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Itinerant Half-Metal Spin-Density-Wave State on the Hexagonal Lattice

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We consider electrons on a honeycomb or triangular lattice doped to the saddle point of the band structure. We assume the system parameters are such that spin density wave (SDW) order emerges below a temperature $T_N$ and investigate the nature of the SDW phase. We argue that at $T \equiv T_N$, the system develops a uniaxial SDW phase whose ordering pattern breaks $O(3) \times Z_4$ symmetry and corresponds to an eight-site unit cell with nonuniform spin moments on different sites. This state is a half-metal—it preserves the full original Fermi surface, but has gapless charged excitations in one spin branch only. It allows for electrical control of spin currents and is desirable for nanoscience.

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Introduction.—The electronic properties of single-layer graphene have been the subject of considerable experimental and theoretical interest [1]. Near half-filling, a description in terms of noninteracting Dirac electrons captures the essential physics, since interactions effects are suppressed by the low density of states (DOS). A sharply different behavior arises when graphene is strongly doped to 3/8 or 5/8 filling [2]. At this filling, a divergent density of states and nested Fermi surface (FS) conspire to produce weak coupling instabilities to an extensive buffet of ordered states, including spin density waves (SDW) [3–5], Pomeranchuk metals [6], and d wave superconductors (SC) [7–9]. A similar situation arises on a triangular lattice at 3/4 filling [10,11].

It has recently been established using renormalization group (RG) methods [7] that the two most relevant instabilities at weak coupling are toward SDW and a d-wave SC. Other potential instabilities, like a charge-density wave, have much smaller susceptibilities. The SDW vertex is the largest at intermediate RG scales, but superconducting vertex eventually overshoots it, making d-wave superconductivity the leading weak coupling instability at the van Hove filling. The SC state has a $d + id$ gap structure and breaks time-reversal symmetry [7]. Upon doping away from van Hove filling, the Cooper and SDW channels decouple at a scale set by doping, and the RG flow is altered. In this situation, the SDW, which is the largest at intermediate RG scales, may become the dominant instability, and numerical functional RG studies found [8] that SDW is indeed the leading instability in substantially wide doping range away from 3/8 or 5/8. Previous work on SDW order argued that the SDW state is noncoplanar and has nonzero spin chirality [3,5,10]. Such a state gaps out the entire Fermi surface (FS).

We argue that the situation is more complex than originally thought, and the chiral SDW state is present only at the lowest temperatures. Over a wide intermediate range of temperatures, a different SDW state emerges in which SDW order develops simultaneously at three inequivalent wave vectors $Q_i$, but the three vector order parameters are all aligned along the same axis. This state has an eight-site unit cell with nonuniform spin moments and zero net magnetization [Fig. 1(b)]. Such a state cannot be accessed starting from a spin Hamiltonian for local moments with a fixed length and can only be accessed starting from a model of itinerant fermions. We show that in this state, unlike in any other known SDW state, the chemical potential shifts proportionally to the SDW order parameter, preserving the original Fermi surface for one spin branch and gapping out the other spin branch. The uniaxial SDW state is therefore a “half-metal” that allows for electrical control of spin currents. Such a state is highly desirable for nanoscience applications.

SDW order quadruples the unit cell to a unit cell with eight sites on the other six. The total spin on each unit cell is zero.

FIG. 1 (color online). (a) The Fermi surface at the doping level of interest is a hexagon inscribed within a hexagonal Brillouin zone (BZ), for both honeycomb and triangular lattices. The FS has three inequivalent corners, which are saddle points of the dispersion, marked by a vanishing Fermi velocity and a divergent density of states. The three inequivalent saddle points $M_i$ are connected by three inequivalent nesting vectors $Q_i$, each of which is equal to half a reciprocal lattice vector, such that $Q_i = -Q_i$. (b) Spin structure for the uniaxial SDW state. The SDW order quadruples the unit cell to a unit cell with eight sites (shaded). The enlarged unit cell has a large spin moment $\Delta$ on two sites and a small spin moment $-\Delta$ on the other six. The total spin on each unit cell is zero.
The model.—For definiteness, we focus on doped graphene at 3/8 filling. Our point of departure is the tight binding model [12], with the nearest-neighbor dispersion

