Neutron scattering study of collective triplet excitations in graphene based systems

Motivated by our analytical and numerical study of many-body excitations in graphene and graphite, we investigate the role of small spectral gap in the collective excitation spectra of graphene. We find that the single-particle gap parameter facilitates the formation of two collective states which are of singlet and triplet nature.

Graphene is a single layer of carbon atoms where $2p_z$ electrons form symmetric spectrum of negative energy and positive energy states, described by the Dirac equation in 2+1 dimensions. Such a peculiar cone-like dispersion relation gives rise to plenty of intriguing phenomena in graphene which differs from their conventional metallic counterparts. The nature of particle-hole excitations in the semi-metallic state of graphene is also significantly different from the corresponding particle-hole continuum (PHC) in metals [1]. In analogy with the plasmonic excitations of metals, where (long range) Coulomb forces bind the particle-hole pairs to form collective states, within the equation of motion approach we find that a very similar treatment gives rise to bound state formation in the triplet particle-hole channel, albeit as a result of short range part of the Coulomb interactions [2].

The so obtained triplet branch of collective excitation below the incoherent continuum of particle-hole excitations in pristine graphene (Fig. 1) whose band structure is given by a clean cone-like dispersion turns out to pose challenges for the observation by neutron scattering experiments. The first challenge deals with the ~1eV energy scale associated with this branch of excitations, which requires very high energy incident neutron beam, such that the momentum transfer falls beyond the first Brillouine zone, where the rapidly decaying atomic form factor of spatially fat $2p_z$ orbitals kills the neutron scattering signal [3]. On the other hand, if one focuses on the small energy parts of the spectrum, where lower energy incident neutrons are required, the expected coherent peak is so close to the incoherent PHC that in practice it does not seem easy to isolate the peak corresponding to such a collective state.

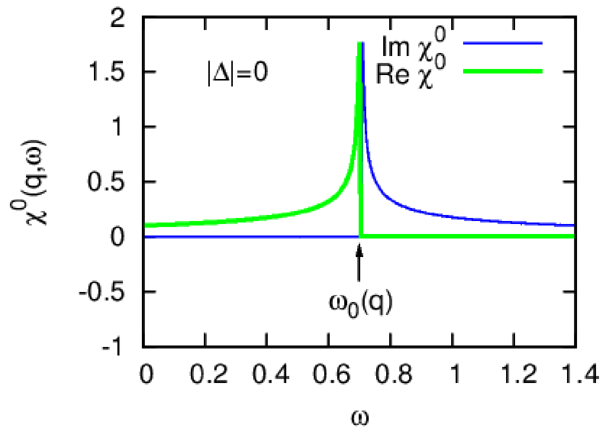

Fig. 1: The lower edge of the PHC is where the imaginary part of the non-interacting susceptibility (blue line) becomes non-zero. Energy scales is in units of the hoping t~2.8 eV of pi electrons.

In this visit as suggested by my host, Professor K. Yamada, we examined the following question: what happens if for some reason, a single-particle gap is opened in the spectrum of Dirac fermions in grahpene? As can be seen in Fig. 2, we find that as expected quite intuitively, the first role of gap opening is to push the lower edge of PHC to higher energies (where the blue line representing imaginary part becomes non-zero) and thereby to separate the incoherent part of the spectrum from the expected peak corresponding to collective excitations. However, we find that one more opportunity appears [4]; that is the density of particle-hole excitations is re-arranged in such a way that the real part (green line) displays a simple pole structure near the energy scale $\omega_0(q)$ i.e. at the lower edge of the gapless spectrum. Therefore the intersection of the green plot will bepossible with both 1/U and -1/U which corresponds to collective excitations in triplet and singlet channels, respectively. Therefore the non-zero value of the gap parameter provides a room for the formation of an additional singlet (charge) collective mode. Our finding shows that these two modes disperse linearly as a function of their momentum with two different velocities [4].

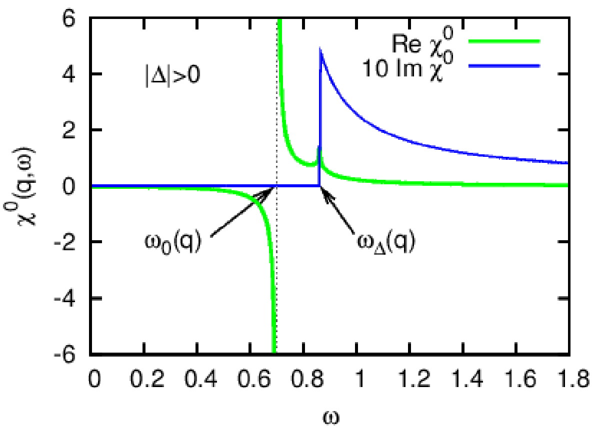

Fig. 2: The blue line is the onset of PH pair creation. As can be seen, gap opening pushes the edge of PHC to higher energies, but leaves behind a simple pole for the real part at the initial edge of the PHC.

The difference in the velocities is interpreted as the sign of spin-charge separation in the spirit of luttinger liquids. The spin mode turns out to move faster than the charge mode. Beyond a critical value of short-range interactions the velocity of the charge mode becomes zero. We identify this as the onset of Mott transition where the charge excitations become localized, while low-energy spin excitations are still possible. This qualifies the gapped graphene as a candidate for a realization of spin liquids, where low-energy spin excitations are possible both in strong and weak coupling regimes. The prediction of the present study for the neutron scattering experiments in gapped Dirac systems (including graphene, highly oriented pyrolitic graphite etc) is that we expect two resonant peaks corresponding to singlet and triplet collective states [4]. The one with lower energy is the singlet state, and the one at slightly higher energy is the triplet state. Moreover the energy difference between them, provides a direct measure of the on-site Coulomb repulsion U of the material.

From an experimental point of view the gapped-graphane or Dirac-cone system is very attractive because of the existence of low energy magnetic and charge excitations which can be studied by using neutron and synchrotron beams. In the near future we will perform neutron and X-ray inelastic scattering experiments to detect low energy spin and charge excitations found by the present theoretical work.

References

[1] G. Baskaran and S. A. Jafari, Phys. Rev. Lett. **89,** 016402 (2002).

[2] S. A. Jafari, G. Baskaran, J. Phys. Condens. Matter **24** , 09560 (2012).

[3] S. A. Jafari, G. Baskaran, Eur. Phys. Jour. B **43,** 175 (2005).

[4] S. A. Jafari, arxiv:1202.6499 (submitted for publication, 2012)

Key Words

Gapped Dirac system, Spin-charge separation, Neutron scattering

Contact to

Seyed Akbar JAFARI (Department of Physics, Sharif University of Technology, Tehran, Iran)

E-mail: jafari@physics.sharif.edu

http://physics.sharif.ir/~jafari