Stoner ferromagnetic phase of graphene in the presence of an in-plan magnetic field

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CENTRO DE CIENCIAS DE BENASQUE PEDRO PASCUAL

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Exchange instability in EGS

What is the order of any possible ferromagnetic instability?

-It could be a second order (Stoner instability)
-It could be a first-order (Bloch ferromagnetic)

$$r_s = \frac{<V>}{<T>} \propto (n)^{-1/d}$$

Stoner instability: i. e. Short-range interaction between e-e

E. C. Stoner, *Proc. R. Soc. London, Ser. A* ***169,*** 339 (1938).

Bloch ferromagnetic: i. e. Hartree-Fock approximation

F. Bloch, *Z. Phys.* ***57,*** 545 (1929). $r_s \approx 5.45\,(3D)$ $r_s \approx 2(2D)$

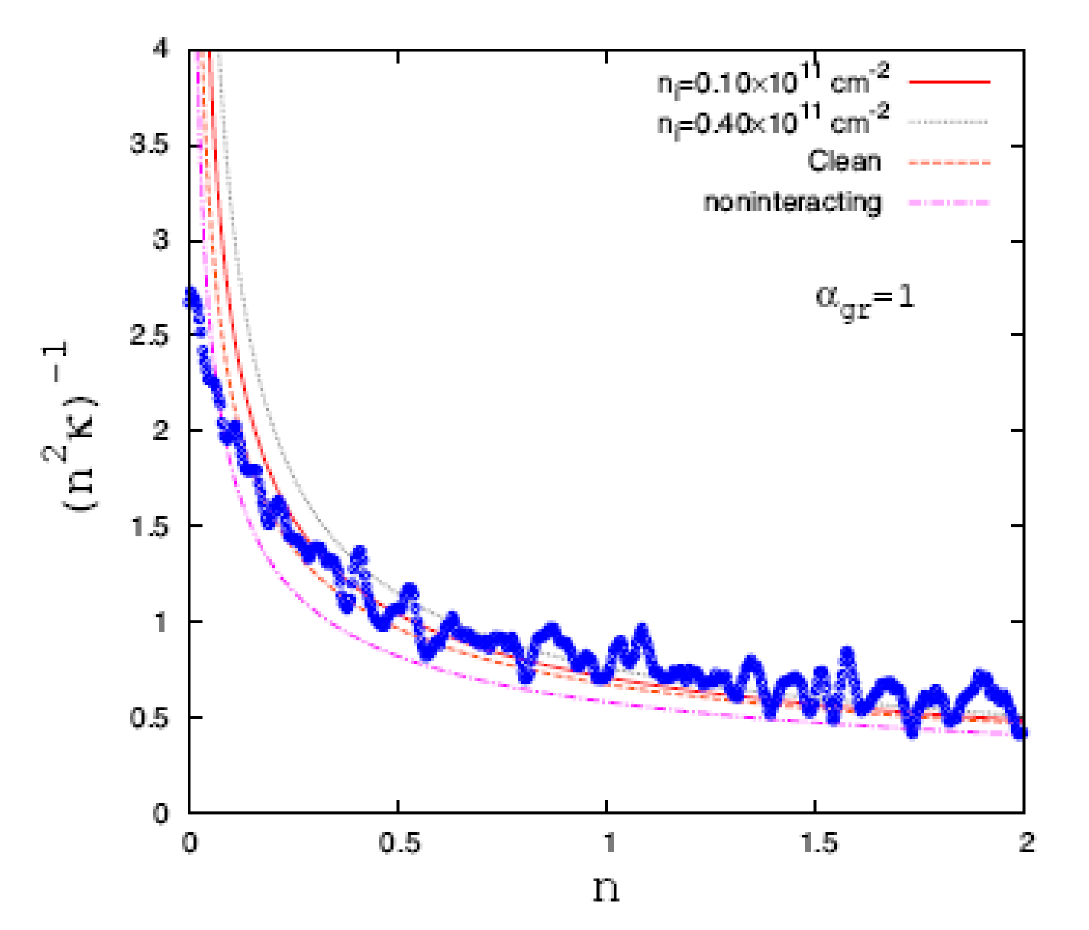
-It turns out that the first-order approximation is quantitatively incorrect

Exchange instability: Gapless graphene !

