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Strongly coupled Graphene on the Lattice

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The two-dimensional carbon allotrope graphene has recently attracted a lot of attention from researchers in the disciplines of Lattice Field Theory, Lattice QCD and Monte Carlo calculations. This interest has been prompted by several remarkable properties of the conduction electrons in graphene. For instance, the conical band structure of graphene at low energies is strongly reminiscent of relativistic Dirac fermions. Also, due the low Fermi velocity of $v_F \simeq c/300$, where c is the speed of light in vacuum, the physics of the conduction electrons in graphene is qualitatively similar to Quantum Electrodynamics in a strongly coupled regime. In turn, this opens up the prospect of the experimental realization of gapped, strongly correlated states in the electronic phase diagram of graphene. Here, we review the experimental and theoretical motivations for Lattice Field Theory studies of graphene, and describe the directions that such research is likely to progress in during the next few years. We also give a brief overview of the two main lattice theories of graphene, the hexagonal Hubbard theory and the low-energy Dirac theory. Finally, we describe the prospect of extracting response functions, such as the electric conductivity, using Lattice Field Theory calculations.

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1. Introduction

Graphene is a novel two-dimensional carbon nanomaterial with unusual electronic properties. These deviate from the standard theory of conduction due to the linear dispersion of the charge carriers [1]. In spite of the "relativistic" energy-momentum relation, the electrons in graphene move non-relativistically. This is evidenced by the low Fermi velocity of $v_F \simeq c/300$, where c denotes the speed of light in vacuum. While the band structure of graphene is classified as semimetallic, the material conducts electricity better than silver and outperforms the carrier mobility in silicon due to its high resistance to impurities and chemical damage. Most importantly, graphene is inspiring technological innovations and improvements, such as graphene-based transistors and integrated circuits, transparent conducting electrodes, solar cells and ultracapacitors. The discovery of this revolutionary material in 2004 was awarded the Nobel Prize in physics in 2011.

Compared to Quantum Electrodynamics (QED), the electron-electron coupling α_g in graphene is enhanced by a factor of c/v_F, and is thus roughly 300 times larger than the fine-structure constant $\alpha \simeq 1/137$ [2]. Moreover, as the screening length diverges at the neutral point, the Landau picture which admits the mapping of a strongly interacting electronic liquid onto a gas of non-interacting fermions breaks down. In this situation, the electrical conductivity is of particular interest, as it is under intense study in suspended graphene, which can be routinely manufactured and electrically contacted. The temperature- and frequency dependence of the conductivity is also a central design parameter in nanoelectronic applications, such as transistors and current switches.

Graphene, as a strongly interacting quantum mechanical many-body system, ranks among the most challenging problems in theoretical and computational physics to date. Other prominent examples where complex behavior emerges in many-body systems at strong coupling include, to name a few, high-T_c superconductivity, superfluidity in ultracold atomic gases, and the formation of hadrons in QCD. While significant progress has been made in the theoretical sector using analytical approaches (such as perturbative, renormalization group and self-consistent treatments), non-perturbative methods which take full account of quantum mechanical fluctuations offer the best prospect for a complete, *a priori* solution. A great driving force behind our understanding of strongly coupled quantum systems is Lattice QCD, whereby the properties of QCD are computed from first principles on a discretized space-time lattice. Due to advances in algorithmics as well as in computer power, Lattice QCD is able to predict the properties of hadrons (such as the masses of baryonic resonances) to percent-level accuracy. The discovery of graphene has also promoted the adoption of Lattice QCD methods, in particular the Hybrid Monte Carlo (HMC) algorithm, in condensed matter physics [3, 4, 5, 6]. In turn, the HMC algorithm has lead to great progress in the closely related area of Hubbard-like models in atomic physics, in particular for the strongly interacting Fermi gases in the unitarity limit [7].

2. Graphene at strong electron-electron coupling

Graphene is often described both as a strongly interacting many-fermion system, and as an "ultimate system of non-interacting electrons". Recent experiments with suspended graphene have provided increasing evidence for the "missing" electron-electron interaction. While the spontaneous breakdown of the semimetallic phase is yet to be detected, observed phenomena include

the fractional quantum Hall effect [8] in an external magnetic field, and a strong upward renormalization of the Fermi velocity at the neutral point [9]. Also, a resistive state in a suspended graphene bilayer has recently been reported at zero magnetic field [10], and hypothesized to be of interaction-driven origin. Taken together, these developments suggest that an investigation of emergent strong-coupling phenomena in graphene is timely, which should also clarify the question whether the electron-electron interaction in graphene is key to our understanding of the electronic phase diagram and transport, or whether such effects can safely be neglected. The combination of Lattice Field Theory and MC calculations, formulated either in terms of a hexagonal Hubbard model based on the tight-binding description of graphene, or in terms of a low-energy theory of Dirac fermions, is a promising way to proceed as it captures the physics of strong electron-electron interaction without uncontrolled approximations. Below is a (by no means exclusive) list of objectives that are likely to be central in the application of Lattice Field Theory to graphene in the near future:

