Triplet excitations in graphene-based systems

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Abstract – In this paper we investigate the excitations in a single graphene layer and in a single-walled carbon nanotube, i.e. the spectrum of magnetic excitations is calculated. In the absence of interactions in these systems there is a unique gap in the electron-hole continuum. We show that in the presence of Coulomb correlations bound states, magnons, appear in this forbidden region. The Coulomb interaction is examined in the context of the Pariser-Parr-Pople (PPP) model which takes into account the long-range nature of the interaction. The energy of the new bound states depends on the strength of the Coulomb forces. The calculations are performed for arbitrary electron-hole (e-h) momentum \( q \). In the end, this work finally settles the discussion about the existence of triplet excitations in graphene which has been lasting for a decade in the literature.

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Introduction. – Since the first isolation of graphene [1], a single two-dimensional (2D) atomic layer of graphite, it has attracted a lot of attention of both experimentalists and theoreticians. Such a property as high conductivity makes graphene a candidate for a variety of modern nanoelectronics applications. Mainly, graphene differs from usual 2D materials in that electrons have a linear relativistic-like dispersion law and zero band gap. Because of these unusual properties a number of new effects appear in this material.

Thus, one of the examples of such unusual behavior are graphene plasmons. They are collective oscillations of electronic density which can be found only in a spin singlet state. Currently, plasmons in graphene are under intense investigation [2,3]. There are a lot of works showing that dispersion law and properties of plasmons for Dirac electrons differ markedly from the plasmons in conventional 2D materials. For instance, in 2D semiconductors at long wavelength the plasma frequency \( \omega_p \sim n^{1/2} \), whereas in graphene \( \omega_p \sim n^{1/4} \). This is a direct consequence of the quantum relativistic nature of graphene [4–6]. Another significant feature of the graphene plasmons is the long lifetime caused by the peculiar way of damping [7,8]. Unlike conventional 2D materials, Landau damping occurs due to interband transitions in graphene. The edges of this region can be moved by manipulation of the doping level. As the authors of [9] claim, for sufficiently large doping values low plasmon losses are possible in graphene.

During the last decade there has been a discussion about the existence of a neutral spin triplet mode in a graphene sheet [10–12]. Some authors using the random phase approximation (RPA) showed the existence of a spin-1 collective mode in undoped graphene [10]. However, the authors of [11] argued that the tensor character of the susceptibility was not considered in [10] and such solution was not found.

Therefore, the issue remains open. In the present article using the variational method we prove that the triplet particle-hole excitations, magnons, do exist both in undoped and doped graphene. This method takes into account all the matrix elements of the Hamiltonian and the full dispersion law of graphene. We carry out a full analysis of the magnons spectrum properties which allows us to find conditions for the existence of the spin-1 mode in the system. It is shown that magnons are formed only in the presence of the Coulomb interaction. We compare the results obtained with the Hubbard and PPP models and show that they differ, especially, when screening effects are not too strong. In addition, our calculations allow to get information about the effective mass and velocity of magnons.

Although, in the original work Baskaran and Jafari denoted this type of excitations “spin-1 mode”, in this work the term “magnon” will be used more often.

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Model. – We consider a semiempirical Pariser-Parr-Pople (PPP) model [13,14] known as an extended Hubbard model in the condensed-matter literature. It has successfully been used in different π-conjugated polymers [15,16], as well as in SWCNTs and graphene nanoribbons [17–20]. The advantages of such approach were discussed in [19] in detail. This model takes into account both local and nonlocal Coulomb repulsion between the π-electrons and the Coulomb attraction of the screened ionic charge. The PPP Hamiltonian describing our system is written in the following way:

\[
\hat{H} = \hat{H}_{tb} + \hat{H}_{U} + \hat{H}_{V}.
\]

The tight-binding term is expressed as

\[
\hat{H}_{tb} = \sum_{ij} \sum_{\alpha_1 \sigma_1 \alpha_2 \sigma_2} (t^{\alpha_1 \alpha_2}_{ij} \hat{c}_{i\alpha_1\sigma_1} \hat{c}_{j\alpha_2\sigma_2} + \text{h.c.}),
\]

where operators \( \hat{c}_{i\sigma}^\dagger \) create (annihilate) an electron with spin \( \sigma \) in the unit cell \( i \) on the atom belonging to the \( \alpha \) sublattice. \( t^{\alpha_1 \alpha_2}_{ij} \) is the hopping amplitude between nearest-neighbor sites.

