CECAM Workshop Scientific Report

Workshop: Graphene: from band structure to many-body physics

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I. Summary/Scope of the workshop

The workshop “Graphene: from band structure to many-body physics” was held at the University of Bremen, Germany from September 3rd to 7th 2012. In total, 66 participants from France, Germany, Italy, The Netherlands, Norway, Ukraine, Spain, USA, UK, Denmark, Belgium, Potugal, Iran, Saudi Arabia, Luxembourg, South Korea, India, Turkey, South Africa, Sweden, Switzerland attended the workshop.

The programme consisted of 30 invited lectures, one poster session presenting 31 posters and many events (reception / conference dinner) to allow for informal exchange. The lectures were scheduled to last 40 min, including 5-10 min discussion time. In addition to this extended time for discussion, the chairpersons were instructed to introduce the subject of the session and to actively participate in the discussion. This “Gordon-conference-style” was essential to guarantee a vivid discussion. The organizers ensured that well-established scientists acted as invited speakers and chairpersons.

Concerning the poster session, we accepted only 31 posters to allow for an intense exchange of ideas at each single poster. Here, we encouraged in particular the young scientists to ask questions. The participation of PhD students was supported by partly covering local accommodation costs.

Due to the compact organization and accommodation in one hotel only all participants were staying together for the whole time of the conference, which additionally enforced the scientific discussion which was mandatory since scientists from various fields, i.e. Quantum Monte-Carlo, many-body perturbation theory, DFT, diagrammatic techniques such as dual fermions or renormalization group approaches etc. were attending the meeting to merge ideas and formulate a common goal for future directions and method developments. By having theorists and experimentalists from the fields of scanning probe techniques, electron transport, magnetometry and photoemission spectroscopy together at the workshop a vivid exchange between theory and experiment has been fostered.

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II. Scientific content, main outcome of key presentations, selected discussions

Electrons in graphene (should) behave like massless Dirac quasiparticles and in absence of doping the Fermi surface shrinks to two Fermi points. In the simplest low energy model, graphene presents a realization of two dimensional quantum electrodynamics (QED) but with large effective fine structure constant $\alpha \approx 1$ instead of $\alpha = 1/137$ in usual QED. Thus, graphene is very likely not a weakly interacting electron system leading to the fundamental question of how the electronic system in graphene and related materials is controlled by many electron correlation phenomena. A central issue of the workshop thus was to understand manifestations of Coulomb interactions in graphene and to discuss open questions including whether and how the electrons in graphene might be driven into insulating, magnetic, exotic quantum-disordered or topologically non-trivial strongly correlated phases.

Various sessions have been related to the topics (a) screening in graphene, (b) defects and edges, (c) many body effects in transport, (d) many body effects in multilayers, (e) many body instabilities, (f) electronic and lattice response, (g) electronic excitations.

The strength of Coulomb interactions in graphene is controlled and can be quantified through the material's dielectric constant, which has been a matter of controversy for the past few years. Several presentations addressed this issue: M. van Schilfgaarde showed that using the quasiparticle self-consistent GW approximation the fully screened dielectric constant of graphene tends to $\varepsilon \sim 4$ in the long wavelength limit which is in agreement with the Dirac electron model. However, unusually strong local field effects appear at intermediate wavelengths.

The critical value of the impurity charge for the relativistic collapse is also dependent on the screened coupling constant and allows for an estimation of the latter. This issue has been addressed in the talks given by L. Levitov about the theoretical prediction of the atomic collapse and the experimental verification by M. Crommie by scanning probe techniques. It has been demonstrated that the response of Dirac fermions to a Coulomb potential differs significantly from how non-relativistic electrons behave in traditional atomic and impurity systems. Electron-like and hole-like Dirac fermions were reported to respond differently to a Coulomb potential and comparison of the experiments to theoretical simulations has allowed to test predictions for how Dirac fermions behave near a Coulomb potential as well as to extract graphene's intrinsic dielectric constant $\varepsilon = 3.0 \pm 1.0$. This value of ε indicates that electron–electron interactions can contribute significantly to graphene properties, is in line with the Dirac electron model and the quasiparticle self-consistent GW approximation. So, there is good evidence for $\varepsilon \sim 3\text{-}4$ (at $q \rightarrow 0$) both from experiment and theory, now.

The several talks (experimental by E. Rotenberg and theoretical by S. Louie, L. Reinig, C. H. Park, and M. Polini) at the workshop reported manifestations of many body effects on the spectral and dynamical properties of graphene at energy scales related to optical excitations (on the order of a few eV). Many-body perturbation theory within the GW-BSE framework showed that the $\pi\pi^*$-plamson peak in the optical absorption spectra of graphene deviates ~0.5eV in energy from the value expected from LDA calculations due to an intricate balance of self-energy and excitonic effects. For highly doped graphene ARPES lineshapes are well explained by GW calculations if proper screening of the substrates is accounted for. Electron-plasmon interactions were clearly demonstrated to manifest in broadened momentum distribution curves near plasmonic resonances and "plasmaronic" side bands in

ARPES were proven to occur. Going to undoped graphene, the situation becomes more intricate: both experimental photoemission spectra and GW calculations revealed a doping dependent *increase* of the charge carrier velocities by up to a factor of ~2 due to electron-electron interactions. Indeed, a logarithmic divergence of the Fermi velocity and marginal Fermi liquid behavior (Im $\sum(\omega) \sim |\omega|$) when approaching charge neutrality are expected theoretically due to the long range tails of the Coulomb interaction. These expectations are now confirmed experimentally.