$$\varepsilon_k = -t_1 \sqrt{1 + 4 \cos \frac{k_y \sqrt{3}}{2} \cos \frac{3k_x}{2} + 4 \cos^2 \frac{k_y \sqrt{3}}{2} - \mu},$$

where $\mu = -t_1$ at 3/8 filling. The FS then forms a perfect hexagon inscribed within a hexagonal BZ [Fig. 1(a)]. The perfect nesting of the FS in doped graphene is quite robust—it is broken only by third and higher neighbor hoppings, which are generally quite small. The Fermi velocity vanishes near the hexagon corners $M_1 = (\pi/3, \pi/\sqrt{3})$, $M_2 = (2\pi/3, 0)$, $M_3 = (\pi/3, -\pi/\sqrt{3})$, which are saddle points of the dispersion:

$$\varepsilon_{M_1 + k} = \frac{3t_1}{4} (k_y^2 - 3k_x^2),$$

$$\varepsilon_{M_3 + k} = -\frac{3t_1}{4} 2k_y(k_y + \sqrt{3}k_x),$$

where each time $k$ denotes the deviation from a saddle point. Saddle points give rise to a logarithmic singularity in the DOS and control the SDW instability at weak coupling. There are three inequivalent nesting vectors connecting inequivalent pairs of saddle points [see Fig. 1(a)]:

$$Q_2 = (0, 2\pi/\sqrt{3}), \quad Q_{1,3} = (\pm \pi/3, -\pi/\sqrt{3}).$$

(3)

Each $Q_i$ is equivalent to $-Q_i$, modulo a reciprocal lattice vector.

For the interactions, we use the low energy model from [7], which provides an exact description of the system in the weak coupling limit. This model contains four interactions: density-density, exchange, pair-hopping, and forward scattering, labeled $g_1$, $g_2$, $g_3$, $g_4$, respectively. Of these, the interactions $g_4$ and $g_1$ do not couple to spin density waves [7] and may be safely ignored [13]. The SDW physics is controlled by the density-density interaction $g_2$ $(|k, k + Q_1| \rightarrow |k, k + Q_1|)$ and the umklapp pair-hopping interaction $g_3$ $(|k, k' \rightarrow |k + Q_2, k' + Q_2|)$. The partition function in the SDW sector can be written as $Z = \int D[\psi^\dagger, \psi] \exp(-S[\psi^\dagger, \psi])$, where $S = \int d^2 k (L(k, \tau)$ and

$$L = \sum_\alpha \psi_{a,a}(\partial_\tau - e_k + \mu)\psi_{a,a}$$

$$- \sum_\alpha g_3 \psi_{a,a}^\dagger \psi_{a,b}^\dagger \psi_{b,b} \psi_{b,a}$$

$$- g_2 \psi_{a,a}^\dagger \psi_{b,b} \psi_{a,a}$$

where the action is written in terms of electron operators, $a$, $b$ are patch labels, and $a$, $b$ are spin components.

Each nesting vector $Q_i$ is associated with it an SDW order parameter $\Delta_i = \Delta_{a,b} = \pm \frac{1}{\sqrt{3}} \sum_\Delta (\psi_{a,a}^\dagger \sigma_{a,b} \psi_{b,a})$. The condition for the emergence of each $\Delta_i$ is the same: $(g_2 + g_3)/t_1 \log^2 t_1/T_N = O(1)$ [7], leaving a large number of SDW states as potential candidates. We study the selection of the SDW order within Ginzburg-Landau theory and by comparing different SDW solutions in the mean-field approximation for Eq. (4) at arbitrary $T < T_N$.

Ginzburg-Landau theory.—To construct the Ginzburg-Landau theory, we decouple the quartic interaction terms by restricting the interaction to the spin channel and a Hubbard-Stratonovich transformation to collective spin variables $\Delta_i$. Note that the Hubbard Stratonovich transformation is exact and does not introduce any approximation. We integrate out the fermions in the Matsubara frequency representation and obtain an action in terms of $\Delta_i$ in the form

$$L = T \sum_{n = -\infty}^{\infty} \int \frac{d^2 k}{(2\pi)^2} \left[ \frac{2}{g_2 + g_3} \sum_i (\Delta_i)^2 \right] + \text{Tr} \ln \left( i\omega_n - e_k - \sum_i \Delta_i \cdot \sigma \right).$$