- **The zero-temperature electronic phase diagram of graphene.** What is the critical value of the electron-electron coupling α_g where the semimetallic properties of graphene break down? Is suspended graphene above or below this critical coupling at zero temperature? Is it possible to induce an insulating state by a technologically feasible amount of strain (increasing the lattice constant of graphene by a few tens of percent) to reduce the probability for the electrons to tunnel between neighboring carbon atoms? What are the critical exponents of the semimetal-insulator transition? How is the Fermi velocity v_F renormalized by interactions? To what extent is the critical coupling and the associated exponents affected by screening of the electron-electron interaction?

- **Finite temperature and gapped phases in graphene.** The effects of finite temperature on gapped strong-coupling phases in graphene are especially interesting, as the Mermin-Wagner theorem prohibits spontaneous breaking of a continuous symmetry in a two-dimensional system. However, there is considerable evidence from MC studies by Hands *et al.* [4] that suspended graphene undergoes a Kosterlitz-Thouless (KT) transition into a gapped phase at a finite temperature, which is currently poorly known. How is the zero-temperature phase diagram of graphene reflected in the finite-temperature properties? What is the critical temperature of the putative KT transition?

- **The electrical conductivity of graphene.** How does the electron-electron interaction affect the conductivity $\sigma(\omega, T)$ as a function of frequency ω and temperature T? To what extent is the minimal DC conductivity $\sigma(\omega = 0, T)$ determined by the electron-electron interaction, and how can the measured (see Ref. [9]) temperature dependence of the minimal conductivity at low T be explained? How close is suspended graphene (and graphene on a dielectric substrate) to a quantum critical point where the semimetallic phase breaks down?

- **The viscosity of the electrons in graphene.** Theoretical estimates [11] of the ratio of shear viscosity to entropy density η/s have put forward the possibility that the viscosity in graphene is unusually small, which was interpreted as an indicator of complex fluid dynamics, observable on length scales of $\simeq 1$ μm. What is the magnitude and temperature

dependence of the viscosity in the presence of interactions? How does the appearance of spontaneously gapped phases affect the viscosity? Within a MC calculation, can sufficient statistics be obtained to find a clear signal for the viscosity?

- **Superfluidity in a graphene bilayer.** In a bilayer with equal populations of electrons and holes on the respective layers, the attractive electron-hole interaction induces pair formation of electrons and holes. What is the critical temperature T_c for superfluidity of electron-hole pairs in a such a graphene bilayer? Depending on the amount of screening, T_c has been suggested to be as high as 300 K, while $T_c \simeq \mu$K in a more pessimistic scenario [12]. If the system is imbalanced (more electrons than holes or *vice versa*), T_c will decrease. What is the critical imbalance where T_c reaches zero?

- **Ultracold fermionic atoms in a hexagonal optical lattice.** What similarities exist between the electronic properties of graphene and the analogous observables of ultracold fermionic atoms (such as potassium-40) confined to a hexagonal optical lattice? The tunneling amplitude and the interparticle coupling can be controlled over a wide range on an optical lattice, the latter using the Feshbach resonance technique [13]. In real graphene, such tuning can in principle be achieved using tension and dielectric materials, albeit in a much more cumbersome and limited way. Significantly, the interparticle coupling on optical lattices can be increased beyond $\alpha_g \simeq 2$, providing access to physics that may only occur in an "unphysical" parameter range in real graphene.

3. Hubbard theory of graphene

Graphene can be described as a tight-binding model with (non-local) electron-electron couplings. The corresponding (non-relativistic) Hamiltonian is

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle,\sigma} \psi^{\dagger}_{\mathbf{i},\sigma} \psi_{\mathbf{j},\sigma} - t' \sum_{\langle\langle \mathbf{i},\mathbf{j} \rangle\rangle,\sigma} \psi^{\dagger}_{\mathbf{i},\sigma} \psi_{\mathbf{j},\sigma} + U_{00} \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} + \frac{1}{2} \sum_{\mathbf{i} \neq \mathbf{j},\sigma,\sigma'} U_{\mathbf{ij}}\, n_{\mathbf{i},\sigma} n_{\mathbf{j},\sigma'}, \qquad (3.1)$$