N. M. R. Peres*, F. Guinea, and A. H. Castro Neto, Phys. Rev. B* ***72***, 174406 (2005)

- Inclusion of the correlation suppresses the spin-polarized phase

Do we need exchange & correlation terms ?



$$\alpha_{gr} = g_v g_s \alpha_{ee}$$

-Demonstrate the importance of including XC effects together with disorder effects

Martin *et al*. Nature Physic **4**, 144 (2007)

R. Asgari, *et al* PRB **77**, 125432 (2008)

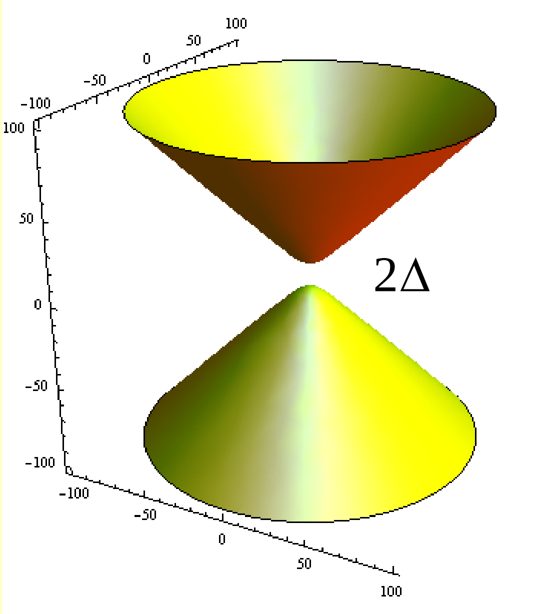
A gap opening in the electronic spectrum

1) Breaking of the sub-lattice symmetry
   - ✓ Different density of particles on the A and B sub-lattices
   - ✓ Kekule distortion
2) Spin-orbit coupling
   - ✓ Rashba interaction
   - ✓ Intrinsic spin-orbit interactions
3) Finite size effect
   - ✓ Armchair Graphene nano-ribbons: Electron confinement
   - ✓ Zigzag Graphene nano-ribbons: Edge states
4) …

Low energy model Hamiltonian

$$\hat{H} = \hat{H}_0 + \frac{1}{2S}\sum_{\mathbf{q}\neq 0} v_q(\hat{n}_{\mathbf{q}}\hat{n}_{-\mathbf{q}} - \hat{N}),$$

$$\mathcal{H}_0 = \begin{pmatrix} \Delta & \hbar v\hat{k}^* & 0 & 0 \\ \hbar v\hat{k} & -\Delta & 0 & 0 \\ 0 & 0 & -\Delta & -\hbar v\hat{k}^* \\ 0 & 0 & -\hbar v\hat{k} & \Delta \end{pmatrix}$$



$$\hat{H}_0 = \sum_{\mathbf{k},\sigma} \Psi^\dagger_{\mathbf{k},\sigma}\mathcal{H}_0\Psi_{\mathbf{k},\sigma}$$

$$E_k = \pm\sqrt{\varepsilon_k^2 + \Delta^2}$$

$$E_k \to \begin{cases} \varepsilon_k & \Delta \prec\prec \varepsilon_F \\ \dfrac{\varepsilon^2{}_k}{2\Delta} & \Delta \succ\succ \varepsilon_F \end{cases}$$