The second term describes on-site Coulomb repulsion:

\[
\hat{H}_{U} = U_0 \sum_{\alpha} \hat{n}_{i\alpha \sigma} \hat{n}_{i\alpha \sigma},
\]

where \( U_0 \) is the strength of on-site interaction and \( \hat{n}_{i\alpha \sigma} = \hat{c}_{i\alpha \sigma}^\dagger \hat{c}_{i\alpha \sigma} \).

Finally, the last term is a long-range interaction term defined by

\[
\hat{H}_{V} = \sum_{ij} \sum_{\alpha_1 \alpha_2} V^{\alpha_1 \alpha_2}_{ij} (\hat{n}_{i\alpha_1} - 1)(\hat{n}_{j\alpha_2} - 1),
\]

where \( V^{\alpha_1 \alpha_2}_{ij} \) is the number of electrons on the site \( i \) and \( \alpha_1 \alpha_2 \) is the value of the off-site Coulomb interaction. The prime in the second sum means that \( \alpha_1 \neq \alpha_2 \) when \( i = j \). There are various ways to interpolate the long-range part of the interaction. In this paper we use the Ohno interpolation formula [21]:

\[
V^{\alpha_1 \alpha_2}_{ij} = \frac{U_0}{\sqrt{1 + |R^{(\alpha_1)}_{ij} - R^{(\alpha_2)}_{ij}|^2/\sigma^2}},
\]

where \( R^{(\alpha)}_{ij} \) determines the position of the \( i\alpha \) atom and \( \sigma \) is a numeric parameter determined by the correct \( \frac{1}{k} \) behavior [22]. In a long-range limit \( V_{ij} = \frac{U_0}{|R_{ij} - R|} \). In contrast, at small distances \( V_{ij} \) approaches the on-site interaction \( U_0 \). Wherefrom for the expression for \( a \) can be written as

\[
a = \frac{\epsilon^2}{4\pi \epsilon_0 U_0 e^2},
\]

where \( e \) is an electron charge and \( \epsilon_0 \) is the vacuum permittivity. Here \( e_\alpha \) is an effective dielectric constant. It includes the substrate contribution as well as the intrinsic one. However, the screening effects will be governed, mostly, by the substrate because the majority of the field lines lie outside of the graphene layer.

From the expressions (4) and (5), obviously, we see that if \( i = j \) and \( \alpha_1 = \alpha_2 \), then \( V_{ii} = U_0 \) and we obtain the Hubbard term.

The main advantage of this approximation is that for a specified value of \( e_\alpha \), there is only one parameter \( U_0 \) in the Hamiltonian which makes it much easier to analyze the properties of the system.

In this paper the band structure of graphene is described by the nearest-neighbor tight-binding model, from which it is known that \( \varepsilon(k) = \beta |f(k)| \), where \( f(k) = 1 + e^{ika_1} + e^{ika_2} \) and \( \beta = +/− \) denotes either conduction or valence bands, respectively. At the same time one can also include the effects of a next-nearest-neighbor hopping. The transformation between the real space and the momentum representations is

\[
\varepsilon_{i\alpha \sigma} = \frac{1}{\sqrt{N}} \sum_{k\beta} e^{-i\mathbf{k}\mathbf{R}_i} U^{-1}_{k\beta\alpha} c_{k\beta \sigma},
\]

where \( U^{-1}_{k\beta\alpha} \) are the matrix elements of the unitary matrix:

\[
\varepsilon_{k\beta\alpha} = \frac{1}{\sqrt{2}} \begin{pmatrix} U_{kA+} & U_{kB+} \ \ U_{kA-} & U_{kB-} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & e^{-i\phi_k} \\ e^{i\phi_k} & 1 \end{pmatrix},
\]

and \( \phi_k = \arg(f(k)) \). These matrix elements are similar to overlap factors studied in many works [4,23,24]. The consideration of them is crucial in our calculations because they encode both band and sublattice structures, contrary to the previous works, where the overlap factor depended on the band index only.

Because of a magnon being a bosonic excitation, it must be described by bosonic operators. For these purposes, unlike [25], we introduce three new operators creating triplet \( e \) pairs with different projections of spin, \( S_z = +1, \ 0, \ -1 \), respectively:

\[
\begin{align*}
(B^+_{2,1})^\dagger &= c_{21}^\dagger c_{11}, \\
(B^0_{2,1})^\dagger &= \frac{1}{\sqrt{2}} \begin{pmatrix} c_{21}^\dagger c_{11} - c_{21}^\dagger c_{11} \\ c_{21}^\dagger c_{11} + c_{21}^\dagger c_{11} \end{pmatrix}, \\
(B^-_{2,1})^\dagger &= c_{21}^\dagger c_{11}
\end{align*}
\]

and one operator which creates a singlet \( e \) pair:

\[
(A^0_{2,1})^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} c_{21}^\dagger c_{11} + c_{21}^\dagger c_{11} \end{pmatrix}.
\]

