Realistic Fractional Quantum Hall Energy Gaps in Graphene via Monte Carlo Simulations

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***Abstract*— Quasi-two-dimensional electron systems can be transformed into a new state of matter exhibiting the fractional quantum Hall effect (FQHE) when held at a low temperature in a strong, perpendicularly applied magnetic field. The role of electricity and magnetism (EM) in the derivation of this phenomenon will be discussed. The work done on incorporating Landau level mixing (LLM) in the ground state of a real-space Hamiltonian for FQHE states in graphene is discussed, as well as the desire to generalize this model to higher Landau levels (LLs) and other materials.**

I. Introduction: the fractional quantum Hall effect

The information presented in this section will largely be derived from "The Quantum Hall Effect" lectures by David Tong [1]. We will begin our discussion of the FQHE with a brief derivation of the classical Hall effect. In a material where charges are restricted to motion in the (x, y) plane, a potential difference in the x-direction and applied magnetic field in the z-direction will create a potential difference in the y-direction, called the Hall voltage V_H as shown in Fig. 1.

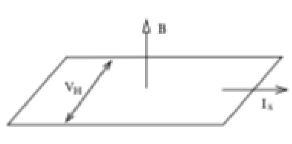

Fig. 1. The classical Hall effect [1]

To understand the origin of this phenomenon, let us consider the Lorentz force. In class, we used the EM Lagrangian to derive the Lorentz force in covariant form. We just need the 3-vector form for our purposes, adding on an additional term from the Drude model that incorporates the scattering of charge carriers off lattice sites with mean free time τ

$$m\frac{d\vec{v}}{dt} = -e(E + \vec{v} \times \vec{B}) - \frac{m\vec{v}}{\tau}$$

The solution of the Lorentz force equation for position yields a cyclotron frequency

$$\omega_B = \frac{eB}{m}$$

We saw the cyclotron frequency in class when we were learning about how relativistic beaming must be considered when measuring radiation in a cyclotron. For our purposes, we are interested in what is happening to the system once it has reached equilibrium ($\vec{v} = \vec{0}$). We can substitute the velocity for the current density using the following relation

$$\vec{J} = -ne\vec{v}$$

We can use this to find the following relationship between the current density and the electric field

$$\begin{pmatrix} 1 & \omega_B\tau \\ -\omega_B\tau & 1 \end{pmatrix} \vec{J} = \frac{e^2 n\tau}{m}\vec{E}$$

Or, simply, $\vec{J} = \sigma\vec{E}$. We are interested in the off-diagonal entries of the resistivity matrix, the inverse of this conductivity matrix. We can define a new variable, the Hall coefficient R_H

$$R_H = -\frac{E_y}{J_x B} = \frac{\rho_{xy}}{B}$$

And plug in our variables from the Lorentz force equation to obtain the following expression for the component of the resistivity that resists current in the x-direction due to the Hall voltage in the y-direction

$$\rho_{xy} = \frac{B}{ne}$$

We would then expect a plot of ρ_{xy} vs. B to be a linear, but instead we see the plot below in Fig. 2.

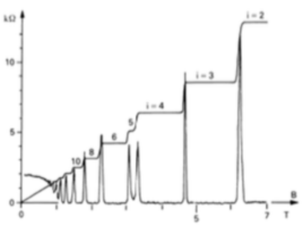

Fig. 2. A plot of ρ_{xy} vs. B displaying the integer quantum Hall effect [1]

At each plateu, the resistivity has a value of

$$\rho_{xy} = \frac{2\pi\hbar}{e^2}\frac{1}{\nu},\ \nu \in \mathbb{Z}$$

And the center of each plateau is at the value

$$B = \frac{2\pi\hbar}{e}\frac{n}{\nu} = \Phi_0\frac{n}{\nu}$$

Where Φ_0 is the flux quantum, or the values of the magnetic field at which the first LLs are filled. As we decrease the disorder in the system, more, shorter plateaus emerge in such a way that a complete lack of disorder would correspond to the classical linear plot for ρ_{xy} vs. B. A state with more, shorter plateaus with plateaus at fractional values of ν can be reached, as shown in Fig. 3.