Non-interacting polarization function

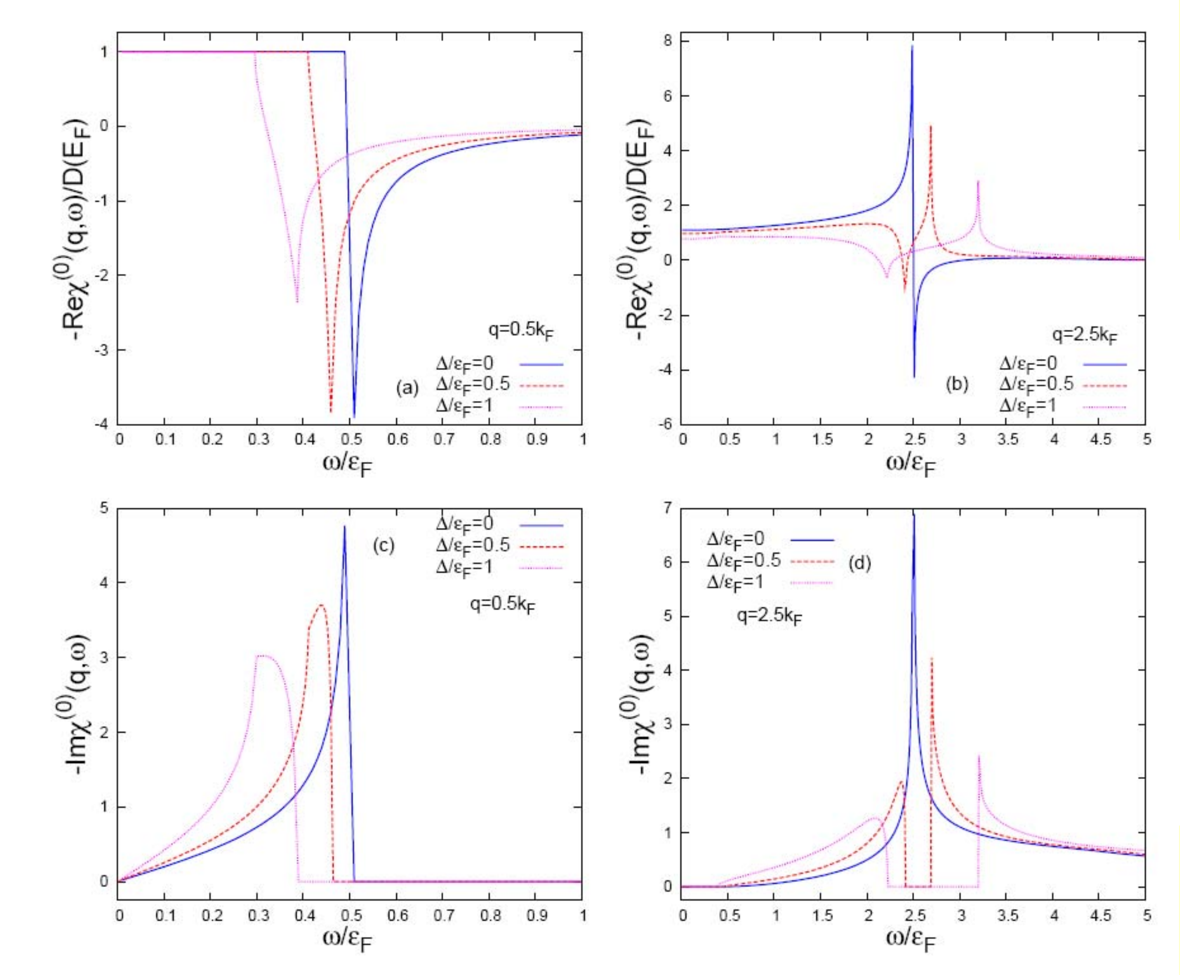
$$\chi^{(0)}(\mathbf{q},\Omega,\mu) = -i\int\frac{d^2\mathbf{k}}{(2\pi)^2}\int\frac{d\omega}{2\pi}\mathrm{Tr}[i\gamma_0 G^{(0)}(\mathbf{k}+\mathbf{q},\omega+\Omega,\mu)i\gamma_0 G^{(0)}(\mathbf{k},\omega,\mu)]$$

