Spin density wave formation in graphene facilitated by the in-plane magnetic field

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We suggest that by applying a magnetic field lying in the plane of graphene layer one may facilitate an excitonic condensation of electron-hole pairs with opposite spins and chiralities. The provided calculations yield a conservative estimate for the transition temperature $T_c \sim 0.1\ B$.

Charge Density Wave (CDW) and Spin Density Wave (SDW) formation in graphene is an intriguing possibility which has been discussed in the literature [1],[2],[4]. Even more so since the reduced dimensionality of graphene will strongly affect the character of the corresponding ordered state probably making it critical. It was also pointed out that magnetic field perpendicular to the graphene layers may facilitate formation of the CDW [1],[2]. The CDW order parameter discussed in these papers establishes different population densities on the two sublattices of graphene (we will call them u and v ones). This corresponds to a site-centered CDW. In this paper we suggest that by applying a magnetic field in the graphene plane or a Weiss exchange field [3] one can facilitate a formation of a bond-centered spin density wave. The corresponding order parameter has $\mathrm{U}(1)\times\mathrm{Z}_2$ symmetry and combines fermion operators with opposite spins and chiralities.

The tight binding Hamiltonian is

$$H_0 = -t\sum_{\mathbf{r},i\sigma} u^+_\sigma(\mathbf{r})v(\mathbf{r}+\mathbf{b}_i) + H.c. \tag{1}$$

where $\mathbf{r}$ belong to a triangular lattice (see Fig. 1).

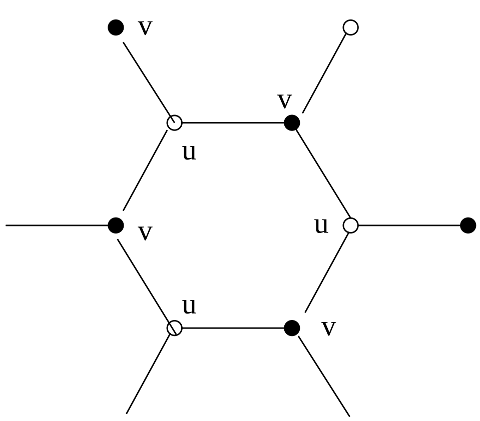

FIG. 1: Crystalline lattice of graphene.

Tunneling on next nearest neighbours generates the so-called trigonal warping of the spectrum. We will not discuss this small deformation of the spectrum since it does not destroy the nesting between the bands of different chirality and therefore will not have any adverse effect on the phenomena discussed in this paper.

The Hamiltonian describing states close to the tips of the Dirac cones is

$$\omega\hat{I} - \hat{H}_0 = \tag{2}$$
$$\sum_{\sigma=\pm1}\Psi^+_\sigma \begin{pmatrix} \omega-\sigma B & vk & 0 & 0 \\ v\bar{k} & \omega-\sigma B & 0 & 0 \\ 0 & 0 & \omega+\sigma B & -v\bar{k} \\ 0 & 0 & -vk & \omega+\sigma B \end{pmatrix}\Psi_\sigma,$$
$$\Psi^+ = \big(u^+_\sigma(\mathbf{k}+\mathbf{Q}), v^+_\sigma(\mathbf{k}+\mathbf{Q}), u^+_{-\sigma}(\mathbf{k}-\mathbf{Q}), v^+_{-\sigma}(\mathbf{k}-\mathbf{Q})\big)$$

Here u, v operators annihilate electrons on different sublattices and $k = k_x + \mathrm{i}k_y$, $\mathbf{Q} = (1, 1/\sqrt{3})2\pi/a\sqrt{3}$. Since magnetic field B lies in the plane, it affects only spin (the same effect can probably be achieved by the exchange field when one brings graphene sample in a close proximity to a ferromagnet). The in-plane magnetic field leads to Zeeman splitting of the bands (see Fig. 2). The predominant interaction is the Coulomb one:

