Pis'ma v ZhETF, vol. 111, iss. 4, pp. 242 – 243

Bilayer, hydrogenated and fluorinated graphene: QED vs SU(2) QCD theory

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Submitted 3 January 2020
Resubmitted 3 January 2020
Accepted 4 January 2020

DOI: 10.31857/S0370274X20040074

The electron spectrum of standard graphene with weakly correlated *sp*-orbitals is described in terms of Dirac fermions corresponding to one-electron band cones with a gap which occurs owing to spin-orbit interaction. Thus the system has properties of a topological insulator. In some cases graphene systems demonstrate strong electron correlations, including twisted magic-angle bilayer system [1] and monolayer graphene intercalated by gadolinium [2].

In the strongly correlated regime the excitation spectrum may change drastically. At the same time, the model still includes Dirac fermions at the nodal points. Such a spectrum occurs in the mean-field approximation corresponding to the deconfinement spinon picture [3]. The corresponding non-magnetic Dirac spin liquid (DSL) [4] is characterized by a quantum topological order. However, the stability of DSL should be further examined and is more probable in frustrated systems. In [5], the spinon picture was applied to bilayer graphene; here we investigate the corresponding models in more detail.

In [6], a frustrated ground state for single-side hydrogenated (C_2H) and fluorinated (C_2F) graphene was predicted, which sheds light on the absence of a conventional magnetic ordering in defective graphene demonstrated in experiments despite presence of magnetic moments. This suggests a highly correlated magnetic behavior at low temperatures offering the possibility of a quantum spin-liquid state.

In the present work, we apply to this problem the gauge-field formalism of quantum electrodynamics (QED) and chromodynamics (QCD) [7] and treat the spin-liquid state in terms of U(1) QED and parent SU(2) QCD theories. The former theory describes deconfinement situation and Dirac spin liquid. The latter theory includes a monopole operator which carries trivial quantum numbers and the Neel to valence bond solid (VBS) quantum phase transition at the quantum critical point [7]. Such an approach enables us to trace the hierarchy of symmetries – from SU(2) to U(1) and Z_2 spin liquids, the latter being the most stable one.

In the low energy infrared (IR) limit, the Lagrangian of Quantum Electrodynamics in 2+1 dimensions, QED_3, reads [8]:

$$\mathcal{L} = i\sum_{j=1}^{4} \bar{\psi}_j \not{D}_a \psi_j, \tag{1}$$

where $\not{D}_a = \gamma^\mu D_{a,\mu}$ is the gauge covariant Dirac operator, ψ_j is a two-component Dirac fermion with four flavors ($N_f = 4$) labeled by j, $\bar{\psi} = \psi^\dagger \gamma^0$, a_μ is a dynamical $U(1)$ gauge field. The theory assumes that the $U(1)$ gauge flux, i.e., the total flux of the magnetic field, is conserved. This noncompact $N_f = 4$ QED_3 theory flows to a stable critical fixed point in the IR limit.

For bipartite lattices, in the mean field approximation one can continuously tune the Hamiltonian, without breaking any symmetry or changing the low-energy Dirac dispersion, to reach a point with particle-hole symmetry [8]. This theory will then have a larger gauge symmetry of $SU(2)_g$,

$$\mathcal{L} = \sum_{v=1,2} i\bar{\psi}_v \gamma^\mu (\partial_\mu - i a_\mu)\psi_v, \tag{2}$$

where a is an SU(2) gauge field, and $\psi_{1,2}$ are two SU(2)-fundamental fermions. This theory has an SO(5) symmetry.

In an alternative theory, the SU(2) gauge symmetry in QCD_3 is lowered to U(1) owing to the Higgs phenomenon [7].

$$\mathcal{L} = \sum_{i=1}^{4} i\bar{\psi}_i \gamma^\mu (\partial_\mu - i a_\mu)\psi_i + (\lambda \mathcal{M}_a + \text{h.c.}), \tag{3}$$

where a_μ is now a U(1) gauge field, and the term $\mathcal{M}_a$ represents instanton tunneling.

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The flavor symmetry of QCD_3 at $N_f = 2$ is SO(5). In both the theories (2) and (3), the Dirac fermions transform in the spinor representation of the SO(5) group, the SO(5)-vector operators being time-reversal invariant mass operators. None of the duality field theories possesses the full SO(5) symmetry (combining antiferromagnetic and VBS order parameters) explicitly, the symmetry being at best emergent in the IR limit. One assumes that at least one of the theories (2) and (3) will flow to the deconfined critical point in the IR limit [7].

The most probable scenario for the QCD_3 theory (tuned to an SO(5) symmetric point) describes the deconfined critical point, and perturbing it drives it into either the VBS phase or the Neel phase [7].

The Dirac spin liquid can be unstable with respect to proliferation of monopoles, and different ordered states can be reached from DSL, the symmetry properties of the magnetic monopoles being different on different lattices [4]. For bipartite lattices, there is always one monopole operator which transforms trivially under all microscopic symmetries owing to the existence of a parent SU(2) gauge theory. This is a spin singlet which carries no non-trivial quantum numbers and therefore provides an allowed perturbation to the Hamiltonian, destabilizing DSL. On the non-bipartite lattices such a destabilization does not occur.

Thus the situation for bipartite (honeycomb) and non-bipartite (triangle) lattices is different. For bipartite situation, there is no additional topological symmetry since the flux of SU(2) gauge field (unlike that of U(1) field) is not conserved [8]. For the non-bipartite lattice, monopoles do not prevent stability of spin liquid (DSL is transformed to Z_2 spin liquid by inclusion of the Higgs field). For frustrated bipartite lattices, spin liquid is expected to exist at the quantum critical point only, but the quantum critical behavior can be observed at finite temperatures.

As discussed in [9], experimental data for twisted bilayer graphene indicate that the electron charge density is concentrated on a moire triangular lattice, so that the consequences of local correlations should be similar to those on the triangular lattice. On the other hand, symmetry and topological aspects of the band structure require that the model should be formulated using the Wannier orbitals of a honeycomb lattice. Besides the minimal phenomenological model of antiferromagnetism on the triangular lattice, the authors of [9] considered the model where the spin density is centered on the bonds of the dual bipartite honeycomb lattice. The half-filled triangular lattice model and the quarter-filled honeycomb-lattice model can be consistent with experimental observations. The half-filled honeycomb-lattice model requires the additional Kekule VBS order which is in agreement with the Monte Carlo calculations.

Triangular versus honeycomb lattice problem for bilayer graphene was considered in [10]. Although the charge density is concentrated on the triangular lattice sites of the moire pattern, the Wannier states of the tight-binding model must be centered on different sites which form a honeycomb lattice.

Generalized triangular lattice Hubbard models have been proposed to describe flat moire bands in twisted van der Waals transition metal dichalcogenide heterobilayers [11]. Recently a heterostructure of ABC-stacked trilayer graphene and boron nitride, which also forms a triangular moire superlattice even at zero twist angle, was studied [12].

An effective Heisenberg model was built in [6] for the C_2H and and C_2F systems, which includes competing exchange interactions on different p-orbitals and combines features of honeycomb and triangle lattices. The case of C_2H turns out to be more complicated due to the presence of the two nonequivalent magnetic sublattices comprising the honeycomb lattice. Thus frustration can lead to a DSL state provided that monopoles are irrelevant.

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364020040013

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