Citation for published version


DOI

https://doi.org/10.1088/1742-6596/334/1/012048

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Search for non-Abelian statistics in half-filled Landau levels of graphene

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Abstract. We have employed large scale exact numerical diagonalization in Haldane spherical geometry in a comparative analysis of the correlated many-electron states in the half-filled low Landau levels of graphene and such conventional semiconductors as GaAs, including both spin and valley (i.e., pseudospin) degrees of freedom. We present evidence that the polarized Fermi sea of essentially non-interacting composite fermions remains stable against a pairing transition in both lowest Landau levels of graphene. However, it undergoes spontaneous depolarization, which in (ideal) graphene is unprotected for the lack of a single-particle pseudospin splitting. These results point to the absence of the non-Abelian Pfaffian phase in graphene.

1. Introduction
The fundamental properties of the enigmatic incompressible quantum liquid formed by the quasi-two-dimensional electrons in a half-filled second Landau level (LL) of such conventional semiconductors as GaAs, and thus responsible for the fractional quantum Hall (FQH) effect observed at the LL filling factor \( \nu=5/2 \) [1] in such materials, continue to attract attention. A somewhat trivial reason is that \( \nu=5/2 \) is unique as the only known even-denominator FQH state observed so far. More importantly, although the nature of the \( \nu=5/2 \) FQH state is not yet decisively proven, in light of the accumulating evidence [2] it has become commonly believed that this state is adiabatically connected to the so-called Pfaffian wave function introduced by Moore and Read [3]. The Pfaffian wave function represents a condensed paired state of composite fermions (CFs) in the absence of an effective magnetic field \( B^* \) (the CFs are weakly interacting quasiparticles formed by the electrons through capturing vortices of the many-body wave function and thus experiencing a reduced effective field \( B^* \) [4]). It has been almost immediately realized that the quasihole (QH) excitations of the Pfaffian ground state obey fractional and nonabelian braiding statistics [5]. More recently, it has been suggested that employing the statistical degeneracy of the multi-QH states for encoding quantum information might pave the way to the essentially error-free topological quantum computation [6]. One of the problems with the practical realization of this idea is a small excitation gap of this state measured in the actual GaAs structures (of the order of hundreds of mK) [7] and not much larger values predicted theoretically for the idealized systems (defined by the absence of disorder, vanishing layer thickness, etc.). It is therefore natural to extend the search for the nonabelian Pfaffian phase to other materials, where the excitation gap might be enhanced either due to a higher overall Coulomb energy scale or due to a more favorable form of the pseudopotential (defined as the dependence of the interaction energy \( V \) of a pair of electrons inside a given LL on their relative pair angular momentum \( m \) [8]), to which the half-filled ground state is known to be sensitive.
In this work, we investigate the possibility of a hypothetical non-abelian Pfaffian phase appearing in half-filled LLs of graphene [9], characterized by a significantly (up to an order of magnitude) larger Coulomb energy scale than GaAs due to a lower dielectric constant (down to unity, the precise value depending on the coupling to the background) and literally atomic layer width [10]. This question has been earlier considered theoretically [11-13] and now became more realistic in view of experimental demonstration of the ν=1/3 FQH effect in graphene [14]. Our results come from exact diagonalization or the largest systems studied so far and using a more accurate form of the Coulomb pseudopotential.

Emergence of the Pfaffian state requires a particular form of the interaction among the electrons in a given LL. In addition to supporting the formation of CFs, it must also induce an effective (residual) interaction among them – such as to lead to the Cooper pairing instability of the CF Fermi sphere at $B^* = 0$. Hence, a broader question we address in this paper is that of CF dynamics in different LLs of graphene. The lack of immediate analogy between graphene and the (better explored) two-dimensional GaAs is the consequence of the differing single-particle orbitals defining all but the lowest LL (caused by the presence of two atomic sublattices spanning the crystallographic structure of graphene), and of an additional “pseudospin” degree of freedom associated with the valley degeneracy in graphene. Our main conclusions are that the CF-CF interaction in graphene is insufficient to induce pairing at $B^* = 0$, and that the polarized compressible CF Fermi sea is unstable toward the depolarization of pseudospin.