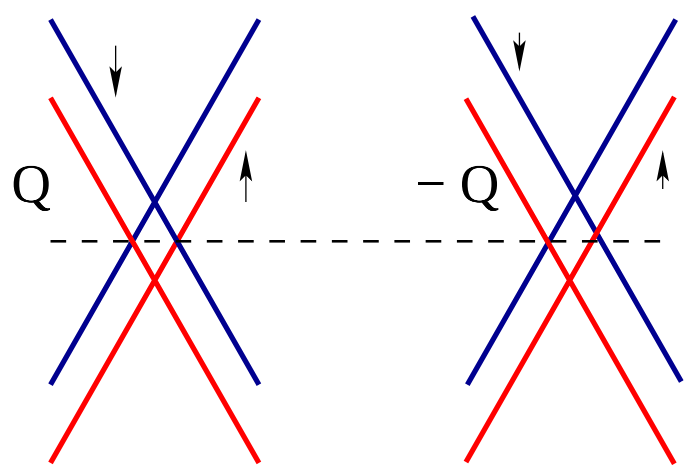

FIG. 2: Graphene bands split by the in-plane magnetic field.

$$V=\frac{1}{2}\sum_{k,k',q;\tau=\pm1}[u^+_\sigma(k'+q+\tau Q)u_\sigma(k+q+\tau Q)+v^+_\sigma(k'+q+\tau Q)v_\sigma(k+q+\tau Q)]\frac{2\pi e^2}{|\mathbf{k}-\mathbf{k}'|}$$
$$\times[u^+_{\sigma'}(k+\tau'Q)u_{\sigma'}(k'+\tau'Q)+v^+_{\sigma'}(k+\tau'Q)v_{\sigma'}(k'+\tau'Q)] \quad (3)$$

The bare Coulomb interaction in graphene is fairly strong $e^2/\hbar v\approx 2$, but it is screened:

$$V(q)=\frac{2\pi e^2}{|q|-2\pi e^2 N\Pi(\omega,q)} \quad (4)$$

where $N=4$ is the number of fermion species (valley and spin). Assuming that the self-consistent interaction is weak we can get an estimate of this interaction by substituting there the polarization loop $\Pi(\omega,q)$ for bare electrons. Then the effective interaction can be approximated as

$$V(q)=\frac{1}{N}[\rho(\epsilon_F)]^{-1}\left\{\begin{array}{c}1,\quad |q|<B\\ B/C|q|,\quad |q|>B\end{array}\right\} \quad (5)$$

where $\rho(\epsilon_F)=k_F/2\pi$ and $C(N)\sim 1$ is constant (according to [1] $C(\infty)=\pi/4$).

The energetics selects order parameters where electrons pair with holes of the opposite spin and chirality. There are two complex order parameters:

$$\Delta^\sigma_{14}(k)=\sum_{\mathbf{k}'}\langle u_\sigma(\mathbf{k}'+\mathbf{Q})V(|\mathbf{k}-\mathbf{k}'|)v^+_{-\sigma}(\mathbf{k}'-\mathbf{Q})\rangle,$$
$$\Delta^\sigma_{23}(k)=\sum_{\mathbf{k}'}\langle v_{-\sigma}(\mathbf{k}'+\mathbf{Q})V(|\mathbf{k}-\mathbf{k}'|)u^+_\sigma(\mathbf{k}'-\mathbf{Q})\rangle \quad (6)$$

As we shall see, on the mean field level these order parameters have equal amplitudes independent of spin: $\Delta^\sigma_{14}(k)=\Delta^{\sigma'}_{23}(k)=\Delta(k)$. Plugging (6) into (3) we obtain the mean field Hamiltonian:

$$\omega\hat I-\hat H_{MF}= \quad (7)$$
$$\sum_{\sigma=\pm1}\Psi^+_\sigma\begin{pmatrix}\omega-\sigma B & vk & 0 & \Delta(k)\\ v\bar k & \omega-\sigma B & \Delta(k) & 0\\ 0 & \Delta(k) & \omega+\sigma B & -v\bar k\\ \Delta(k) & 0 & -vk & \omega+\sigma B\end{pmatrix}\Psi_\sigma$$

