Dirac points, spinons and spin liquid in twisted bilayer graphene

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Twisted bilayer graphene is an excellent example of highly correlated system demonstrating a nearly flat electron band, the Mott transition and probably a spin liquid state. Besides the one-electron picture, analysis of Dirac points is performed in terms of spinon Fermi surface in the limit of strong correlations. Application of gauge field theory to describe deconfined spin liquid phase is treated. Topological quantum transitions, including those from small to large Fermi surface in the presence of van Hove singularities, are discussed.

1. Introduction

Heterostructures of two-dimensional (atomically-thin) materials attract great attention of scientists owing to their ability to provide novel electronic properties. Recently, correlated flat band has been observed in a graphene bilayer system \(^{1)}\). This band results from the superlattice modulation in the moire structure of two graphene sheets twisted by an angle which is close to the theoretically predicted “magic angle”. The temperature dependence of the amplitude of the Shubnikov-de Haas oscillations demonstrated large electron effective masses and small Fermi velocities.

The unique properties of twisted bilayer graphene (TwBLG) open up a new basis for many-body quantum phases. The accessibility and gate tunability of the flat bands through twist angle may provide the way to a number of exotic correlated systems, including unusual superconductors and quantum spin liquids. In particular, for carrier concentration near half of the superlattice density, \( n = \pm n_s/2 \) (which corresponds to half-filling in the effective Hubbard model) the flat band strongly correlated system is Mott-like insulating phase arising from electron localization in the moire superlattice. The metal-insulator transition at about 4 K is confirmed by measurements of transport properties (conductance) \(^{1)}\). This behavior is qualitatively different from previously reported zero-field insulating behavior which occurs at an integer multiple of \( \pm n_s \).

In a typical Mott insulator, the ground state usually has an antiferromagnetic spin ordering which is not observed in our system. Thus we have a Mott paramagnetic ground state that can be described within modern theoretical concepts. This singlet ground state can be treated as a spin liquid. From this point of view, the TwBLG system is somewhat similar to copper-oxide systems with square lattice, but the situation is even more favorable: suppression of antiferromagnetic ordering owing to frustrations on a triangular lattice is surely justified, unlike cuprates where competition of long-range electron hoppings in the \( t - J \) model should be introduced \(^{2)}\).

In the present paper we discuss possible field-theoretical approaches to describe the TwBLG system with especial attention to topological aspects.

2. Moire and Dirac points

Consider first the Dirac points in TwBLG within the one-electron picture (neglecting correlations). Two close graphene layers yield a moire superlattice which modifies the graphene electron dispersion and opens gaps both at the primary Dirac point and the moire-induced secondary Dirac point in the valence band \(^{1)}\) \(^{3)}\) \(^{4)}\).

To zeroth order, the low-energy band structure of TwBLG can be considered as two sets of monolayer graphene Dirac cones (each is four-fold degenerate due to valley and spin) rotated about the \( \Gamma \) point by the twist angle. The difference between the two wave vectors at the point \( K \) (or \( K' \)) gives rise to the mini Brillouin zone (MBZ) \( \sim \) a small hexagon, which is reciprocal to the moire superlattice \(^{1)}\). The Dirac cones near the same valley mix through interlayer hybridization, whereas interactions between distant Dirac cones are suppressed, so that the valley itself is a good quantum number.

The Dirac cones are characterized by a renormalized Fermi velocity \( v_F \). At \( v_F \to 0 \) there exist three additional Dirac points with opposite winding numbers \((-1)\) to the main Dirac point \((+1)\). For \( v_F = 0 \) when all four Dirac points merge, the winding number is \(-2\), since the total winding number cannot change \(^{5)}\). At exactly the first magic angle, the Dirac point at each corner of the MBZ \( (K_s \text{ and } K'_s) \) becomes a parabolic band touching with winding number \(-2\), similar to bilayer graphene with Bernal stacking (except that the two corners have the same winding number) \(^{1)}\).

