_{l=1}^{qN_\Phi} \psi_l(\boldsymbol{r}) c_l, \tag{2}$$

where c_l is canonical fermion annihilation operator. In the zero energy Landau levels, the valley, sublattice, and layer indices all coincide; henceforth we will refer to this as a valley index, and it can take two values. The fermion operators also carry a spin index with two possible values, and we do not explicitly display the spin or valley indices.

We now introduce Pauli matrices $\sigma^{x,y,z}$ which act on the spin space, and a second set $\rho^{x,y,z}$ which acts on the valley space (here we follow the conventions of Ref. [18]). In terms of these matrices, the three-component AF order is measured by $(\rho^z\sigma^x, \rho^z\sigma^y, \rho^z\sigma^z)$ while the two-component VBS order parameter is (ρ^x, ρ^y).

It is convenient to write the above matrices as

$$\Gamma_1 = \rho^z\sigma^x, \qquad \Gamma_2 = \rho^z\sigma^y, \qquad \Gamma_3 = \rho^z\sigma^z,$$
$$\Gamma_4 = \rho^x, \qquad \Gamma_5 = \rho^y$$

and to notice that the 5 Γ_a matrices anticommute and square to unity; indeed these are the 5 Dirac gamma matrices. Their 10 products $i\Gamma_a\Gamma_b$ $(a \neq b)$ realize the Lie algebra of SO(5), and the 15 matrices Γ_a and $i\Gamma_a\Gamma_b$ realize the Lie algebra of SU(4).

Next, we introduce a five-component unit vector $n_a(\boldsymbol{r}, \tau)$, where $\boldsymbol{r} = (x, y)$ are the spatial coordinates and τ is imaginary time, representing the combined spacetime fluctuations of the AF and VBS orders. Then the imaginary time Lagrangian of the electrons projected to the zero energy Landau levels is

$$\mathcal{L} = \sum_{l=1}^{qN_\Phi} c_l^\dagger \frac{\partial c_l}{\partial \tau} - \lambda \int d^2\boldsymbol{r} n_a(\boldsymbol{r}, \tau) \Psi^\dagger(\boldsymbol{r}, \tau) \Gamma_a \Psi(\boldsymbol{r}, \tau), \tag{3}$$

where λ is the coupling of the electrons to the AF and VBS orders, and there is an implicit sum of a over five values, and also over the spin and valley indices. The λ term arises from a decoupling of the electron-electron interactions specified in Refs. [13,17,18].

Now we can state our primary result. We integrate over the c_l electrons in $\mathcal{L}$ and obtain an effective action for unit vector $n_a(\boldsymbol{r}, \tau)$. Apart from the usual terms of the O(5) nonlinear sigma model considered in Ref. [17] (and anisotropies due to the Zeeman coupling, electron-electron interactions, and a possible transverse electric field for bilayers), the effective action has a topological WZW term at level q,

$$\mathcal{S}_{\rm WZW} = 2\pi i q W[n_a],$$
$$W[n_a] = \frac{3}{8\pi^2} \int_0^1 du \int d^2\boldsymbol{r} d\tau \epsilon_{abcde} n_a \partial_x n_b \partial_y n_c \partial_\tau n_d \partial_u n_e. \tag{4}$$

Here we have introduced the extra coordinate u, and $n_a(\boldsymbol{r}, \tau, u)$ is any function which smoothly extrapolates from the physical $n_a(\boldsymbol{r}, \tau)$ at $u = 1$ to a fixed value (say) $n_a = (1, 0, 0, 0, 0)$ at $u = 0$. The choice of the extrapolation can only change $W[n_a]$ by integers, and so $e^{2\pi i q W}$ is well defined.

In the case of graphene in zero magnetic field and weak interactions, the same WZW term between the Néel and VBS orders is also present [37]. However, for the experimentally important case of bilayer graphene, there is no such WZW term for the AF and VBS orders at zero field and weak interactions [18,38] (although, E.-G. Moon has noted such a term for the quantum spin Hall order [38]); so, in this case the zero energy Landau level projection is crucial for obtaining the topological coupling.