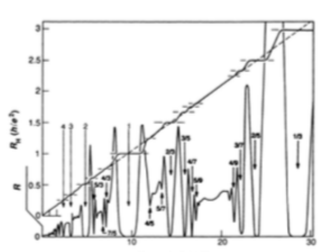

Fig. 3. The fractional quantum Hall effect [1]

The integral quantum Hall effect has free electrons as charge carriers, but the FQHE has composite charge carriers that can posses different, well-defined rational fractions of the electron's charge. We derived the Hall effect classically, but discussing the FQHE requires second quantization formalism, which we discussed in class in regards to quantum electrodynamics. As we did with many of our class problems, we start with the Lagrangian for a particle with charge $-e$ in a magnetic field (although, we only need 3-vectors for this discussion as opposed to the Lagrangian 4-density we worked with in class)

$$\mathcal{L} = \frac{1}{2}m\dot{\vec{x}}^2 - e\dot{\vec{v}}\cdot\vec{A}$$

This Lagrangian yields a canonical momentum

$$\vec{p} = m\dot{\vec{x}} - e\vec{A}$$

And Hamiltonian

$$H = \frac{1}{2m}(\vec{p} + e\vec{A})^2$$

We can find the commutator for our mechanical momentum

$$\vec{\pi} = \vec{p} + e\vec{A} \Rightarrow [\pi_x, \pi_y] = -ie\hbar B$$

and define the raising and lowering operators

$$a = \frac{1}{\sqrt{2e\hbar B}}(\pi_x - i\pi_y) \text{ and } a^\dagger = \frac{1}{\sqrt{2e\hbar B}}(\pi_x + i\pi_y)$$

This leaves us with the Hamiltonian for a quantum harmonic oscillator

$$H = \hbar\omega_B\left(a^\dagger a + \frac{1}{2}\right),\ n \in \mathbb{N}$$

With energy eigenstates

$$E_n = \hbar\omega_B\left(n + \frac{1}{2}\right)$$

These energy eigenstates are our LLs. Since we have a magnetic field in the z-direction, $\nabla \times \vec{A} = B\hat{z}$, we can choose the Landau gauge $\vec{A} = xB\hat{y}$. We learned in class about how using gauges can simplify problems or illuminate interesting physics. We worked with the Coulomb gauge, Lorentz gauge, and velocity gauge. Now, in the Landau gauge, our Hamiltonian becomes

$$H = \frac{1}{2m}\left(p_x^2 + (p_y + eBx)^2\right)$$

Which shows us that only the y-component of the momentum has the canonical Poisson structure that we saw before. This causes a shift in our wave-function that changes the expression for the energy eigenstates which explicitly yields a velocity

$$v_y = -\frac{E}{B}$$

We have gone from describing the Hall effect in the language of classical electrodynamics to describing the quantum Hall effect in the language of second quantization, a gap in formalism for which this class built a bridge.

II. Realistic fractional quantum Hall energy gaps in graphene via Monte Carlo simulations

Now that we have seen the crucial role that electrodynamics played in the formation of the topic of my research, let us discuss the current state of this research and what needs to be done. In this discussion, we have not yet considered the effect that LLM has on the Hamiltonian. LLM occurs when strong electron-electron interactions propels electronss into higher LLs. The FQHE was historically discovered experimentally in GaAs semiconductor heterostructures which have a parabolic electron dispersion that suppresses LLM in large magnetic fields. However, graphene has a linear dispersion, so any Hamiltonian expecting to yield results that match up with experiment must incorporate LLM.

To make calculations more palatable, Arciniaga mapped a Hamiltonian including LLM for FQHE states in graphene to the Haldane sphere [2]. In this topological space, these pseudopotentials have no injective mapping to real-space potentials, so Getachew worked on a scheme for mapping pseudopotentials in the Haldane sphere to candidate real-space potentials [3]. Hernandez used a mapping to a real-space potential to approximate the ground state FQHE energy in graphene [4].

I will be continuing the work of these three previous M.S. theses, starting with utilizing Monte Carlo methods to approximate the energy gaps in FQHE states that incorporate LLM and comparing these results to experiment. I hope to then work on developing a real-space potential that incorporates three-body, particle-hole symmetry breaking terms, so that the model can be generalized to higher LLs and materials other than graphene. This more general model for FQHE energy states might provide clues for ways to experimentally demonstrate fractional statistics and non-abelian quasiparticles which could be the key step in building a topologically protected quantum computer.

III. Conclusion

My research will incorporate many of the concepts and skills I have learned during my time in this course. We saw how this course bridged the gap between the classical formalism of the Hall effect and the second quantization formalism required to work with the FQHE. I am so thankful to Dr. Jaikumar for his excellent teaching and encouragement in this class and I look forward to using what I have learned to advance our ability to model the FQHE in realistic systems as one step toward the physicist's ultimate technological dream, practical quantum computing.

References

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[3] Getachew, Y 2017, Constructing Realistic Real-Space Potentials on the Haldane Sphere for the Fractional Quantum Hall Effect M.S. Thesis, California State University, Long Beach.

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