When crossing the van Hove energy with doping the topology of the Fermi surface changes \(^{6)}\). The winding number drops from \(-1\) or \(+1\) (depending on the conduction band) to 0 since higher energy contours encircle

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the MBZ $\bar{\Gamma}$ symmetry point where no Berry curvature exists. Thus we have a topological transition in the presence of van Hove singularities.

3. Mott transition in TwBLG

According to the experimental data [1], at $|n| > n_f/2$ the Shubnikov-de Haas oscillation frequencies in TwBLG correspond to straight lines which extrapolate to zero at the half-filling densities. The authors of [1] suppose that this may mean small Fermi pockets resulting from charged quasiparticles near a Mott-like insulator phase, and the halved degeneracy of the pockets might be related to the spin-charge separation in the Mott insulator, similar to the situation in cuprates [2]. In other words, we have a partial Mott transition in the localized spin states subsystem (formation of the Hubbard subbands violating the Fermi liquid picture). Note that in this sense the narrow band Hubbard $(t-J)$ model can be effectively represented as a two-band $s$-$d$ exchange model [7].

Thus we have a situation of strong correlations. As concluded in [1], a theoretical treatment of the TwBLG problem can be performed within a two-band Hubbard model (including the valley degrees of freedom) on a frustrated triangular lattice. Then we have to use the SU(4) basis [8]. However, these two valleys can be treated as independent in zero order consideration.

To treat the metal-insulator (Mott-Hubbard) transition, one represents conventionally the electron annihilation operator as a product of a charged boson $b_i$ and a neutral spinful fermion (spinon) $f_{i\sigma}$, so that in the rotor representation (see [9, 10])

$$c_{i\sigma} = b_i f_{i\sigma}. \quad (1)$$

With increasing the Hubbard $U$, the spinless boson system at an odd-integer band filling undergoes a superfluid-to-Mott insulator transition. In a mean field description, the spinons are free (non-interacting), despite strong correlations in the electronic system. If the boson $b_i$ is condensed ($\langle b \rangle \neq 0$) we get the Fermi liquid (FL) phase of the physical electrons: when replacing $b$ by its $c$-number average $\langle b \rangle$, the $f_{i\sigma}$ fermions acquire the same quantum numbers as the initial electrons, so that the $f_{i\sigma}$ Fermi surface describes a conventional metal. If the boson is gapped and consequently uncondensed, a spin liquid Mott insulator occurs, where Fermi surface of neutral fermionic excitations (spinons) survives. The Mott insulator for the bosons is also an insulator state for the electrons with a gap to all charged excitations, and there is a continuous transition to an insulator with a “ghost” spinon Fermi surface. Thus we have the situation of deconfinement where charge and spin degrees of freedom are separated, and the gauge field can play an important role. Away from half-filling, the Bose holon operators should be introduced using other slave particle representations, see [2].

The flat band situation with large effective mass is somewhat similar to that in heavy fermion (Kondo) systems where $f$-electron states become delocalized and take part in the Fermi surface even in the absence of “direct” hybridization [11, 12].

4. Dirac points and spinons in the strongly correlated case

The Mott transition on the honeycomb lattice corresponding to graphene (the situation on the bilayer graphene triangular lattice is similar) has been investigated in Refs. [13, 14]. In this case the correlated metallic state is a semimetal containing gapless electronic excitations at isolated Fermi points in the Brillouin zone only. These points are essentially the Fermi surface of electrons.

The states near the Fermi points have a Dirac-like spectrum, and the problem can be analyzed within the corresponding relativistic formalism. The low energy action for the neutral Dirac spinons $\Psi$ in the insulating phase has the structure

$$S = \int d^3 x \sum_{\mu} \sum_{\sigma=1}^{N} \bar{\Psi}_\sigma (\partial_\mu - i a_\mu) \gamma_\mu \Psi_\sigma \quad (2)$$

where integration is performed in 2+1 dimensions, $\gamma_\mu$ are the Dirac matrices, $\bar{\Psi}_\sigma = \Psi_\sigma \gamma_0$, and $a_\mu$ is an emergent gauge field associated with the spinon-boson decomposition of the electron operator (1). Note that the Dirac excitation spectrum can be formed even if the bare lattice electron dispersion does not lead to such a spectrum (e.g., for the square and kagomé lattices) [10].