At lowest energies the behavior of mono- and also multilayer graphene appears very intricate and there were several discussions focusing on various types of instabilities (spin-liquid, nematic, charge-density waves etc.). Quantum Monte Carlo simulations of the Hubbard model on the honeycomb lattice reported by A. Muramatsu indicate transitions from a Dirac material to a gapped phase at $U/t \sim 3.5$ but the onset of antiferromagnetic order only for $U/t > 4.5$. The intermediate phase in the range $3.5 < U/t < 4.5$ has been proven by A. Muramatsu to be very likely a spin liquid. However, the question of which aspects of graphene physics could be described in terms of a Hubbard model with on-site interaction only is still unclear. As pointed out in the presentation of S. Blügel, cRPA calculations show that both local ($U \sim 3.3t$) and non-local Coulomb interactions in graphene are large. The interplay of long- and short range Coulomb interactions can lead to non-trivial superconducting phases as has been pointed out in the talk of F. Guinea.

The realistic description of strong local and non-local Coulomb interactions requires novel computational tools. The “Dual Boson Approach” explained in the presentation of A. Lichtenstein can be a very promising in this respect. Similarly, functional renormalization group methods can be very helpful to judge the possibilities of many body instabilities in the case on strong local and non-local Coulomb interactions being effective at the same time. As demonstrated by C. Honerkamp in bilayer graphene the interplay of local- and non-local Coulomb terms puts the system in close proximity to a transition line between a quantum spin Hall phase and an antiferromagnetic phase. Several sessions and discussions on strong correlations in graphene showed that further interfacing of ab-initio and quantum field theoretical methods is needed. As pointed out by S. Sharapov, measurements of the optical Hall effect can help to distinguish between different gapped states of graphene.

Edges and defects in graphene can exhibit localized states and resonances near the Fermi level which make the system susceptible to magnetic or other instabilities. This issue has been addressed in several theoretical and experimental talks. On the experimental side magnetic moments in fluorinated graphene revealed by SQUID magnetometry were reported by I. Grigorieva and STM spectroscopy by C. Gomez-Rodriguez demonstrated the appearance of midgap resonances in irradiated graphite. The latter type of resonances are believed trigger the formation of magnetic moments. A joint theoretical (O. Yazyev) and experimental study (M. Crommie’s group) on edge magnetism of unzipped chiral graphene nanoribbons reported the formation of a spectral gap of ~25meV which could be understood in terms of a mean field Hubbard model but with $U/t \sim 0.5$. The spectral properties of the mean field model qualitatively agree with numerically exact ground state QMC simulations of graphene nanoribbons reported by S. Wessel. These calculations also revealed tendencies towards long range strong ferromagnetic ordering. In so far, a consistent picture has emerged. What however still remains to be clarified is how screening (for instance from the metallic substrate of the unzipped CNT) and the interplay of local and non-local Coulomb interactions finally leads to an effective $U/t \sim 0.5$.

This problem is indeed closely related to the issue graphene hybrid structures. The presentation of L. Ponomarenko reporting Coulomb drag measurements and possibly a gapped phase in Graphene-hBN-Graphene structures demonstrated that that these heterostructures hold the interesting promise to engineer the strength of Coulomb interactions – an interesting option that should be explored in future research.

III. Assessment of the results and impact on future direction of the field

The goal of this workshop was to bring people from separate scientific communities together especially those doing density functional based simulations and beyond and those employing quantum lattice models. In particular, we wanted to promote the dissemination of information, scientific discussion with mutual benefits, and future collaborations amongst participants. To stimulate the active participation of younger participants (PhD students and postdocs), they were asked to present their recent research results as posters. We were successful in attracting the excellent speakers that we invited. Both the invited speakers and the regular participants contributed to a lively discussion. The unusual mixture of experimentalists, people doing classical molecular dynamics, ab initio calculations and quantum dynamics gave rise to exciting and fruitful discussions and new perspectives.

The proposed workshop has become a forum to discuss about possible solutions of the interacting electron problem in graphene related materials. We have been able to achieve the following key objectives:

1) To identify the major problems in our current understanding of electron correlation phenomena in graphene. To this end the communication between experiment and different theoretical communities and related combined results have shown predictive power and general understanding of electron correlation phenomena in graphene based materials. Overview talks have been given by distinguised experimentalists from different parts of the field (transport, STM, ARPES).

2) In various talks the main advantages and shortcomings of currently theoretical available techniques to model the interacting electron gas in this material have been dicussed. The techniques considered comprise (but not be limited to): density functional theory (LDA, GGA, LDA+U, etc), many body perturbation theory (GW and related quasiparticle methods), renormalization group (e.g. RPA based RG and more general functional RG), and Quantum Monte Carlo methods (determinantal quantum Monte Carlo, fixed node variational wave function Monte Carlo).

3) Presently there is an ongoing merging of different (complementary) theoretical approaches (experts in DFT based computational material science, numerical and analytical approaches to correlated electron systems). The workshop has identified possible contact points between. The speakers are convinced that the combination of complementary approaches like density functional based band structure methods with field theoretical or lattice model many body approaches including many body perturbation theory, renormalization group or Quantum Monte Carlo methods presents a very promising way to address the problem of interacting electrons in graphene.

4) The workshop has set the basis for scientific collaborations between the participants in order to foster methodological advances with respect to the state of the art as well as establishing new collaborations between theory and experiment.

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The Organizers