Such a WZW term has a strong impact in the interplay between the order parameters. As we will review below, it topologically links AF order to defects of the VBS order, and vice versa.

Derivation.—We provide two derivations of Eq. (4).

First, pick any three of the five n_a components, say $a = u, v, w$, and set the other two to zero. Then we have unit 3-vector field $\vec{N} = (n_u, n_v, n_w)$. Now consider a static Skyrmion texture in $\vec{N}(\boldsymbol{r})$. Then by a computation parallel to that in Section III.B of K. Moon *et al.* [39] (and its generalization to $q = 2$ [40]), the Skyrmion acquires a "charge." In the present situation the charge is measured by $i\Gamma_u\Gamma_v\Gamma_w$ and its spatial density is [41]

$$\langle \Psi^\dagger(\boldsymbol{r}) i\Gamma_u\Gamma_v\Gamma_w \Psi(\boldsymbol{r}) \rangle = \frac{q}{2\pi} \vec{N} \cdot (\partial_x \vec{N} \times \partial_y \vec{N}), \tag{5}$$

where the angular brackets represent the expectation value over the occupied states in the zero energy Landau level perturbed by the texture in $\vec{N}$ as in $\mathcal{L}$. (A similar relationship has been noted in monolayer graphene in zero magnetic field [42]; however, no such relationship applies to bilayer graphene in zero field.) Now consider a VBS vortex, i.e., a 2π vortex in (n_4, n_5) applied to $\mathcal{L}$. For a two-component order, the core of the vortex has a singularity, but this can be relieved by orienting n_a in a third direction, say $(\pm 1, 0, 0, 0, 0)$. Now the VBS vortex is equivalent to a half-Skyrmion in $\vec{N} = (n_1, n_4, n_5)$, and after integrating Eq. (5) over all space, this vortex has $\langle \sigma^x \rangle = \pm q$. Similarly, vortex cores in the directions $(0, \pm 1, 0, 0, 0)$ and

$(0,0,\pm 1,0,0)$ yield $\langle \sigma^y \rangle = \pm q$ and $\langle \sigma^z \rangle = \pm q$. So we reach the important conclusion that the VBS vortex has total spin $S = q/2$, and has an associated $(q+1)$-fold degeneracy. For $q = 1$, note that this is precisely the situation considered in Ref. [43] for quantum spin models (see also Ref. [44]). Alternatively, we can examine the fate of $\mathcal{S}_{\rm WZW}$ in the presence of such VBS vortices: following a computation by Grover and Senthil [36], we find that the WZW term reduces to the quantum Berry phase of a single spin with $S = q/2$. From this we conclude that Eq. (5) implies Eq. (4).

For a second derivation of the WZW term from Eq. (3), we examine a diagrammatic expansion of $\mathcal{L}$. Consider a situation where n_a is polarized near, say, (0,0,0,0,1). Then, we can write $n_a = (\pi_1, \pi_2, \pi_3, \pi_4, 1)$ where $|\pi_i| \ll 1$ for $i = 1, \ldots, 4$. Then to zeroth order in the π_i, the c_l operators in $\mathcal{L}$ have the Green's function

$$G = (i\omega + \lambda \Gamma_5)^{-1}, \tag{6}$$

where ω is the frequency of the electron propagator. We now proceed to integrate out the electrons, and derive an effective action for the π_i. At fourth order in the π_i, we consider the box diagram in Fig. 2; this can be evaluated by methods similar to those in Ref. [18], but with the G above, and the vertices contributing the factors implied by Eq. (3). A computation described in the Supplemental Material [41] yields the contribution

$$\mathcal{S}_\pi = \frac{i3q}{16\pi} \int d^2\mathbf{r} d\tau \epsilon_{ijkm} \pi_i \partial_x \pi_j \partial_y \pi_k \partial_\tau \pi_m. \tag{7}$$

It can be checked that Eq. (4) reduces to $\mathcal{S}_\pi$ for $n_a = (\pi_1, \pi_2, \pi_3, \pi_4, 1)$, and so $\mathcal{S}_{\rm WZW}$ is the explicitly SO(5) invariant form of $\mathcal{S}_\pi$.