Finally, the third quartic term and sixth order terms are equivalent to $-\Delta_i/T_N$. It is useful to define the expansion coefficients

$$Z_i = \sum_{\omega_n} \int \frac{d^2 k}{(2\pi)^2} \xi_i,$$

where the integrands $\xi_i$ are expressed in terms of fermionic Green functions $G = ((i\omega_n - e_k - \mu)^{-1}$, $G_i = ((i\omega_n - e_k + Q_i - \mu)^{-1}$, and $G_{i+j} = (i\omega_n - e_k + Q_i + Q_j - \mu)^{-1}$ as

$$\xi_1 = G^2 G_3,$$

$$\xi_2 = G^2 G_3 G_1,$$

$$\xi_3 = G G_3 G_1 G_{1+3}, \quad \xi_4 = G G^2 G_3 G_1.$$ (7)

Diagrammatically, $Z_1$-$Z_3$ are given by “square” diagrams with four fermionic propagators and $\sigma_{a,b}$ in the vertices, and $Z_4$ is given by a “hegagonal” diagram with six fermionic propagators, (see Fig. 2). The free energy evaluated at $T = T_N$ can be expressed in terms of these coefficients as

$$L = \alpha(T - T_N) \sum_i \Delta_i^2 + Z_1 (\Delta_1^2 + \Delta_2^2 + \Delta_3^2)^2$$

$$+ 2(Z_2 - Z_1 - Z_3) (\Delta_1^2 \Delta_2^2 + \Delta_3^2)^2$$

$$+ 4Z_3 ((\Delta_1 \cdot \Delta_2)^2 + (\Delta_3 \cdot \Delta_1)^2 + (\Delta_1 \cdot \Delta_3)^2)$$

$$- 4Z_4 \Delta_1 \cdot \Delta_2 \times \Delta_3 + \cdots$$

(8)

where $\alpha$ is an inessential positive constant.

The quadratic term and the first quartic term in (8) set the overall magnitude of $\Delta_0^2$ but do not differentiate between different SDW states. The second quartic term in (8) determines whether SDW order develops only at one nesting vector or at all three (depending on the sign of $Z_2$-$Z_1$-$Z_3$). Finally, the third quartic term and sixth order term control the relative orientation of the vector order parameters, if SDW order develops at multiple wave vectors. Close to $T_N$, the expansion to order $\Delta_i^4$ is generally sufficient, but we include the sixth order term because $Z_3$ is suppressed by an extra factor of $T_N/t_1$, which is exponentially small in the weak coupling limit. The relative smallness of $Z_3$ arises because in the integrals for $Z_1$, $Z_2$, and $Z_4$, all fermions can be simultaneously brought to the saddle points, whereas in the integral for $Z_3$, three fermions can be
The smallest signs and relative magnitudes of \( C_1 \) smaller by \( TN = t \) order parameters is controlled by the sign of the state). Meanwhile, the relative orientation of the three order simultaneously at all three nesting vectors (the bagonal diagrams are shown above. The integrals are dominated produced by “hexagonal diagrams.” Sample square and hexagonal diagrams are represented diagrammatically by square diagrams. The diagrams for \( Z_2 \) and \( Z_3 \) correspond to patterns \( \Delta_3, \Delta_1, \Delta_1, \Delta_1 \) and \( \Delta_3, \Delta_1, \Delta_1, \Delta_1 \), respectively. The sixth order chirality sensitive term is represented by \( H = \delta_\mu \).

FIG. 2. The terms quartic in \( \Delta \) are produced by processes \( \Delta_1, \Delta_1, \Delta_1, \Delta_1 \) and \( \Delta_3, \Delta_1, \Delta_1, \Delta_1 \), respectively. The sixth order chirality sensitive term is represented by \( H = \delta_\mu \).

The positivity of \( Z_1 \) guarantees a second order phase transition, with the type of SDW order depending on the signs and relative magnitudes of \( Z_2, Z_3, \) and \( Z_4 \). Since \( Z_3 \) is smaller by \( T_N / t_1 \) than \( Z_{1,2} \), and \( Z_2 \) is smaller by \( \log T_N / t_2 \) than \( Z_1 \), it follows that \( Z_2, Z_{1,2}, Z_3 \), and \( Z_4 \) are negative and favor the nonchiral SDW order with the three \( \Delta_i \), all aligned along the same axis.

