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Magnetic Catalysis in Graphene Effective Field Theory

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We report on the first calculation of magnetic catalysis at zero temperature in a fully nonperturbative simulation of the graphene effective field theory. Using lattice gauge theory, a nonperturbative analysis of the theory of strongly-interacting, massless, $(2+1)$ -dimensional Dirac fermions in the presence of an external magnetic field is performed. We show that in the zero-temperature limit, a nonzero value for the chiral condensate is obtained which signals the spontaneous breaking of chiral symmetry. This result implies a nonzero value for the dynamical mass of the Dirac quasiparticle.

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INTRODUCTION

Graphene, a novel material consisting of a single layer of Carbon atoms arranged in a hexagonal lattice, constitutes one of the most fascinating recent developments in condensed matter physics [1]. This new field has seen tremendous growth due to the interest of both theorists and experimentalists in graphene's extraordinary electronic and mechanical properties [2, 3]. Furthermore, there exists great hope for technological applications of graphene in electronic devices [4].

The electronic structure of graphene can be described by a valence and conduction band which touch at two inequivalent corners of the Brillouin zone. Near these so-called “Dirac points”, the dispersion is linear, and thus the quasiparticles can be described by two species of massless Dirac fermions.

Recent studies have shown a complex phase structure of the theory with the existence of both an insulating antiferromagnetic (AFM) and a charge-density wave (CDW) phase in addition to the semimetal phase [5, 6]. In these studies, an on-site Hubbard interaction along with realistic nearest- and next-nearest-neighbor interactions [7] were introduced in addition to the long-range Coulomb tail characterized by $\alpha_g = 2e^2/(4\pi v_F(\epsilon + 1))$. At small α_g , graphene undergoes a transition from the semimetal phase to the AFM phase when the on-site interaction satisfies $U > U_{cr}$. For small U , the theory exhibits a phase transition from the semimetal phase to the CDW phase when $\alpha_g > \alpha_g^{cr}$. In this work, we simulate at half-filling for $U = 0$, where we can construct a real, positive-definite action.

In the presence of an external magnetic field, graphene exhibits a series of quantum-Hall plateaus that can be understood within a single-particle picture for Dirac fermions [8]. However, as the magnetic field increases ($B \geq 20$ T), new plateaus appear at filling factors $\nu = 0, \pm 1, \pm 4$ [9–11]. These plateaus result from the spontaneous breaking of the four-fold degeneracy of the Landau levels and the dynamical generation of a mass for

the Dirac quasiparticle. Although Zeeman splitting accounts for the plateau at $\nu = \pm 4$, this “magnetic catalysis” phenomenon is offered as an explanation for the other plateaus [12, 13]. The gap for the $\nu = 0$ state exhibits a crossover from linear [14] to $\sqrt{eB}$ scaling [11, 15] which is interpreted to be the result of the screening of the on-site interaction due to the substrate [13]. Here, with no on-site interaction, we also find a $\sqrt{eB}$ dependence of the gap.

Magnetic catalysis is a striking example of dynamical symmetry breaking whereby an external magnetic field induces fermion-antifermion pairing for any attractive interaction [16–18]. Previous approaches to magnetic catalysis in graphene relied on perturbative, self-consistent techniques [19, 20], and thus one would also like a fully nonperturbative approach. Although previous lattice studies examined magnetic catalysis at finite temperature [21, 22], this is the first lattice study of the phenomenon at zero temperature. In the present article we expand on the preliminary results which first appeared in [23] by characterizing the behavior of both the dynamical mass and the chiral condensate as a function of the external magnetic flux.

GRAPHENE EFT

Starting from a tight-binding description of graphene, one can expand in momentum around the Dirac points which gives, at lowest order, the Dirac Hamiltonian. Thus, in the low-energy approximation, graphene is described by two species of massless Dirac fermions, arising from the points K and K' , each having an additional degree of freedom coming from the spin of the original electron [24]. These charged particles interact via the Coulomb interaction which is mediated by the scalar potential A_0 . This approximation is reasonable due to the fact that the Fermi velocity of the quasiparticles satisfies $v_F/c \approx 1/300$. The Euclidean effective field theory

(EFT) describing these excitations reads

$$S_E = \int dt d^2x \sum_{\sigma=1,2} \bar{\Psi}_\sigma \not{D}[A_0] \Psi_\sigma + \frac{(\epsilon+1)}{4e^2} \int dt d^3x (\partial_i A_0)^2, \quad (1)$$

where ϵ is the dielectric constant of the substrate on which graphene resides, and the Dirac operator reads

$$\not{D}[A_0] = \gamma_0 (\partial_0 + ieA_0) + v_F \sum_{i=1,2} \gamma_i \partial_i. \quad (2)$$

Our four-component Dirac spinors are organized in the following basis

$$\Psi_\sigma^\top = (\psi_{KA\sigma}, \psi_{KB\sigma}, \psi_{K'B\sigma}, \psi_{K'A\sigma}), \quad (3)$$

where K, K' refer to the Dirac points, A, B refer to the sublattices, and σ refers to the electron's spin projection. The graphene EFT possesses an internal $U(4)$ symmetry that is a consequence of the Dirac approximation. The generation of different mass terms allows for several patterns of SSB.