Theoretical consequences.—We now turn to a discussion of the theoretical consequences of the WZW term for the vicinity of the AF-VBS transition. For $q = 1$, it has been

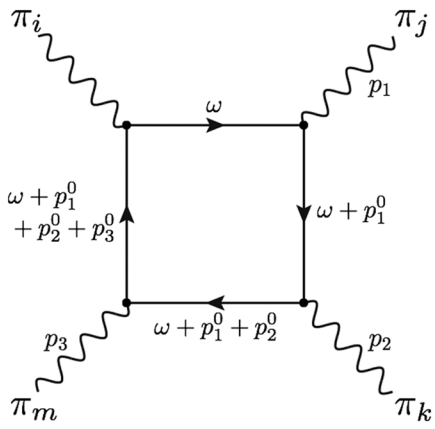

FIG. 2. Box diagram leading to $\mathcal{S}_\pi$. The full lines are the Green's function in Eq. (6) at the labeled frequencies, and the vertices are the λ term in Eq. (3).

demonstrated in Refs. [35,36,43] that the O(5) nonlinear sigma model with $O(3) \times O(2)$ anisotropy and a level 1 WZW term is equivalent to the CP^1 model in $2+1$ dimensions. This is the same model appearing in the AF-VBS transition of SU(2) quantum spin models [21,22], and is a relativistic field theory with a U(1) gauge field and a two-component complex scalar z_α. In terms of these fields, the AF order is $z_\alpha^* \sigma^s_{\alpha\beta} z_\beta$, with $s = x, y, z$; so the vector AF order has been "fractionalized" into spinons z_α. Alternatively, we can also view the z_α quanta as representing the vortices or antivortices in the VBS order [43] which, as we have just seen, carry spin $S = 1/2$.

Presently, the experimentally accessible case of the AF-VBS transition is in bilayer graphene, so we focus now on the $q = 2$ case. With a level 2 WZW term, the VBS vortices carry spin $S = 1$, and therefore we need complex scalar fields with three components: we write these as Z_s, with $s = x, y, z$. The field theory of the Z_s quanta is now the CP^2 model with anisotropic quartic terms; such a field theory was considered in Ref. [45] in a different context:

$$\mathcal{L}_{cp} = |(\partial_\mu - iA_\mu) Z_s|^2 + g|Z_s|^2 + u_1(|Z_s|^2)^2 + u_2(Z_s^2)(Z_t^{*2}).$$

Here μ is a spacetime index, A_μ is the emergent U(1) gauge field, g is the coupling which tunes the AF to VBS transition, and $u_{1,2}$ are quartic couplings. In terms of the degrees of freedom in $\mathcal{L}_{cp}$, the three-component AF order parameter is now $i\epsilon_{stu} Z_t^* Z_u$, while the complex VBS order $\langle \rho^x + i\rho^y \rangle \sim e^{i\theta}$ is the monopole operator in the U(1) gauge field [20,22].

For both the CP^1 and CP^2 models mentioned above, both first and second order transitions are possible between the AF and VBS states. A recent numerical study [17] on a single layer model indicates a first order transition for the parameters studied.

Experimental implications.—Finally, we turn to experimental consequences for bilayer graphene. The defining characteristic of deconfined criticality is the presence of a gapless "photon" excitation of an emergent U(1) gauge field [21]. This is associated with the A_μ above, and can also be interpreted as a "spin-wave" excitation involving fluctuations of the angle θ. Our definition of θ shows that it is the angular phase associated with off-diagonal-long-range order (ODLRO) in valley space. The valley anisotropy terms in graphene are very small [13,17], because it is suppressed by powers of the lattice spacing to the magnetic length; so we expect a nearly gapless θ spin-wave mode to be present (and most of the remarks below to also apply) even in the case of a first-order transition.