Depending upon the details of the lattice, $a_\mu$ can be a U(1) or SU(2) gauge field. For a large number of flavors $N$ (determined by the number of the Dirac points in the Brillouin zone), the action $S_D$ describes a conformal field theory (CFT). Thus we have a scale-invariant, strongly interacting quantum state with a power-law spectrum for all excitations, well-defined quasiparticles being absent. This state is labeled as an algebraic spin liquid (see [10, 2]). Note that one of the ways to obtain a deconfined phase is to include gapless excitations which carry gauge charges. These excitations can screen the gauge interaction to make it less confining [2].

Unlike true deconfined phases where noninteracting quasiparticles become free at low energies, here deconfinement means only that the gapless charged particles remain gapless, but are not quite free. The corresponding gapless spin liquids are obtained from the staggered flux liquid (sfL) and uniform RVB (uRVB) phases. The
The FL phase contains boson condensation which restores the quasiparticle picture. Therefore the low-energy excitations in the FL phase are described by electron-like quasiparticles and this phase corresponds to a FL phase of electrons.

The dynamics for the \( U(1) \) gauge field arises owing to screening by bosons and fermions, both carrying gauge charge. In the low doping case one can take into account screening by fermions only. After integrating out \( \Psi \) in (2) the effective partition function for the \( U(1) \) gauge field reads

\[
Z = \int \cd a_\mu \exp \left(-\frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} a_\mu(q) \Pi_{\mu\nu} a_\nu(-q) \right),
\]

\[
\Pi_{\mu\nu} = \frac{N}{8} \sqrt{q^2} \left( \delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \right).
\]

The polarizability \( \Pi \) makes the gauge coupling \( a_\mu j^\mu \) a marginal perturbation at the free fermion fixed point.

Consider the electron Green’s function. In the leading order in \( 1/N \), it was found that

\[
G(x) = \langle b^\dagger(x)b(0) \rangle_0 \langle f(x)f^\dagger(0) \rangle \exp \left(i \int_0^x dx \cdot a \right)
\]

where \( \int_0^x dx \) is the integration along the straight return path and \( \langle \cd \cd \rangle \) stands for integrating out the gauge fluctuations \( \Psi \). Then one obtains

\[
G(x) \propto (x^2)^{-(2-\alpha)/2}
\]

with the exponent \( \alpha \sim 1/N \) being the anomalous dimension; for the square-lattice antiferromagnet \( \alpha = 32/(3\pi^2 N) \). These results describe a partial confinement of spinons and bosons coupled by the gauge field. The conductivity is determined by the contributions of both fermions and bosons which cannot be considered as independent quasiparticles \[16, 2\].

5. Topology of Lifshitz transitions

The electron states in a strongly correlated system need not to have purely quasiparticle nature. They can be described by both poles and branch cuts of the Green’s function, cf. Eq. 3. If the suppression of the quasiparticle residue \( Z \) is strong, the pole in the Green’s function can be even transformed to the zero, \( G(E) \propto E + \varepsilon(k) \), which means formation of the energy gap and takes place, e.g., for the Mott transition \[17\]. The violation of the standard Fermi-liquid picture can be described in terms of the formation of the Luttinger surface which is the surface of zeros of the electron Green’s function \[18\].