2. Interaction matrix elements and pseudopotentials on a sphere

Interaction in an isolated LL is completely determined by its pseudopotentials $V_m$, which (except for the lowest LL) are different in graphene and GaAs. Their analytic expressions for an arbitrary (nth) LL in the planar geometry have been derived earlier [11]. These “planar” pseudopotentials $V_{\text{plane},n,m}$ were used in (to our best knowledge) all previous many-body calculations (e.g., [13]) even though these calculations were most often carried out in a more convenient spherical geometry (with $N$ electrons confined to the surface of a sphere and exposed to a magnetic flux $2Q \hbar c/e$). The series $V_{\text{plane},n,m}$ were simply truncated at $m=N_0$, where $N_0=2(2Q+n)$ represents the magnetic flux of a corresponding system in the lowest LL, with the same LL degeneracy of $N_0+1$. This approach has an obvious disadvantage in the disconnection of $V_m$ from the Coulomb potential $V(r) \sim 1/r$ from which it ought to be derived. This is especially problematic at a longer range $r$, comparable to the sphere radius $R=Q^{1/2}$ (in units of the magnetic length $\lambda=(\hbar c/eB)^{1/2}$), i.e., for $m$ not much smaller than $Q$. Therefore, in the following we instead adopted a direct analytical solution of the Dirac problem on a sphere provided by Jellal [15].

In the excited LLs of graphene, the single-particle states $\langle |n,m\rangle \rangle$ are spinors, whose two components represent standard LL wave functions, with equal angular momenta $m$ but different LL indices: $|n,m\rangle$ and $|n-1,m\rangle$. It is essential that in the spherical geometry both components of $\langle |n,m\rangle \rangle$ must have the same LL degeneracy (i.e., equal $N_0$) and thus different flux $2Q$ (i.e., different magnetic length scales $\lambda$). Using this convention for the meaning of “$|n,m\rangle\rangle$”, the Coulomb matrix elements of graphene $\langle \langle \ldots \rangle \rangle$ take the form of simple averages over the corresponding two-body matrix elements of GaAs $\langle \ldots \rangle$ [16].

The “spherical” pseudopotentials $V_m$ (describing graphene in the spherical geometry and correctly linked to the Coulomb potential $\sim 1/r$) are then obtained from the above matrix elements by standard diagonalization of the two-electron problem; cf. Fig. 1. Comparison of pseudopotentials of different LLs of graphene with the “reference” ones of the first and second LL of GaAs (for which the ground state at a half-filling is known/believed to be the nearly free CF Fermi sea and the paired CF superfluid described by the Pfaffian, respectively) is best illustrated in Fig. 2, in which we present the symmetric first-order differences defined as $\Delta^{(1)}V_m=V_m-(V_{m+s}+V_{m-s})/2$. For $s=2$ (top frames), $\Delta^{(2)}V_m$ considered for the odd values of $m$ (as appropriate for the spin-polarized electrons) reveals the deviation of $V_m$ from a straight line, which is its most important feature in producing the particular form of the pair electron correlation in a spin-polarized ground state [17]. Clearly, the pseudopotentials in the lowest two LLs of graphene appear similar in this respect. It is also remarkable that none of the LLs of graphene has a pseudopotential similar to that of the second LL of GaAs. For $s=1$ (bottom frames), $\Delta^{(1)}V_m$ considered for the even values of $m$ tells about the stability of the ground state against spin depolarization. Here,
we find that the lowest two LLs of graphene behave similarly (again), while the pseudopotential for $n=2$ in graphene resembles that of $n=1$ in GaAs (for $s=2$ these two differed in the sign of the leading term, $\Delta^9(V)$. This suggests that none of the graphene LLs is analogous to the second LL of GaAs.

3. Many-electron ground states with full spin and pseudospin polarization

We begin by studying the polarized $N$-electron ground states at different $N_f=2N-\sigma$ (corresponding to a half-filled LL). An extended incompressible liquid is represented on a sphere by a series of uniform (i.e., having zero total angular momentum, $L=0$) finite-size states $(N, N_\sigma)$ with a constant shift $\sigma$ (e.g., $\sigma=3$ for the Pfaffian). The correlation energy, pair correlation function, etc. should depend smoothly on $N$ along the series (and extrapolate properly to the plane). Using an efficient Lanczos method we were able to diagonalize Hamiltonians of up to $N=20$ electrons, with dimensions of the order of $10^7$.