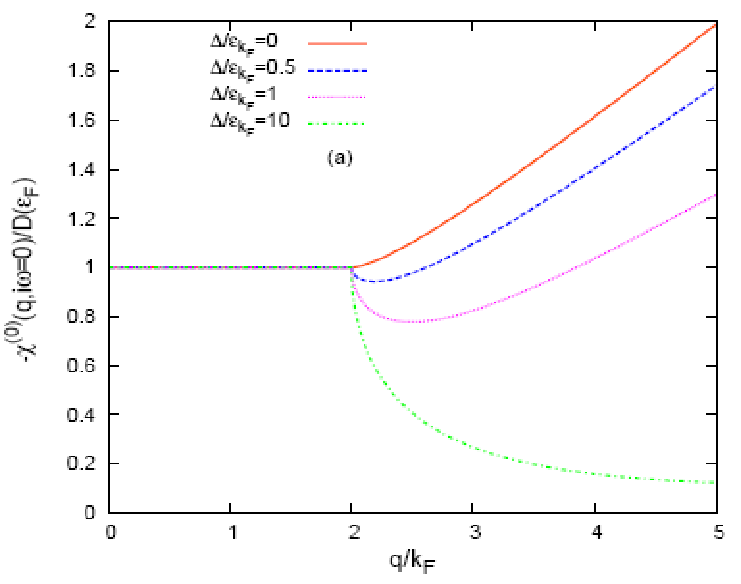
$$G^{(0)}(\mathbf{k},\omega,\mu) = i\frac{-\gamma_0\omega+\hbar v\gamma\cdot\mathbf{k}+i\Delta}{-\omega^2+\hbar^2v^2k^2+\Delta^2-i\eta} - \pi\frac{-\gamma_0\omega+\hbar v\gamma\cdot\mathbf{k}+i\Delta}{\sqrt{\hbar^2v^2k^2+\Delta^2}}\delta(\hbar\omega-\sqrt{\hbar^2v^2k^2+\Delta^2})\theta(k-\mathrm{k_F})$$

$$\begin{aligned}
\chi^{(0)}(\mathbf{q},i\omega,\mu) \;=\; & -\frac{g}{2\pi v^2}\{\mu-\Delta+\frac{\varepsilon_q^2}{2}\left[\frac{\Delta}{\varepsilon_q^2+\hbar^2\omega^2}+\frac{1}{2\sqrt{\varepsilon_q^2+\hbar^2\omega^2}}(1-\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})\tan^{-1}(\frac{\sqrt{\varepsilon_q^2+\hbar^2\omega^2}}{2\Delta})\right] \\
& - \frac{\varepsilon_q^2}{4\sqrt{\hbar^2\omega^2+\varepsilon_q^2}}\Re e\left[(1-\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})\{\sin^{-1}(\frac{2\mu+i\hbar\omega}{\varepsilon_q\sqrt{1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2}}})-\sin^{-1}(\frac{2\Delta+i\hbar\omega}{\varepsilon_q\sqrt{1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2}}})\}\right] \\
& - \frac{\varepsilon_q^2}{4\sqrt{\hbar^2\omega^2+\varepsilon_q^2}}\Re e\left[(\frac{2\mu+i\hbar\omega}{\varepsilon_q})\sqrt{(1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})-(\frac{2\mu+i\hbar\omega}{\varepsilon_q})^2}\right] \\
& + \frac{\varepsilon_q^2}{4\sqrt{\hbar\omega^2+\varepsilon_q^2}}\Re e\left[(\frac{2\Delta+i\hbar\omega}{\varepsilon_q})\sqrt{(1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})-(\frac{2\Delta+i\hbar\omega}{\varepsilon_q})^2}\right]\}\,,
\end{aligned}$$

A. Qaiumzadeh & R. Asgari, Phys *.Rev. B* ***79***, 074414((2009)

Numerical results





$\Delta = 0$: B. Wunch et al. NJP **8**, 318 (2006), E. H. Hwang & Das Sarma, PRB **75**, 205418 (2007)

$\Delta \neq 0$: Y. Barlas et al, PRL **98**, 236601 (2007), A. Qaiumzadeh & R. Asgari, P *R B* *79*, 074414(2009), Pyatkovskiy, JPC **21**, 025506 (2009)