The Lifshitz transitions (in particular, those discussed in Sect. 2) can be viewed as quantum phase transitions with change of the topology of the Fermi surface (FS), but without symmetry breaking. The topology of FS is characterized not only by its shape. FS itself is the singularity in the Green’s function, which is topologically protected: it is the vortex line in the frequency-momentum space \[17, 19\]. Formally, in the Mott insulating phase FS does not exist. However, the topology of FS is preserved if we take into account the Luttinger contribution. Then the Luttinger theorem (the conservation of the volume enclosed by FS independently of the interaction strength) is still valid \[17, 12\]. It should be noted that the Fermi surface combined from the poles and zeros is a whole object which cannot have holes and edges \[17\]. A similar picture occurs in cuprates where the Fermi points are stretched into arcs to form a large closed Fermi surface \[2\].

As for the non-Fermi liquid behavior, the flat band can be also treated as the Khodel-Shaginyan fermion condensate caused by electron-electron interaction \[21\], where all the states have zero energy.

The Lifshitz transition for bilayer graphene is governed by the conservation of the topological charge \( N_2 \). Merging of the two conical points with \( N_2 = 1 \) leads to formation of the Dirac node with quadratic dispersion and the topological charge \( N_2 = 2 \). Interaction between the layers may lead to several possible scenarios of the geometry of the fermionic spectrum in bilayer graphene. In particular, the \( N_2 = 2 \) Dirac point can split into four Dirac conical points with \( N_2 = \pm 1 \) (trigonal warping). The total topological charge is conserved, \( N_2 = 1 + 1 + 1 - 1 = 2 \) \[17\].

Thus the topological treatment may provide an interpolation from the one-electron Dirac points to the Dirac fermions (spinons) at the Fermi points in the strongly correlated Hubbard \((t-J)\) model.

6. Superconductivity

Many features of TwBLG are similar to those of the cuprate high-\( T_c \) materials where superconductivity occurs in a close vicinity of Mott insulator state after passing small antiferromagnetic region with doping. Here the transition may occur through complicated states, including incommensurate charge and magnetic order, stripes and magnetic phase separation. Doping is supposed to frustrate the ground state Neel order so that the system is pushed across the transition where the Neel order is lost and a spin liquid state arises \[2\]. Thus the transition to the superconducting state goes continuously via quantum critical point, a pseudogap state forming at finite temperatures in the quantum critical regime. The critical point can have a deconfinement na-
ture. At the same time, in TwBLG the situation seems to be even more clear since antiferromagnetism is totally suppressed by frustrations of triangular lattice.

Introducing exchange interactions in the narrow band system enables one to treat exotic topological phases and superconductivity [2]. In particular, the d-wave superconducting phase contains both the boson and fermion-pair condensate.

The superconducting properties can change in the deconfinement situation. The conventional and strongly correlated superconductors (being topologically ordered states) can be distinguished by flux quantum which equals $hc/(2e)$ in the former case (fermion pairing) and $hc/e$ in the latter case (Bose condensation in the spin-gap state) [2].

Recently, the value $hc/(4e)$ was found in Ref. [8]. These authors proposed topologically protected gapless edge states and half-vortices carrying half the usual superconducting flux quantum (effective 4e charge superconductor). The flat band superconductivity has been also discussed in Ref. [20].

7. Conclusions

According to estimations in Ref. [1], we have in TwBLG strong coupling or intermediate coupling situation (the Hubbard $U$ is larger or of order of effective electron bandwidth). We have considered above the strong correlation limit in TwBLG system in terms of spinon-boson deconfinement. At the same time, occurrence of spinons and fractionalized Fermi liquid (FL*) state with non-Fermi-liquid features can take place also in the intermediate coupling regime described by the spin-fermion model with suppressed magnetic ordering [22, 7]. The transition from small to large Fermi surface can be connected with the change in statistics of spinons [22].

With increase of doping, the Fermi level crosses the van Hove singularity in the nearly flat band [6] and we come to a new strongly correlated state. A similar situation in cuprates (pinning of the Fermi level to the van Hove singularity and the formation of flat bands in the two-dimensional $t - t'$ Hubbard model) was considered in Ref. [23]. The corresponding theoretical treatment for TwBLG requires further investigations.

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