TWO DIMENSIONAL PERIODIC MAGNETIC MODULATION: HOFSTADTER BUTTERIES AND CONDUCTANCES IN MONO AND BILAYER GRAPHENE

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by

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Dedicated to my loving parents..

CERTIFICATE

This is to certify that the thesis entitled **Two dimensional periodic magnetic modulation: Hofstadter butterflies and conductances in mono and bilayer graphene**, being submitted by **Manisha Arora** to the Department of Physics, Indian Institute of Technology Delhi, for the award of degree of **Doctor of Philosophy**, is a record of bonafide work carried out by her under my supervision and guidance. The results reported in this thesis have not been submitted, either in part or in full, to any other University or Institute for award of any degree or diploma.

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Abstract

The primary focus of the proposed thesis is to investigate the electronic and transport properties of monolayer and bilayer graphene system under two dimensional periodic magnetic field. Quantization of Hall conductivity for non relativistic 2DEG and relativistic system, such as monolayer graphene, under uniform transverse magnetic field is quite well known. The emphasis here is to analyze the behaviour of MLG and BLG systems under the periodic modulation and to see if quantization of Hall conductivity still survives along with evaluation of diagonal conductivity for the modulated MLG system.

We begin with providing a theoretical model for the applied 2D periodic magnetic field having square lattice symmetry. The energy spectrum of massless Dirac fermions in monolayer graphene under such modulation is then calculated. It is shown that the translation symmetry of the problem is similar to that of TKNN problem and in the weak field limit the tight binding energy eigenvalue equation is indeed given by Harper Hofstadter Hamiltonian. Due to its magnetic translational symmetry the Hall conductivity can be identified as a topological invariant and hence quantized. Hence the idea of Quantum Hall Effect is extended to magnetically modulated two dimensional electron system. It is demonstrated that the calculations and the results can be generalized to any arbitrary magnetic modulation periodic in two dimensions. Apart from this, possible experimental set ups are indicated where the results may be verified.

We proceed to extend our analysis to the system of bilayer graphene subjected to the periodic modulation. We evaluate eigenvalues of the modulated bilayer system by obtaining connection between eigenvalues of modulated BLG and MLG system. We further obtain the Harper equation for the BLG system which enables us to solve for corresponding eigenstates. The studies are performed for both four band and two band models of BLG. An interesting feature of the work comprises of the success in obtaining variation in the band gap of the energy

spectrum due to changing interlayer coupling strength. The survival of topological quantization of Hall conductivity is rigorously verified along with obtaining Diophantine equation for the system to evaluate associated Chern numbers.

We further go on to evaluate the diagonal conductivity for monolayer system under the described 2D magnetic modulation. We plot both the diffusional and collisional conductivity components of the total diagonal conductivity, for linear responses and weak scattering potentials, as a function of magnetic field strength. It is observed that both these components contribute significantly. Apart from this, extensive numerical computation is performed for calculation of wavefunctions and DOS for the modulated MLG system. The wavefunctions are also analyzed to an extent in an attempt to have a better understanding of the transport properties of the system.

सार

प्रस्तावित थीसिस का प्राथमिक फोकस दो आयामी आवधिक चुंबकीय क्षेत्र के तहत मोनोलेयर और द्वि परत ग्राफीन प्रणाली के इलेक्ट्रॉनिक और परिवहन गुणों की जांच करना है। गैर-सापेक्ष 2 डी ई जी और सापेक्षतावादी प्रणाली के लिए हॉल चालकता की मात्रा, जैसे मोनोलेयर ग्रैफेन, समान लंबवत चुंबकीय क्षेत्र के तहत काफी प्रसिद्ध है। यहां पर जोर आवधिक मॉडुलन के तहत एमएलजी और बीएलजी सिस्टम के व्यवहार का विश्लेषण करने पर है और यह देखने के लिए कि मॉड्यूलेटेड एमएलजी सिस्टम के लिए विकर्ण चालकता के मूल्यांकन के साथ हॉल चालकता का परिमाणीकरण अभी भी जीवित है या नहीं।