In the definitions above 1 and 2 are general quantum numbers. In general, these operators do not describe bosons. However, with respect to the ground state, the Fermi Sea state, and considering that the operator \( c_{2\sigma}^\dagger \) creates an electron with spin \( \sigma \) above the chemical potential, \( \mu \), while
$c_{1\sigma}$ creates a hole with spin $-\sigma$ below the chemical potential, the usual commutation relations are fulfilled. Therefore, it can be shown that the on-site interaction term of the Hamiltonian, $H_U$, can be presented in the invariant form:

$$H_U = \frac{U_0}{2N} \sum_{1'2'}^{21} \varphi_{122'}^{11'} \left( -K_{22'}^\dagger \cdot K_{11'} + \frac{1}{2} \left( A_0^{22'} \right)^\dagger A_0^{11'} \right),$$

where, just for simplification, $2 = \{k/\beta_1\}$, $1 = \{k - q/2\}$, $1' = \{p - q/3\}$, $2' = \{p/4\}$, $\varphi_{122'}^{11'} = \sum_\alpha U_{1\alpha} (U_{2\alpha})^* U_{1'\alpha} (U_{2'\alpha})^*$ and

$$K_{ij}^\dagger = \left( \begin{array}{c} B_{ij}^{1j} \dagger + B_{ij}^{1j} \dagger \\ \frac{2}{\sqrt{2}} \left( B_{ij}^{1j} \dagger - B_{ij}^{1j} \dagger \right) \end{array} \right).$$

The same procedure could be done with $H_V$:

$$H_V = \frac{1}{N} \sum_{1'2'}^{21} \varphi_{122'}^{11'} \left( -K_{22'}^\dagger \cdot K_{11'} - \frac{1}{2} \left( A_0^{22'} \right)^\dagger A_0^{11'} \right),$$

where the following notations were introduced:

$$\varphi_{122'}^{11'} = \sum_{\alpha_1\alpha_2} V_{\alpha_1\alpha_2}^* U_{1\alpha_1} (U_{2\alpha_2})^* U_{1'\alpha_2} (U_{2'\alpha_2})^*,$$

$$V_{\alpha_1\alpha_2}^* = \sum_j V_{j\alpha_1\alpha_2} e^{-iqR_j}.$$

Here the spectrum of triplet excitations with $S_z = +1$ is computed. It can be done without loss of generality because the Hamiltonian is invariant under rotation in the spin space. The variational method is used in this work. Consequently, to construct a trial wave function we look at a subspace of the total many-body Hilbert space which consists only of such excitations. The states of the subspace are specified as a superposition of $S_z = +1$ e-h pairs:

$$\left| \psi_q^{(T)} \right> = \sum_{k\beta\beta'} a_{k\beta\beta'} \left( B_{+}^{k\beta',k-q\beta'} \right)^\dagger |FS\rangle,$$

where $a_{k\beta\beta'}$ are the coefficients which in general are complex. Similarly, it is possible to construct a wave function describing singlet excitations of graphene corresponding to the plasmon mode:

$$\left| \psi_q^{(S)} \right> = \sum_{k\beta\beta'} a_{k\beta\beta'} \left( A_0^{k\beta',k-q\beta'} \right)^\dagger |FS\rangle.$$

Therefore, within the variational method the computation of the excitation spectrum reduces to solving the Schrödinger equation $H|\psi_q^{(T)}\rangle = E_q|\psi_q^{(T)}\rangle$ in the reduced subspace, where $E_q$ is the energy of a magnon with the momentum $q$. Then, the excitation energy is $\hbar \omega_q = E_q - E_0$, where $E_0$ is the energy of the filled Fermi Sea.

A piece of graphene chosen for our calculations is composed of 1225 unit cells (or 2450 carbon atoms). We determined such size of the sample to eliminate the impact of size quantization effects. So, to obtain the spectrum of magnons the eigenvalues problem for the square $(1225 \times 1225)$ matrix has to be solved.

**Results and discussion.** — First of all, let us consider the case of the undoped graphene sheet. Without Coulomb correlations the $e$-$h$ continuum consists only of the interband transitions. However, the Coulomb interaction couples an electron and a hole which can lead to the appearance of bound states. This situation is presented in fig. 1. There is a curve beneath the region of $e$-$h$ excitations, which corresponds to magnons. Thus, our calculation confirms the Baskaran and Jafari proposal in [10] on the existence of a magnetic collective mode. However, in their work it was claimed the existence of a critical value of Coulomb interaction $U_c \approx 2.23t$ above which the bound states were not found, while our calculations do reveal this effect. This is because in [10,26] the overlap factors were not taken into account, which, together with the RPA, gave the wrong position of the pole of the spin susceptibility. At the same time, in our calculations all the matrix elements (8) were considered properly.