where $\psi_{\mathbf{i},\sigma}$ annihilates an electron at lattice site $\mathbf{i}$ with spin $\sigma \in \{\uparrow,\downarrow\}$ and $n_{\mathbf{i},\alpha} \equiv \psi^{\dagger}_{\mathbf{i},\alpha} \psi_{\mathbf{i},\alpha}$. The tunneling amplitudes between nearest- and next-to-nearest neighbor sites are $t \simeq 2.5$ eV and $t' \simeq 0.1$ eV, respectively. If only the on-site repulsion U_{00} is accounted for, the phase diagram of Eq. (3.1) has been computed using the Quantum Monte Carlo (QMC) approach of Ref. [14]. In such a treatment, graphene exhibits a semimetallic phase (SM) at weak coupling, a gapped spin-liquid phase (SL) at intermediate couplings and an antiferromagnetic Mott insulator (AFMI) at strong coupling. As $U_{00}/t \simeq 3.3$ in suspended graphene, such systems are tantalizingly close to the critical coupling $U_{00}/t \simeq 3.5$ for a semimetal-insulator transition into the SL phase.

At least two mechanisms exist which can change this picture. First, U_{00}/t increases under the application of strain, due to the decreased overlap of the carbon orbitals. A technologically feasible amount of strain, increasing the lattice constant of graphene by a few percent, may then suffice to induce the SL state. Second, the non-local couplings in Eq. (3.1) should not be neglected at low densities, where the electron-electron interaction remains unscreened. Indeed, the couplings $U_{\mathbf{ij}}$ have been computed in density functional theory (DFT) by Ref. [15], which yielded $U_{01}/t \simeq 2.0$

with further sizeable contributions at longer ranges. A particularly interesting question is in what way such non-local couplings affect the electronic phase diagram, in particular the critical coupling for the SL state. Notably, the Hybrid Monte Carlo (HMC) algorithm [16] which enables global lattice updates, has recently been successfully employed for systems with a Hamiltonian similar to Eq. (3.1), in particular the Unitary Fermi Gas (UFG).

4. Dirac theory of graphene

Relativistic QFT can be applied to graphene, as the electronic dispersion relation becomes linear in the vicinity of the neutral point [2]. The resulting linearized low-energy theory, valid in the vicinity of the "Dirac points" of graphene, can be studied at strong electron-electron interaction using the Lattice Monte Carlo (LMC) framework, and complements the abovementioned Hubbard approach. As in Lattice QCD and Lattice Field Theory in general, Euclidean space-time is used in order to obtain a positive definite probability measure. The resulting low-energy QFT of graphene can then be formulated in terms of the action

$$S_E \equiv \frac{1}{2g^2}\int d^3x\,dt\,(\partial_i A_0)^2 - \sum_{a=1}^{N_f}\int d^2x\,dt\,\bar{\psi}_a D[A_0]\psi_a, \quad D[A_0] = \gamma_0(\partial_0 + iA_0) + v_F\gamma_i\partial_i, \qquad (4.1)$$

where ψ (with $\bar{\psi} \equiv \psi^\dagger\gamma_0$) is a four-component fermion field, and γ_μ denotes the Dirac gamma matrices. A graphene monolayer corresponds to $N_f = 2$, while a bilayer is described by $N_f = 4$ in the absence of interlayer couplings. Interlayer tunneling can be accounted for by introducing two coupled monolayers, giving rise to the characteristic quadratic dispersion of graphene bilayers. The electron-electron interaction is mediated by the instantaneous gauge field A_0, with coupling constant $g^2 \equiv e^2/\varepsilon$. Here ε is the effective permittivity of the medium (for example a hemisphere of SiO_2 substrate). The strength of the electron-electron interaction is controlled by the "fine structure constant" $\alpha_g \equiv e^2/(4\pi\varepsilon v_F)$ (in units where $\hbar = c = 1$), such that low values of $v_F \simeq 1/300$ and $\varepsilon \simeq 1$ translate into a large electron-electron coupling. In the presence of a dielectric substrate, $\varepsilon > 1$ due to the increased permittivity. It should be noted that Eq. (4.1) is an example of a "reduced gauge theory", as the gauge field A_0 propagates in one more spatial dimension than the fermion field ψ, which is confined to a $(2+1)$-dimensional surface.

The LMC treatment of graphene is based on a discretized version of Eq. (4.1) on a lattice of space-time points. Unlike the QMC treatment of graphene, this lattice has no correspondence to the "physical" hexagonal lattice of carbon atoms. Instead, physical predictions are obtained in the continuum limit of vanishing lattice spacing. As the continuum limit can only be approached, a question arises to what extent the space-time lattice distorts the continuum physics. For this purpose, different discretizations of Eq. (4.1) have been developed, which share the same continuum limit but emphasize different aspects of the physics on a lattice. In Lattice QCD, a standard choice is staggered (or Kogut-Susskind) fermions [17], which only partially respect the symmetries of the continuum theory. The use of overlap fermions (see Ref. [18] and references therein), while significantly more computationally expensive, allows for a much closer approach to the continuum limit in studies of emergent strong-coupling phenomena, such as spontaneous chiral symmetry breaking.