Now recall the fact, noted earlier, that in the zero energy Landau levels the valley index coincides with the layer index of bilayer graphene (and also the sublattice index). So ODLRO in valley space is accompanied by ODLRO in the

layer space; i.e., θ is also the angular phase of interlayer excitonic superfluidity. Signatures of excitonic superfluidity have been observed in quantum Hall states in GaAs bilayers [46]. However, in the GaAs bilayers there is negligible tunneling of electrons between the layers, and this crucial to the emergence of a U(1) symmetry which is broken by the excitonic condensate. So it might seem surprising that a similar superfluidity can be present in graphene bilayers, in the presence of very strong tunneling between the layers. The resolution is the identification of the layer and valley indices in the zero energy Landau levels of bilayer graphene: in the absence of intervalley scattering by impurities, and the irrelevancy of valley anisotropy terms to be presented below, there is also an emergent interlayer U(1) symmetry in bilayer graphene.

The counterflow electrical current can be written in terms of the gauge field

$$J_{t\mu} - J_{b\mu} = \frac{4e}{2\pi}\epsilon_{\mu\nu\lambda}\partial_\nu A_\lambda, \tag{8}$$

where J_t and J_b are the currents in the top and bottom layers, and e is the charge of the electron. The factor of 4 is deduced from Eq. (5), which shows that a AF Skyrmion in (n_1, n_2, n_3) has excitonic charge density $\langle \rho^z \rangle = 4$ for $q = 2$. The counterflow conductivity can be computed from Eq. (8) using $\mathcal{L}_{cp}$; at the $g = g_c$ deconfined quantum critical point this implies a universal value of order, the quantum unit of conductance e^2/h.

For $g > g_c$, in the VBS state, the conductivity should be computed using an effective action for θ which includes the influence of monopoles. Now the current is

$$J_{t\mu} - J_{b\mu} = 4e\rho_s \partial_\mu \theta, \tag{9}$$

where ρ_s is the stiffness of the excitonic superfluidity appearing the effective Lagrangian density

$$\mathcal{L}_\theta = \frac{\rho_s}{2}(\partial_\mu \theta)^2 - y_3 \cos(3\theta), \tag{10}$$

with y_3 the fugacity of tripled monopoles which are allowed by the threefold rotational symmetry of the underlying honeycomb lattice [20]. The stiffness vanishes as $\rho_s \sim (g - g_c)^\nu$ by the Josephson relation, where ν is the correlation length exponent. Away from the critical point, the bare value y_3^0 is proportional to the very small threefold valley anisotropy term [13,17]; y_3 has a further suppression [22,47] from the critical fluctuations of $\mathcal{L}_{cp}$ leading to $y_3 = y_3^0 (g - g_c)^{\nu\Delta}$, where Δ is the scaling dimension of the tripled monopole operator. So the effective "interlayer tunneling" term, y_3, is highly suppressed near the deconfined quantum critical point. We also note that numerical studies on square lattice antiferromagnets have provided striking evidence for the emergent U(1) symmetry due to the suppression of monopoles [48], and there is direct evidence for the suppression of monopoles on the honeycomb lattice in the work of Block *et al.* [27].

In GaAs bilayers [46], the excitonic superfluidity is most directly observed in counterflow experiments, where electric currents flow in the opposite direction in the two layers. This would be technically more difficult in bilayer graphene, given the close spacing of the layers, but experiments of this type would be ideal. In the bilayer graphene experiments of Weitz *et al.* [1], there is a Zeeman coupling to the magnetic field (whose consequences have been studied earlier [22]), and an electric field is applied transverse to the layers. The electric field provides a small breaking of the layer-exchange symmetry. In the presence of such a symmetry breaking, there is a coupling between the counterflow and parallel current modes, and a vestige of the counterflow superfluidity would also be present in a measurement of the total current in both layers. Weitz *et al.* observe a phase transition out of the (presumed) AF state, signaled by the enhancement of the conductivity. We propose that this enhancement is due to the coupling to counterflow superfluidity.

We thank D. Abanin, Eun-Gook Moon, E. Shimshoni, T. Senthil, I. Sodemann, and A. Yacoby for useful discussions. This research was supported by the NSF under Grant No. DMR-1360789, the Templeton foundation, and MURI Grant No. W911NF-14-1-0003 from ARO. Research at Perimeter Institute is supported by the Government of Canada through Industry Canada and by the Province of Ontario through the Ministry of Research and Innovation. J. L. is also supported by the STX Foundation.

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