An order parameter of the form \( \Delta(e^{iQ \cdot r} + e^{-iQ \cdot r} \pm e^{0 \cdot r}) \) leads to spin moments on the lattice of the form shown in Fig. 1. A quarter of lattice sites have spin moment \( 3\Delta_i \), the other three quarters have moment \( -\Delta \). Such an order cannot be obtained from any spin Hamiltonian for local moments of constant magnitude on every site. Our result differs from earlier mean-field analysis [11] which found noncoplanar insulating SDW order at weak coupling. We note, however, the \( 3\Delta \) state that we found, with nonequal spin length on different sites, was not considered in that work and other earlier considerations of SDW order. We found analogous results for fermions on a triangular lattice at van Hove filling, which are described by an identical low energy theory provided we neglect further neighbor hopping.

Properties of a uniaxial SDW.—Is the uniaxial SDW state a metal or an insulator? To address this issue we need to compute the fermionic spectrum. Without loss of generality, we take the SDW to be uniaxial along the \( z \) axis, so that \( \hat{S} \) is a good quantum number, and spin-up and spin-down fermions decouple. Consider the state with \( \Delta_1 = \Delta_3 = \Delta = \Delta z \sigma _3 \). Up-spins near the three van Hove points are described by a simple Hamiltonian

\[
H = \begin{pmatrix}
\epsilon_{1,k} - \delta_\mu & \Delta & \Delta \\
\Delta & \epsilon_{2,k} - \delta_\mu & \Delta \\
\Delta & \Delta & \epsilon_{3,k} - \delta_\mu
\end{pmatrix},
\]

where \( \epsilon_1, \epsilon_2, \epsilon_3 \) are the dispersions near the van Hove points, Eq. (2), and \( \delta_\mu \) is the SDW-induced shift of the chemical potential. The \( 3 \times 3 \) Hamiltonian describing the spin-down branch is obtained by taking \( \Delta \rightarrow -\Delta \). At \( k = 0 \) (i.e., at van Hove points) the energies of spin-up excitations \( E_k - \delta_\mu \) are \( -\Delta, -\Delta \), and the energies of spin-down excitations are \( \Delta, \Delta \), and \(-\Delta \). In conventional SDW states (e.g., SDW on a 2D square lattice), \( \delta_\mu/\Delta \neq T_N/E_F \) is negligibly small and can be safely neglected. We find that in our case \( \delta_\mu = -\Delta \), so that gapless excitations arise in the spin-down spectrum.

To see the unexpected shift of the chemical potential, we diagonalize Eq. (10) and the corresponding equation for down spins and inspect six branches of excitations. We find that fixing \( \delta_\mu = -\Delta \) ensures that both in the paramagnetic and in the \( 3Q \) uniaxial SDW state, there are four bands with \( E_k \leq \mu \) and two bands with \( E_k \geq \mu \) for all momenta in the reduced BZ (see Fig. 3). Since the chemical potential is fixed by the constraint that the total number of electrons (equal to the number of states below the chemical potential) must not change between \( \Delta = 0 \) and \( \Delta \neq 0 \) [14], it follows that we must set \( \delta_\mu = -\Delta \). For verification, we computed the thermodynamic potential \( \Omega(\Delta, \mu) \) from (5), numerically solved the simultaneous equations \( \partial \Omega / \partial \Delta = 0 \) and \( \partial \Omega / \partial \mu = -N \), and confirmed that \( \delta_\mu = -\Delta \) to a high accuracy.

Having determined that \( \delta_\mu = -\Delta \), we find from (10) that gapless excitations emerge when \( e_{1,k} e_{2,k} e_{3,k} = 0 \), which has solutions along three lines passing through each van Hove point. Two of them coincide with the original FS; the third is directed towards the center of the BZ. The \( 3Q \) uniaxial SDW state is then obviously a metal. We emphasize, however, that gapless states exist only for the electrons with spin projection along \( \Delta \). The electrons with spin projection along \( \Delta \) are fully gapped. Since a Fermi surface exists for one spin projection only, we dub this state a “half-metal.” We found an analogous “half-metal” spectrum for the \( 3Q \) uniaxial SDW phase on the triangular lattice.