To study the graphene EFT nonperturbatively, we will discretize the continuum action in (1) on a cubic lattice. The gauge sector is described by the “noncompact” $U(1)$ lattice action [25]

$$S_G^{(NC)} = \frac{\beta}{2} \sum_n \sum_{i=1}^3 \left(\hat{A}_0(n) - \hat{A}_0(n+\hat{i}) \right)^2, \quad (4)$$

where $\beta = \xi(\epsilon+1)/(2e^2)$, $\xi \equiv a_s/a_t = 3v_F$ is known as the anisotropy parameter, which controls the ratio of the spatial lattice spacing to the temporal lattice spacing, and $\hat{A}_0(n) = a_t A_0(n)$ is a dimensionless lattice field. The Dirac action is discretized on the lattice staggered fermions [26]. In this formulation, the Dirac spinor structure of the action is diagonalized leaving

$$S_F = \sum_n \left[\frac{1}{2} \hat{\chi}_n \left(U_0(n) \hat{\chi}_{n+\hat{0}} - U_0^\dagger(n-\hat{0}) \hat{\chi}_{n-\hat{0}} \right) + \frac{v_F}{2\xi} \sum_{i=1,2} \eta_i(n) \hat{\chi}_n (\hat{\chi}_{n+\hat{i}} - \hat{\chi}_{n-\hat{i}}) \right], \quad (5)$$

where $\hat{\chi}_n = a_s \bar{\chi}_n$, $\hat{\chi}_n = a_s \chi_n$ are one-component, dimensionless Grassmann fields, $\hat{m} = a_t m$ is the dimensionless bare mass, and $\eta_1(n) = (-1)^{n_0}$, $\eta_2(n) = (-1)^{n_0+n_1}$, are site-dependent phase factors. The interaction of the fermions with the scalar potential is introduced via the link variables $U_0(n) = e^{ie\hat{A}_0(n)}$. Staggered fermions preserve a remnant $U(1) \times U(1)_\epsilon$ symmetry left over from the continuum $U(4)$ symmetry. The $U(1)$ symmetry, which corresponds to fermion number conservation, is given by

$$\chi(x) \rightarrow \exp(i\alpha) \chi(x), \quad \bar{\chi}(x) \rightarrow \bar{\chi}(x) \exp(-i\alpha). \quad (6)$$

The $U(1)_\epsilon$ symmetry, known as the “even-odd” symmetry, is given by

$$\chi(x) \rightarrow \exp(i\beta\epsilon(x)) \chi(x), \quad \bar{\chi}(x) \rightarrow \bar{\chi}(x) \exp(i\beta\epsilon(x)), \quad (7)$$

where $\epsilon(x) \equiv (-1)^{x_0+x_1+x_2}$.

For one species of staggered fermions in two dimensions, there is no controversy that the full chiral symmetry is restored in the continuum limit, and that at nonzero lattice spacing, the exact $U(1)_\epsilon$ symmetry, a subgroup of the full continuum chiral group, is a reliable indicator of the breaking of the full continuum symmetry [27]. Other easily simulated lattice fermion formulations do not have this property, which is the main reason for choosing it for this study. In practice, one explicitly introduces a mass term, $m \sum_n \hat{\chi}_n \hat{\chi}_n$, which breaks the $U(1)_\epsilon$ symmetry, in order to regulate infrared singularities and to investigate SSB. After taking the infinite volume limit one then attempts to extrapolate to the chiral limit, $m \rightarrow 0$.

In our simulations we use an improved version of the action in (5), known as the asqtad action [28]. The improvement removes all $O(a^2)$ discretization errors in both the free lattice Dirac action and in the interaction of the fermions with the $U(1)$ gauge field. The latter is done to remove interactions with high-momentum photons, which are responsible for violations of the symmetry between the two Dirac fermion species which are encoded in the staggered action, along with suppressing vertices in the lattice action which have no continuum analogue. The remaining errors begin at $O(\alpha_g a^2)$ and are expected to be small thus giving us a closer representation of the continuum EFT. We are not, however, interested in explicitly taking the continuum limit of the EFT as this corresponds to sending the cutoff to infinity while the theory is only valid for long wavelengths.