Now, if one dopes graphene, there is a window in the two-particle spectrum and, as stated above, at small momenta and in the presence of the Coulomb interaction we can expect to find new states in it. In fig. 2(a), (b) the magnon spectrum is presented. It was found numerically by solving the Schrödinger equation for the Hubbard model ($V_{ij} = 0$, $U_0 = 10.8$ eV) and for different values of $q$. It is seen that there are two new branches. The first one is almost dispersionless, lying in the long-wavelength
The doping level $\mu$ grapheme (black curve) and for the (5, 5) SWCNT (red curve). The doping level $\mu$ is 0.18$t$ for both systems.

Fig. 3: (Colour on-line) Magnons energy dependence as a function of the strength of the Coulomb interaction for $|q| = 0$ for graphene (black curve) and for (5, 5) carbon nanotube (red curve).

region (panel (a)), while the second one, a high-energy branch, is located at large momenta (panel (b)). For a better insight into the system behavior, it is useful to plot the energy dependence of the bound state from the strength of the Coulomb interaction for a specific momentum value. The black curve in fig. 3 shows that energy of this bound state diminishes with the increase of $U_0$. This is immediately seen from (11). The triplet components of the interaction give a negative contribution to the energy of the excited states, while a singlet one has a positive sign. Therefore, under the influence of the Coulomb interaction low- and high-energy magnon modes are formed by the shift of the states from the interband and intraband transitions regions, respectively. The size of this shift is proportional to the value of $U_0$. Therefore, we can speak of a critical value $(U_0^{crit})_{gr}$ above which the new states could be formed in the initially forbidden area.

Fig. 4: (Colour on-line) PPP spectrum of magnons in the doped graphene for different values of $q$ and $\epsilon_r$.

It is necessary to mention that in [23] the authors also demonstrated the existence a magnon mode. However, it appears at much smaller values of interaction than those in our calculations. Again, as mentioned above, this discrepancy is caused by the matrix elements (8) entering into the Hamiltonian in (11) and (13).

Since the doping level can be controlled by the gate voltage, it is important to know how magnons depend on the doping level. Thus, the triangle window expands as the doping level increases. Because of this, for a fixed value of the Coulomb interaction $U_0$, the magnon energy increases as well. This is in accordance with [23].

Next, we consider carbon nanotubes. We would like to show that there are the same excitations in the metallic single-walled carbon nanotubes (mSWCNTs). The only difference between this case and the one described above consists in different graphene and mSWCNT dispersion laws.

It is known that SWCNT consists of a graphene sheet that is rolled over a chiral vector $C_{nm} = n\mathbf{a}_1 + m\mathbf{a}_2 = (n, m)$, where $n$ and $m$ are some integers. There are three classes of the SWCNTs: armchair $(n, n)$, zig-zag $(n, 0)$ and chiral $(n, m)$. The condition for being metallic is $n - m = 3q$, with integer $q$ [27,28]. In this paper we consider only armchair nanotubes, but the calculations for the zigzag one could be performed in the same manner. In the SWCNTs one of the components of the momentum
Fig. 6: (Colour on-line) (a) Spatial probability distribution of electron localization in the graphene crystal for a fixed position of a hole calculated using the Hubbard Hamiltonian ($\frac{U}{t} = 4$). The radius of the circle is proportional to the probability of finding electron on the site. Blue/red circles are again atoms in sublattices $A/B$. A hole is localized on the atom of type $A$ and is denoted by $\circ$. The numbers are the electron probabilities to be localized on the site. (b) Full probability to find an $e$-$h$ pair in the graphene crystal as a function of the distance between an electron and a hole positions. Blue circles denote the case in which both electron and hole are in the same sublattices. Pink squares describe the case in which an electron and a hole belong to different sublattices. The probabilities were calculated for the Hubbard model ($\frac{U}{t} = 4$). (c) Probability dependence of the localization of both an electron and a hole on the same site as a function of $\epsilon_r$. 