Spin dependence of the polarization function

$$
\begin{aligned}
\chi_\sigma^{(0)}(\mathbf{q}, i\omega, \zeta, \Delta) &= -\frac{g_v}{2\pi\hbar^2 v^2}\{\mu_\sigma - \Delta + \frac{\varepsilon_q^2}{2}\left[\frac{\Delta}{\varepsilon_q^2+\hbar^2\omega^2} + \frac{1}{2\sqrt{\varepsilon_q^2+\hbar^2\omega^2}}(1-\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})\tan^{-1}(\frac{\sqrt{\varepsilon_q^2+\hbar^2\omega^2}}{2\Delta})\right] \\
&- \frac{\varepsilon_q^2}{4\sqrt{\hbar^2\omega^2+\varepsilon_q^2}}\Re e\left[(1-\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})\{\sin^{-1}(\frac{2\mu_\sigma+i\hbar\omega}{\varepsilon_q\sqrt{1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2}}}) - \sin^{-1}(\frac{2\Delta+i\hbar\omega}{\varepsilon_q\sqrt{1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2}}})\}\right] \\
&- \frac{\varepsilon_q^2}{4\sqrt{\hbar^2\omega^2+\varepsilon_q^2}}\Re e\left[(\frac{2\mu_\sigma+i\hbar\omega}{\varepsilon_q})\sqrt{(1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})-(\frac{2\mu_\sigma+i\hbar\omega}{\varepsilon_q})^2}\right] \\
&+ \frac{\varepsilon_q^2}{4\sqrt{\hbar\omega^2+\varepsilon_q^2}}\Re e\left[(\frac{2\Delta+i\hbar\omega}{\varepsilon_q})\sqrt{(1+\frac{4\Delta^2}{\varepsilon_q^2+\hbar^2\omega^2})-(\frac{2\Delta+i\hbar\omega}{\varepsilon_q})^2}\right]\}\ ,
\end{aligned}
$$

A. Qaiumzadeh & R. A, *Phys. Rev. B* ***80,***035429(2009)

Ground state energy: Thermodynamic properties

$$\varepsilon_{tot}(n,\zeta,\Delta,B) = \varepsilon_{kin}(n,\zeta,\Delta) + \varepsilon_x(n,\zeta,\Delta) + \varepsilon_c(n,\zeta,\Delta) + \varepsilon_Z(\zeta,B)$$

$$\varepsilon_{kin}(n,\zeta,\Delta) = \frac{g_v}{6\pi n\hbar^2 v_{\rm F}^2}\{[\hbar^2 v_{\rm F}^2 k_{\rm F}^2(1+\zeta)+\Delta^2]^{3/2} + [\hbar^2 v_{\rm F}^2 k_{\rm F}^2(1-\zeta)+\Delta^2]^{3/2} - 2\Delta^3\}$$

$$\varepsilon_x(n,\zeta,\Delta) = -\frac{1}{4\pi n}\int \frac{d^2\mathbf{q}}{(2\pi)^2} V_q \int_0^\infty d\omega\ [\chi_\uparrow^{(0)}(\mathbf{q},i\omega,\zeta,\Delta) + \chi_\downarrow^{(0)}(\mathbf{q},i\omega,\zeta,\Delta)],$$

$$\varepsilon_c(n,\zeta,\Delta) = -\varepsilon_x(n,\zeta,\Delta) + \frac{1}{2\pi n}\int \frac{d^2\mathbf{q}}{(2\pi)^2}\int_0^\infty d\omega \ln[1 - V_q(\frac{\chi_\uparrow^{(0)}(\mathbf{q},i\omega,\zeta,\Delta) + \chi_\downarrow^{(0)}(\mathbf{q},i\omega,\zeta,\Delta)}{2})],$$