We now introduce a uniform magnetic field perpendicular to the sheet of graphene, described in the continuum by the vector potential $A_\mu = \delta_{\mu,2} B x_1$. On the lattice this necessitates the introduction of static $U(1)$ link variables in the spatial directions

$$U_y(n) = e^{ia_s^2 e B n_x}, \quad (8)$$

$$U_x(n) = \begin{cases} 1 & , n_x \neq N_s - 1 \\ e^{-ia_s^2 e B N_x n_y} & , n_x = N_s - 1 \end{cases}, \quad (9)$$

where $N_s = N_x = N_y$ and $n_x, n_y = 0, 1, \dots, N_s - 1$. The toroidal geometry (periodic boundary conditions in space) requires that $\Phi_B \equiv eB/(2\pi) = N_B/L_s^2$, where $L_s = N_s a_s$, is the lattice extent in the spatial direction and N_B is an integer in the range $0 \leq N_B \leq N_s^2/4$ [29].

RESULTS AND DISCUSSION

The main observable we use in determining SSB is the chiral condensate. In the chiral limit it serves as an order

parameter distinguishing the semimetal phase, where it is zero, from the insulating phase, where it is nonzero. In the continuum, the chiral condensate is defined as follows:

$$\begin{aligned}\langle\bar{\Psi}\Psi\rangle &= \frac{1}{V} \frac{\partial \log Z}{\partial m} \\ &= \frac{1}{V} \frac{1}{Z} \int \mathcal{D}A_0 \text{Tr} (\not{D} + m)^{-1} e^{-S_E^{\text{eff}}[A_0]},\end{aligned}\quad (10)$$

where $S_E^{\text{eff}}[A_0] = S_G[A_0] - \text{Tr} \log (\not{D} + m)$, and the partition function is given by

$$Z = \int \mathcal{D}A_0 e^{-S_E^{\text{eff}}[A_0]}.\quad (11)$$

On the lattice, the equivalent expression is given by

$$\langle\bar{\chi}\chi\rangle = \frac{1}{V} \frac{1}{Z} \int \mathcal{D}A_0 \text{Tr} (\not{D}_{st} + m)^{-1} e^{-S_E^{\text{eff}}[U_0]},\quad (12)$$

where $\not{D}_{st}$ is the asqtad-improved staggered Dirac operator and m is the bare fermion mass.

Our strategy for studying magnetic catalysis is as follows. At zero magnetic field, the graphene EFT is known to undergo a second-order transition as a function of the inverse coupling β [30]. Going to large values of β , corresponding to values of the graphene fine-structure constant less than the critical value of $\alpha_g^{cr} = 2e^2/(4\pi v_F(\epsilon_{cr} + 1)) \approx 1.1$ [30], one is firmly in the semimetal region, characterized by a vanishing chiral condensate. Fixing the coupling and turning on the external magnetic field, one would expect to see the condensate acquire a nonzero value. Our results for the chiral condensate as a function of bare mass at fixed $\beta = 0.80$, which corresponds to $\alpha_g \approx 0.3$, for both zero and nonzero magnetic flux, are shown in Fig. 1. One can see that for zero field, $\sigma \equiv \langle\bar{\Psi}\Psi\rangle$ is approximately linear in the bare mass over the range of values shown. This is a clear indication that we are in the semimetal phase. At nonzero field, one can see that the condensate increases and exhibits strongly nonlinear behavior as a function of m .

For both zero and nonzero magnetic flux, the condensate vanishes as the explicit symmetry breaking parameter is removed. When SSB occurs this may still happen because of the finite spatial extent of the box. We have explicitly checked this is not the case by calculating σ as a function of m for $N_s = 8, 20, 30$. We find no significant dependence on N_s . One can explain this independence at nonzero magnetic field by noting that the magnetic length, $l_B \equiv \sqrt{\hbar c/eB}$, which characterizes the quasiparticle's cyclotron orbit, satisfies $1 < l_B < N_s$, in units of a_s . We have also checked the dependence of the condensate on N_z and found that for $N_z \geq 10$, the finite volume correction is less than 2%.

The finite extent of the box in the Euclidean time direction, N_τ , also plays a role. It is related to the temperature of the system, $T = 1/(N_\tau a_t)$. We vary N_τ to investigate the role of temperature in restoring the symmetry. This is depicted in Fig. 2. We find that when the

FIG. 1: The chiral condensate $\sigma \equiv \langle\bar{\Psi}\Psi\rangle$ as a function of the bare fermion mass at zero field (black points) and at magnetic flux $\Phi_B = 0.125$ (blue points), where flux is measured in units of a_s^2 . We report the volumes in the form $N_s^2 \times N_z \times N_\tau$. The red points depict the chiral limit of σ using the $T = 0$ extrapolated points ($\chi^2 \approx 0.6$) for $\Phi_B = 0.125$. The errors on each point at $T = 0$ were statistical as well as systematical i.e. the choice of model for the zero-temperature extrapolation. The error bars on each point are not visible on this scale.