As anticipated from the analysis of pseudopotentials, the Pfaffian wave function was not found to have high squared overlaps $|\chi|^2$ with the corresponding ($\sigma=3$) exact $N$-electron Coulomb ground states in any LL of graphene. Actually, the oscillations in $|\chi|^2$ as a function of $N$ reveals the emergence of a shell structure of the (essentially) non-interacting CFs at $B^*=0$ (the shells being the effective CF LLs) rather than the formation of a uniform phase, adiabatically connected to the Pfaffian. Specifically, the ground states of $N=6$, 12, and 20, corresponding to the number $v^*=2$, 3, and 4 of completely filled CF LLs all have relatively small $|\chi|^2$ while the other ground states (corresponding to partial filling of the topmost CF LL) all have relatively high $|\chi|^2$. This is illustrated in Fig. 3, presenting also a comparison with the Coulomb eigenstates in the second LL in GaAs (for two different widths $w=0$ and $3\lambda$, as the finite width is known to improve the overlap in such system [18]). Evidently, the decrease of $|\chi|^2(N)$ in graphene is much faster than in GaAs (especially for $w=3\lambda$), where also the $N$-dependence is different. In the case of GaAs, a significant enhancement of $|\chi|^2$ was also recently demonstrated through the LL mixing [19]. However, this effect is not relevant in graphene due to a much smaller (constant) ratio of the inter-LL splitting to the Coulomb energy scale. Fig. 3 also compares the Coulomb energies of the exact Coulomb eigenstates and the Pfaffian states, also showing lack of a Pfaffian phase in graphene.
FQH ferromagnetism is a rare phenomenon (i.e.,
ferromagnetically ordered ground state) associated with
an inverse electron number \( N^{-1} \). The lowest CF state for the
single CF in the
lowest LL (not shown; studied earlier [1]) has a relatively high correlation energy.

The dominant tendency is the CF shell filling, with low values of \( E \) coincident with exact filling of an indicated number of the CF-LLs. Let us illustrate this tendency on a few examples. At the half-filling, the \((NN_f)\) states of strongly interacting electrons map onto the states of nearly non-interacting CFs at \( N_f = N_f - 2(N-1) = 2 - \sigma \) (negative sign meaning the effective magnetic flux acting on the CFs oriented opposite to the original flux \( 2Q \) [20]), with the \( n^*\)th CF-LL degeneracy of \( 12 - \sigma f + 1 + 2n^* \). For \( \sigma = 3 \) and \( N = 20 \), this yields four lowest CF-LLs completely filled (i.e., this finite-size half-filled state is “aliased”)
with an incompressible \( v^* = 4 \) CF state, corresponding to the electron filling factor \( v = 4/7 \), leading to a relatively low correlation energy. For \( \sigma = 4 \) and \( N = 16 \), there are three filled CF-LLs and an additional single CF in the \( n^* = 3 \) level with the single-particle angular momentum equal to \( |N_f^*|/2 + n^* = 4 \), yielding an \( L = 4 \) state (aliased with a single CF-quasiparticle in an incompressible \( v^* = 3 \) state) with a somewhat higher correlation energy than in the case of complete CF-LL filling. Finally, for \( \sigma = 3 \) and \( N = 16 \), there are three full CF-LLs and additional four CFs in an 8-fold degenerate CF-LL with \( n^* = 3 \), leading to a relatively high correlation energy. The above behavior for the second LL in graphene repeats that of the lowest LL (not shown; studied earlier [13]), both hosting a CF Fermi sea rather than a CF liquid.

4. Spontaneous depolarization of pseudospin

Full spin polarization of any FQH state can in principle be enforced by the Zeeman effect. However, in graphene one must also consider an additional “pseudospin” degree of freedom associated with the valley degeneracy. Since valley depolarization is not protected by a pseudospin analog of the single-electron Zeeman splitting (at least, in the absence of external potentials or lattice distortions [10]), we have included in diagonalization the single-electron pseudospin \( (p_z = \pm \frac{1}{2}) \) and classified the \( N \)-electron eigenstates by its total length \( P \) and projection \( P_z \). Dependence of the correlation energy \( E \) on size \( N \) for the pseudospin-uncorrelated states \( (P = 0) \), is shown in Fig. 4(b,c). Especially for \( n = 0 \), the half-filled state evidently undergoes a spontaneous depolarization of pseudospin (e.g., the unpolarized series with \( \sigma = 1, 3 \), and 4 clearly extrapolate to lower energies than any polarized series). This is not unexpected, given that spontaneous FQH ferromagnetism is a rare phenomenon \((v = 1 \text{ and } 1/3 \text{ in the lowest LL})\).
5. Conclusion

We used exact diagonalization to study many-electron ground states at a half-filling of different LLs in graphene, including pseudospin (i.e., valley) degeneracy. We found that even in the subspace of fully polarized spin and pseudospin the Pfaffian state is not realized in graphene. Instead, the Fermi sea of free CFs forms in the lowest two LLs (with non-liquid phases most likely prevailing in higher LLs). We also demonstrated that the CF Fermi sea in graphene undergoes the spontaneous (and unprotected) depolarization of pseudospin. These results point to the absence of a Pfaffian phase in graphene.

The authors thank M. O. Goerbig and N. Regnault for the insightful comments. AW acknowledges support by Marie Curie PIEF-GA-2008-221701 and Polish MNiSW Grant No. N202179538.

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