Total energy
C2DEG vs 2DEG

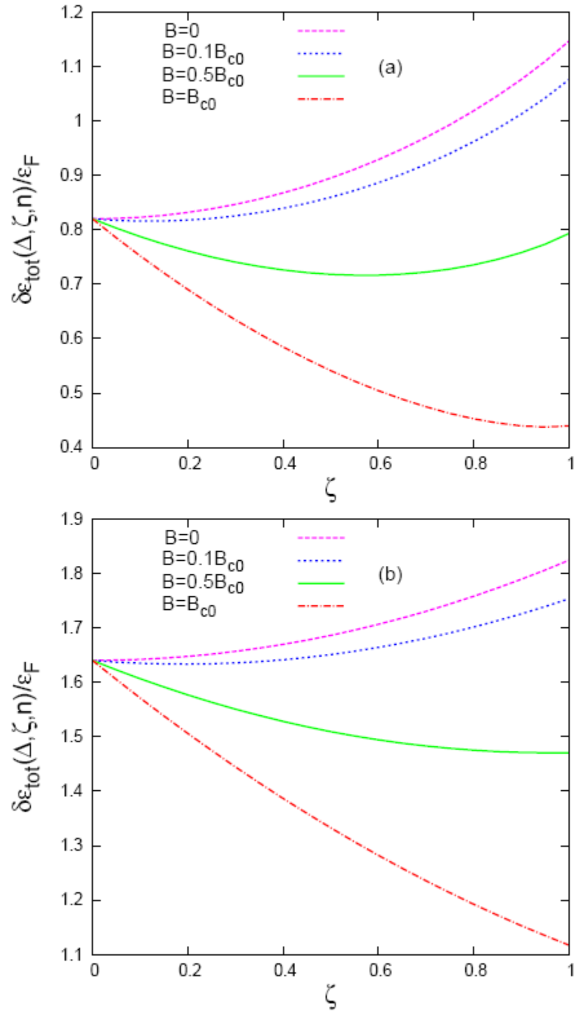


FIG. 3: (color online). Total energy as a function of spin polarization for various magnetic fields for (a): $\Delta = 0$ and (b): $\Delta = 100$meV at $\Lambda = 100$.

$$\Lambda = 10^2 \sqrt{4\bar{n}^{-1}\sqrt{3}/9.09}$$

A. Qaiumzadeh & R. Asgari, *Phys. Rev. B* **80**,035429(2009)

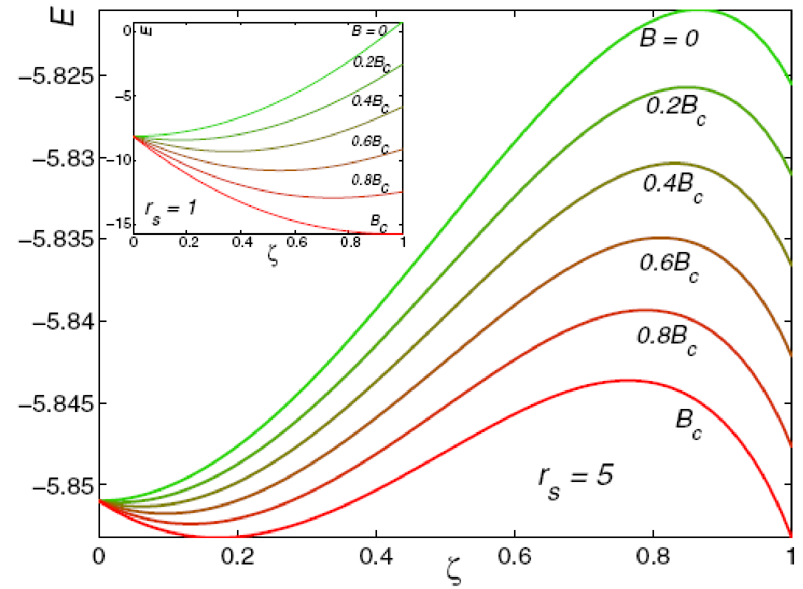


FIG. 1 (color online). Calculated energy E (in arbitrary units) per particle as a function of spin polarization ζ in an applied magnetic field B ranging from 0 to B_c with steps $0.2B_c$ for the $r_s = 5$ 2D electron system. (Note that B_c is a function of r_s.) Inset: The corresponding $r_s = 1$ results.

Y. Zhang & S. Das Sarma, Phys. Rev. Lett. ***96****, 196602 (2006)*

Spin polarization, C2DEG vs 2DEG

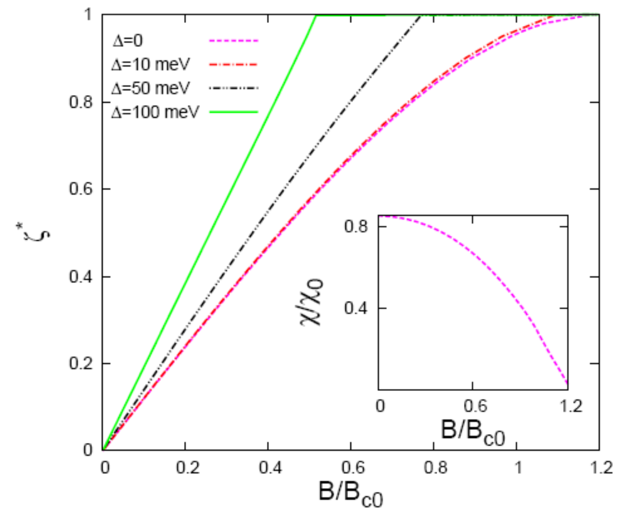


FIG. 4: (color online). Spin polarization as a function of the magnetic field for several energy gap values at $\Lambda = 100$. The inset: The spin susceptibility as a function of the magnetic field for $\Delta = 0$.