The half-metallic nature of the SDW should manifest itself in numerous experiments. For example, in tunneling experiments conducted with electrons spin polarized along the \( z \) axis, a hard gap will be seen for down spins, but a Fermi surface will be seen for up spins. Furthermore, since the low energy charged excitations involve up spins only,
uniaxial state has the lowest Free energy over a wide range of intermediate temperatures, roughly between $T_N/2$ and $T_N$, but undergoes a first order transition at a lower temperature to the insulating chiral SDW state discussed in earlier works [3,5,10]. We show the Free energy profile in Fig. 3(b). We found this behavior both for graphene and for fermions on a triangular lattice. Intuitively, the chiral SDW state wins at the lowest $T$ because it has spin-degenerate excitations and opens a full spectral gap, unlike the half-metal state.

The Free energy profile in Fig. 3(b) is for weak or moderate coupling, when $T_N/t_1 \ll 1$. At $T_N \sim t_1$, the phase diagram is more complex. For completeness, we discuss the forms of $Z_i$ and the phase diagram at $T_N \sim t_1$ in the Supplemental Material [13]. The ordering temperature $T_N$ depends sensitively on the strength of the microscopic interactions. For graphene doped near the saddle point we estimate $T_N \approx 3-30$ K, whereas $t_1 \approx 3$ eV [16]. Thus, at least for doped graphene, we should be decisively in the limit $T_N/t_1 \ll 1$, where our calculations apply.

Conclusion.—We considered in this Letter the SDW instability on the honeycomb and triangular lattices when doped to the saddle points of the dispersion. The SDW instability is subleading to a $d$-wave superconducting instability at weak coupling but becomes the leading instability if superconductivity is suppressed. We found that if the SDW ordering temperature $T_N$ is much smaller than the fermionic bandwidth, then a uniaxial SDW order develops simultaneously at three inequivalent nesting vectors. This has an order parameter manifold $O(3) \times Z_4$ and corresponds to the ordering pattern shown in Fig. 1. Such a state can only be obtained from a model of itinerant electrons with interactions and not from a spin model of local moments. We found that such a SDW state is a half-metal in which gapless excitations exist in one spin branch only. Such a state may be beneficial for nanoscience applications particularly because charge currents will necessarily also be spin currents, which allows for electrical control of the latter.

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FIG. 3 (color online). (a) Excitation spectrum $\varepsilon_k = E_k - \delta \mu$ of the 3$Q$ uniaxial state. Negative $k$ are along the FS, positive $k$ are along the BZ boundary in the original BZ (along $k_4$ in the reduced zone). Placing the chemical potential at $\delta \mu = -\Delta$ ensures that four bands lie below the chemical potential (horizontal dotted line) and two lie above for all $k$, irrespective of the value of $\Delta$. Thus the choice $\mu = -\Delta$ conserves electron number. Excitations with spin projection opposite to $\Delta$ are in blue (solid), along $\Delta$ are in red (dashed) lines. Note that gapless excitations arise in the spin-down branch only. (b) Free energy difference $\delta F = F_{\text{uniaxial}} - F_{\text{chiral}}$ between the 3$Q$ uniaxial SDW state and the chiral state, evaluated in the mean-field approximation for the honeycomb lattice Hubbard model with $g_2 = g_3 = U = 1.7t_1$ ($T_N \sim 0.002t_1$). The 3$Q$ uniaxial state has lower Free energy over a wide range of intermediate temperatures, but at the smallest $T$ the noncoplanar, chiral state, studied in earlier works [3,5,10], has lower Free energy.
In infinite 2D samples, $T_N = 0$, since $O(3)$ symmetry is restored by thermal fluctuations at any nonzero temperature in two dimensions. However, in a sample of finite size $L$, $T_N \approx T_{MF}/\log L/a$, where $T_{MF}$ is the transition temperature neglecting thermal fluctuation effects, and $a$ is the lattice scale. For samples of micron size, $\ln L/a \approx 7$, whereas $T_{MF}$ was estimated in the supplement to Ref. [7] as 20–200 K. Thus, we arrive at our estimate $T_N \approx 3–30$ K.