The spectrum is

$$E^2_\pm=|\Delta(k)|^2+v^2(|k|\pm B)^2 \quad (8)$$

The self-consistency conditions are

$$\Delta_{14}(k)= \quad (9)$$
$$\int\frac{d^2p}{(2\pi)^2}V(|\mathbf{k}-\mathbf{p}|)\left[\Pi_{11,44}(p)\Delta_{14}(p)+\Pi_{12,34}(p)\Delta_{23}(p)\right]$$
$$\Delta_{23}(k)= \quad (10)$$
$$\int\frac{d^2p}{(2\pi)^2}V(|\mathbf{k}-\mathbf{p}|)\left[\Pi_{22,33}(p)\Delta_{14}(p)+\Pi_{21,43}(p)\Delta_{23}(p)\right]$$

where

$$\Pi_{11,44}(p)=\Pi_{22,33}(p)=T\sum_n G^\uparrow_{11}(\omega_n,p)G^\downarrow_{44}(\omega_n,p)$$
$$\Pi_{12,34}(p)=\Pi_{21,43}(p)=T\sum_n G^\uparrow_{12}(\omega_n,p)G^\downarrow_{34}(\omega_n,p)$$

As we said, these equations yield $\Delta_{14}(k)=\Delta_{23}(k)=\Delta(k)$. Summing over the Matsubara frequencies and integrating over angles we get the following equation:

$$\Delta(p)=\int\frac{d^2k}{(2\pi)^2}\frac{V(\mathbf{p}-\mathbf{k})}{2}\times \quad (11)$$
$$\left\{\frac{\tanh[(|k|+B)\beta/2]}{|k|+B}+\frac{\tanh[(|k|-B)\beta/2]}{(|k|-B)}\right\}\Delta(k)$$

In integrating over angles we will adopt the same approximation as in [1] and will replace the resulting elliptic function $K(k/p)$ by 1. In the limit of $N\to\infty$ these equations yield $T_c\sim B\exp(-N)$. We believe that using this formula for $N=4$ substantially underestimates T_c. The approximate equations for the mean field critical temperature $\beta^*=B/2T_c>>1$ is (here $x=p/B$):

$$\Delta(x)=\frac{1}{2N}\int_0^\infty\frac{y\mathrm{d}y}{C\max(x,y)+1}\left\{\frac{\tanh[(y+1)\beta^*]}{y+1}+\frac{\tanh[(y-1)\beta^*]}{y-1}\right\}\Delta(y) \quad (12)$$

We found a good interpolation formula will split the interval of integration into (0,A) and (A,∞) where $A>1$.

At $x < A$ the interaction will be approximated as constant, and at $x > A$ as $(Cx)^{-1}$. We look for the solution of this equation as

$$\Delta(x) = \frac{\Delta_0}{(x+1)^\gamma} \tag{13}$$

where $\gamma = 1/2 + \sqrt{1/4 - 1/CN}$ and

$$T_c \approx B\exp[-(N - 1/\gamma)] \tag{14}$$

Assuming that $C(4) \approx 1$ we get $\gamma(4) \approx 1/2$ and the estimate $T_c \sim 10^{-1}B$.

Few words about the effects of reduced dimensionality. As is well known, in two dimensions continuos U(1) symmetry cannot be spontaneously broken. In this case the second order phase transition is replaced by the Berezinskii-Kosterlitz-Thouless (BKT) one and the low temperature phase is critical. The BKT termperature is determined by the equation

$$T_{BKT} = \frac{\pi}{2}\rho(T_{BKT}) \tag{15}$$

where $\rho(T)$ is the temperature dependent stiffness. $\rho(T)$ vanishes at T_c and reaches some constant value at $T = 0$. Since the system is not strongly interacting, $\rho(0) >> T_c$. Therefore the BKT transition temperature occurs close to the mean field and one should expect to see the effects of fluctuations only in a fairly narrow region around the transition temperature.

Our estimate of the transition temperature indicates that it is not too low and for realistic magnetic fields $B \sim 10 - 20$ T probably lies in the interval 1 K or even larger. In a hypothetical construction a graphene layer is brought into a microscopic contact with a ferromagnetic film; in this case the Weiss fields can probably be made higher by an order of magnitude.

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