5. Computation of transport properties

A brief outline of the extraction of the transport properties of graphene using LMC calculations is given here, in order to provide an idea of the computational intricacies and challenges. An experimentally readily accessible and relevant observable is the minimal DC ($\omega = 0$) conductivity $\sigma(n=0,T)$, which involves the computation of the Euclidean correlator

$$G(\tau) = \int d^2x \langle J^\dagger(\tau,\mathbf{x}) J(0,\mathbf{0})\rangle, \qquad J(\tau,\mathbf{x}) \equiv \sum_{k=1,2} \bar{\psi}(\tau,\mathbf{x})\gamma_k \psi(\tau,\mathbf{x}), \tag{5.1}$$

where $\rho(\omega)$ is obtained from the correlator $G(\tau)$ (which is measured from the MC data) as

$$G(\tau) = \int_0^\infty \frac{d\omega}{2\pi} K(\omega,\tau)\rho(\omega), \qquad K(\omega,\tau) = \frac{\cosh(\omega\tau - \omega/2T)}{\sinh(\omega/2T)}. \tag{5.2}$$

The minimal conductivity is then given by the zero-frequency limit of the spectral function $\rho(\omega)$ according to

$$\frac{\sigma(n=0,T)}{T} = \lim_{\omega\to 0} \frac{\rho(\omega)}{6\omega T}, \tag{5.3}$$

where the temperature T is related to the temporal extent N_τ of the Euclidean space-time lattice by $1/T = aN_\tau$, and a is the temporal lattice spacing. The inversion of Eq. (5.2) is complicated by the fact that $G(\tau)$ is obtained by MC calculation at a discrete set of points τ_i, where the number of data points i is typically $\mathcal{O}(10)$ due to CPU power limitations and algorithm scaling, while $\rho(\omega)$ is in principle a continuous function of ω. As the integration range in ω is discretized into $N_\omega \sim \mathcal{O}(10^3)$ points, a straightforward inversion is ill-defined.

The numerical inversion of expressions similar to Eq. (5.2) has become the focus of intense theoretical and computational efforts. Here, we shall focus on the studies at Swansea University of the behavior of the conductivity in the vicinity of the deconfinement transition in QCD at high temperatures by Aarts *et al.* in Ref. [19]. These efforts have led to the development of a promising algorithm, which allows for a numerically stable calculation of $\rho(\omega)$ using a combination of Bayesian analysis and the maximum entropy method (MEM). In the Bayesian approach, one constructs the "most probable" spectral function by minimizing a conditional probability $P[\rho|DH]$, where D denotes the available data on $G(\tau)$ and H some additional "prior knowledge". In the MEM approach, this additional knowledge is introduced by the "entropy term"

$$P[\rho|DH] = \exp\left(-\frac{1}{2}\chi^2 + \alpha S\right), \quad S = \int_0^\infty \frac{d\omega}{2\pi}\left[\rho(\omega) - m(\omega) - \rho(\omega)\ln\frac{\rho(\omega)}{m(\omega)}\right], \tag{5.4}$$

where χ^2 is the standard likelihood function, and α is a parameter which controls the relative weight of the data and the prior knowledge, which is introduced through the "default model" function $m(\omega)$. Unfortunately, the MEM analysis of current-current correlators in Lattice QCD suffers from numerical instabilities and poor convergence, which make a model-independent determination of σ in the limit $\omega \to 0$ difficult. In this situation, performing the analysis in terms of the new quantities

$$\bar{K}(\omega,\tau) = \frac{\omega}{2T} K(\omega,\tau), \qquad \bar{\rho}(\omega,\tau) = \frac{2T}{\omega}\rho(\omega,\tau), \qquad a^2\bar{m}(\omega) = \bar{m}_0(b + a\omega). \tag{5.5}$$

was found in Ref. [19] to circumvent the numerical instabilities at small ω to a large extent. In the context of Lattice QCD, the zero-frequency conductivity has been shown to be independent of b to an accuracy of $10-20\%$. While such accuracy in itself is sufficient to produce novel and valuable information, it should also be noted that as far as CPU power is concerned, the situation for graphene is more favorable than the situation for QCD, due to the lower dimensionality of the graphene problem. This advantage can be translated to greater MC statistics, but more significantly to a larger extent N_τ in the temporal lattice dimension, which will improve the accuracy and model-independence of the MEM analysis.

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