is quantized, consequently, it is possible to show that the energy dispersion relation for an armchair carbon nanotube is [27]

$$\varepsilon_\nu(k) = \sqrt{4 \cos \left( \frac{ak}{2} \right) \cos \left( \frac{\pi \nu}{n} \right) + 4 \cos^2 \left( \frac{ak}{2} \right) + 1}, \quad (16)$$

where $k$ is the continuous component of the wave vector, while $\nu$ corresponds to the discrete part of the wave vector (band index). Considering $\nu = 0$, we get the particle-hole spectrum similar to graphene. Therefore, it is instinctively clear that there should be a magnon mode, as well (fig. 2(c), (d)). However, there are a number of differences from the graphene magnons. The main one is a lower value of the critical Coulomb interaction. In fig. 3 the red curve shows that the bound state appears in the armchair nanotube at $(U_0^{crit})_{arb} \approx 1.4$, while in graphene $(U_0^{crit})_{gr}$ is twice that value. Another sharp difference is that in the SWCNTs magnons disperse much more strongly than in graphene (fig. 2(d)). That is why, a magnon mode in the tubes is dumped at smaller values of the wave vector.

The Hubbard model studied above considers only purely local interactions. Such a model is well suited to describe CVD graphene grown on metal substrates where the screening is strong [29–31]. However, graphene is often fabricated on silicon oxide or boron nitride substrates with dielectric constants around 4 [32,33]. Hence, in such devices long-range interactions can play a role.

Concentrating only on the low-energy magnons, from fig. 4 it is seen that in the presence of a long-range interaction the bound states are shifted up from their energy, calculated using $V_{ij} = 0$. This energy shift depends on the value of relative permittivity. In the limit of big $\epsilon_r$ we recover the solution obtained using the Hubbard model, while for $\epsilon_r \approx 4$ the energy shift is around 0.08$t$. However, qualitatively, the behavior of the magnon mode remains quite the same. Hence, we consider that long-range Coulomb effects do not play a crucial role and one can solve the Hubbard model problem with an effective on-site repulsion $U^*_{0}$ [34].

As shown above, there is a critical value of the on-site Coulomb interaction below which the bound states are not formed. However, importantly, not only the Coulomb interaction but also doping and screening determine the conditions for the bound state formation. This is presented in a phase diagram (fig. 5). It is seen that the value of doping needed for magnon formation increases with a decrease of the on-site repulsion as well as with the decrease of screening.

From the computed spectrum we can find the magnons dispersion law, velocity and effective mass. Thus, for the curve corresponding to $\epsilon_r = 17.8$ we get that the group velocity $v_{mag} = \frac{\partial \varepsilon}{\partial k} \approx 6 \times 10^4 \frac{m}{s}$, which is three orders less than the Fermi velocity in graphene. The magnon effective mass is $m^* = \left( \frac{\partial^2 \varepsilon}{\partial k^2} \right)^{-1} \approx 1.8m_e$.

Finally, the last thing which is analyzed is how the magnons appear in the real space. To do it one has to calculate the probability to find an $e$-$h$ pair somewhere in the graphene lattice. For instance, if the hole position is fixed and it is localized on the atom of type $\alpha = A/B$, then the probability to find an electron in the position $R_i$ on the same type of atom is

$$P_{\alpha_\alpha} = \left| \frac{1}{2N} \sum_k g_{k\beta\beta}^* e^{-i\mathbf{k} \cdot \mathbf{R}_i} e^{-i\phi_k} \right|^2, \quad (17)$$

and the probability to find an electron on a different type of atom is

$$P_{\alpha_\beta} = \left| \frac{1}{2N} \sum_k g_{k\beta\beta}^* e^{-i\mathbf{k} \cdot \mathbf{R}_i} e^{-2i\phi_k} \right|^2. \quad (18)$$

Evidently, we have $P_{AA} = P_{BB}$ and $P_{AB} = P_{BA}$.
Figure 6(a) shows the spatial probability distribution of finding an electron somewhere in the crystal when the hole position is fixed (its position is marked on the graph as o). One sees that the distribution function has the same symmetry as the graphene lattice. As we can see, there is the largest probability to find an electron on the same site as a hole which corresponds to a spin-flip. This situation is quite similar to that observed in a 1D chain of aligned spins when one spin-flip event causes a magnon. As is shown in fig. 6(b) the probability distribution is exponentially decreasing as we move away from the position of a hole. This fact proves that magnons are really localized in the sample we used for our calculations and that the choice of its size was well founded. Finally, from fig. 6(c) it is seen that the magnons wave function becomes more localized in space with the increase of the screening effects.

Conclusion. – In conclusion, in this paper we investigate magnetic excitations in graphene and in the armchair SWCNT. We confirm that a new mode appears in the gap of the particle-hole spectrum in the presence of Coulomb interactions in these systems. Thereby, the result of this work settles a dispute which has been in the literature for a decade. Finally, it is demonstrated that the variational method used in this paper is more accurate than those used in previous works because it takes into account all the features of graphene lattice and band structures.

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