हम वर्ग जाली समरूपता वाले अनुप्रयुक्त 2D आवर्त चुंबकीय क्षेत्र के लिए एक सैद्धांतिक मॉडल प्रदान करने के साथ प्रारंभ करते हैं। इस तरह के मॉडुलन के तहत मोनोलेयर ग्रैफेन में बड़े पैमाने पर डिराक फर्मियन के ऊर्जा स्पेक्ट्रम की गणना की जाती है। यह दिखाया गया है कि समस्या की अनुवाद समरूपता टीकेएनएन समस्या के समान है और कमजोर चुंबकीय क्षेत्र सीमा में तंग बाध्यकारी ऊर्जा ईजिन मूल्य समीकरण वास्तव में हार्पर हॉफस्टैटर हैमिल्टन द्वारा दिया गया है। इसकी चुंबकीय अनुवादकीय समरूपता के कारण हॉल चालकता को एक टोपोलॉजिकल इनवेरिएंट के रूप में पहचाना जा सकता है और इसलिए इसे परिमाणित किया जा सकता है। इसलिए क्वांटम हॉल इफेक्ट का विचार चुंबकीय रूप से संशोधित दो आयामी इलेक्ट्रॉन प्रणाली तक बढ़ाया गया है। यह प्रदर्शित किया जाता है कि गणना और परिणामों को दो आयामों में किसी भी मनमाने चुंबकीय मॉड्यूलेशन आवधिक के लिए सामान्यीकृत किया जा सकता है। इसके अलावा, संभावित प्रयोगात्मक सेट अप इंगित किए जाते हैं जहां परिणाम सत्यापित किए जा सकते हैं।

हम अपने विश्लेषण को आवधिक मॉडुलन के अधीन द्वि-परत ग्राफीन की प्रणाली तक विस्तारित करने के लिए आगे बढ़ते हैं। हम मॉड्यूलेटेड बीएलजी और एमएलजी सिस्टम के आइजेनवैल्यू के बीच संबंध प्राप्त करके मॉड्यूलेटेड बाइलेयर सिस्टम के आइजनवैल्यू का मूल्यांकन करते हैं। हम आगे बीएलजी प्रणाली के लिए हार्पर समीकरण प्राप्त करते हैं जो हमें संबंधित ईजिन राज्यों के लिए हल करने में सक्षम बनाता है। अध्ययन बीएलजी के चार बैंड और दो बैंड मॉडल दोनों के लिए किया जाता है। काम की एक दिलचस्प विशेषता में इंटरलेयर कपलिंग ताकत बदलने के कारण ऊर्जा स्पेक्ट्रम के बैंड गैप में भिन्नता प्राप्त करने में सफलता शामिल है। संबंधित चेर्न संख्याओं का मूल्यांकन करने के लिए सिस्टम के लिए डायोफैंटाइन समीकरण प्राप्त करने के साथ-साथ हॉल चालकता के टोपोलॉजिकल क्वांटिज़ेशन के अस्तित्व को कड़ाई से सत्यापित किया जाता है।

हम आगे वर्णित 2 डी चुंबकीय मॉडुलन के तहत मोनोलेयर प्रणाली के लिए विकर्ण चालकता का मूल्यांकन करने के लिए आगे बढ़ते हैं। हम चुंबकीय क्षेत्र की ताकत और तापमान के एक समारोह के रूप में, रैखिक प्रतिक्रियाओं और कमजोर बिखरने की क्षमता के लिए, कुल विकर्ण चालकता के विवर्तनिक और संयुग्मन चालकता घटकों दोनों के लिए ग्राफ बनाते हैं। यह देखा गया है कि ये दोनों घटक महत्वपूर्ण योगदान देते हैं। इसके अलावा, मॉड्यूलेटेड एमएलजी सिस्टम के लिए वेवफंक्शन और डॉस की गणना के लिए व्यापक संख्यात्मक गणना की जाती है। सिस्टम के परिवहन गुणों की बेहतर समझ रखने के प्रयास में तरंगों का भी एक हद तक विश्लेषण किया जाता है।

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