dimensionless quantity T/m is large the condensate tends to vanish while for $T/m < 1$ the condensate plateaus towards a finite value. To study magnetic catalysis in the ground state requires first taking the zero-temperature limit. Special attention must be paid to the order of limits by first taking $T \rightarrow 0$ before taking $m \rightarrow 0$ in order to properly isolate the ground state. We have performed this limit by taking points at fixed m near the plateau and extrapolating to $T = 0$ using a polynomial fit form. Using two different fit forms for the extrapolation we have been able to estimate a systematic error associated with this procedure. Previous studies [21, 22] were performed at finite-temperature and did not take this limit.

In Fig. 1 we illustrate the chiral condensate as a function of the bare mass after taking the zero-temperature limit for magnetic flux $\Phi_B = 0.125$. One can see that in the chiral limit a nonzero condensate is obtained. This procedure was then repeated for three other magnetic fluxes. The chirally extrapolated, zero-temperature results are displayed in Fig. 3. We thus have obtained a profile of the condensate as a function of the magnetic flux solidifying the scenario of magnetic catalysis in the graphene EFT.

SSB also has observable consequences for the fermion quasiparticle which acquires a dynamical mass, m_F . In order to study the dynamical mass, we calculate the quasiparticle propagator in the temporal direction at zero

FIG. 2: The chiral condensate σ plotted as a function of T/m for the ensembles with $\Phi_B = 0.125$ and $N_s = 8$.

FIG. 3: The chirally extrapolated, zero temperature values of the chiral condensate σ , plotted as a function of the magnetic flux, $\Phi_B = eB/2\pi$. The points at $\Phi_B = 0.125$ and $\Phi_B = 0.0625$ have a spatial size of $N_s = 8$ while those at $\Phi_B = 0.083$ and $\Phi_B = 0.056$ have a spatial size of $N_s = 12$. The errors on the points were obtained from the chiral extrapolations at $T = 0$. We have fitted the data to a quadratic constrained to pass through the origin ($\chi^2/\text{d.o.f.} \approx 3.6/2$).

spatial momentum

$$G_F^{(\tau)}(\tau; \vec{p} = 0) \equiv \sum_{x,y} \langle \chi(x, y, \tau) \bar{\chi}(0, 0, 0) \rangle, \\ \sim A e^{-m_F \tau}, \quad \text{for large } \tau, \quad (13)$$

where A is a τ -independent constant. The results for the dynamical mass are displayed in Fig. 4. One observes that at a given bare mass, the dynamical mass increases with the magnetic flux. Furthermore, the plot suggests that all four ensembles extrapolate to nonzero values in the chiral limit. Although one expects this to be the case for nonzero magnetic flux, at zero magnetic flux one ex-

FIG. 4: The fermion dynamical mass as a function of the bare fermion mass for all four nonzero magnetic fluxes and zero flux. The curve represents the pole of the fermion propagator ($\Phi_B = 0$) calculated to $O(e^2)$ in lattice perturbation theory.

pects the dynamical mass to vanish in the chiral limit. Perturbative arguments show that at zero magnetic field, the dynamical mass develops negative curvature near the origin and ultimately vanishes as the bare mass is removed [31]. A possible continuation of this work would be the calculation of the quasiparticle propagator at finite momentum in order to study the renormalization of the Fermi velocity v_F .

Extrapolating the dynamical mass to the chiral limit for nonzero magnetic flux, we find a result which agrees with perturbative predictions for magnetic catalysis in $(2+1)$ -dimensional field theories. Namely, we find that the chirally extrapolated quasiparticle mass, m_F , scales linearly with $\sqrt{eB}$. This is illustrated in Fig. 5 giving further confirmation of magnetic catalysis in the graphene EFT.

CONCLUSION

Using nonperturbative methods for the study of the graphene EFT, we have shown the existence of spontaneous symmetry breaking at zero temperature due to an external magnetic field. We have characterized the ground state of the system by performing a zero-temperature extrapolation of our observables followed by a chiral extrapolation. We have also characterized the dynamically generated mass of the Dirac quasiparticles and investigated its dependence on magnetic flux. In a future article we will present results for the time-reversal-odd Haldane condensate as well as the pseudoscalar Nambu-Goldstone boson that results from the spontaneous breaking of chiral symmetry [31].

FIG. 5: The zero-temperature, chirally extrapolated dynamical mass as a function $\sqrt{eB}$. We have included a linear fit which gives an intercept which is consistent with zero ($\chi^2/\text{d.o.f.} \approx 3.7/2$). This is expected due to the fact that the dynamical mass vanishes in the chiral limit in the absence of an external magnetic field.

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