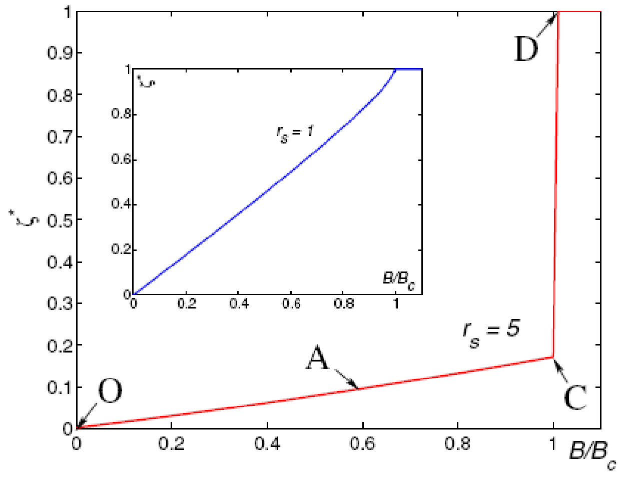


FIG. 3 (color online). Calculated spin polarization as a function of magnetic field B for $r_s = 5$. Inset: The corresponding $r_s = 1$ results. The relevance of O, A, C, and D in defining various susceptibility are discussed in the text.

A. Qaiumzadeh & R. Asgari, *Phys. Rev. B* ***80***,035429(2009)

$$\boxed{\Lambda = 10^2 \sqrt{4\bar{n}^{-1}\sqrt{3}\,/\,9.09}}$$

Y. Zhang & S. Das Sarma, Phys. Rev. Lett. ***96***, *196602 (2006)*

$$\boxed{B_{c0} = \varepsilon_F / \sqrt{2}\mu_B}$$

Critical magnetic field

$$\frac{B_c}{B_{c0}} = \frac{\sqrt{2}}{2\varepsilon_F}\left\{[(2\varepsilon_F^2 + \Delta^2)^{1/2} - \Delta] + 2\frac{\partial\delta\varepsilon_{xc}}{\partial\zeta}|_{\zeta=1}\right\}$$

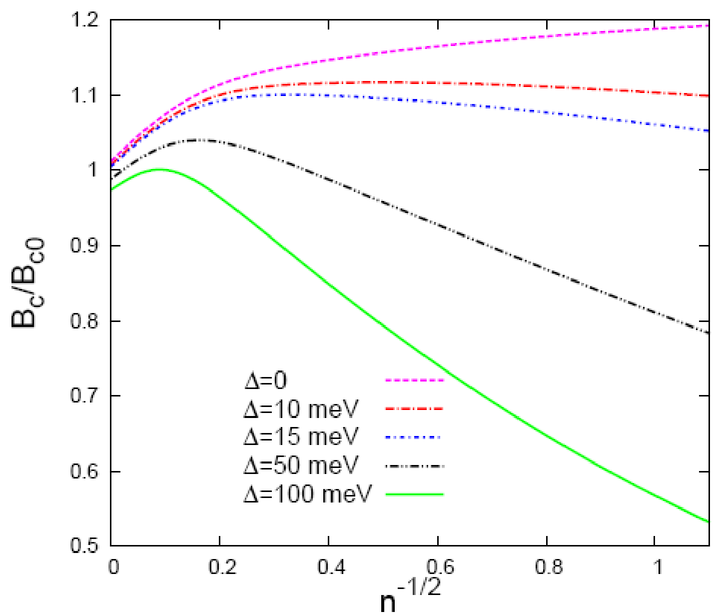


FIG. 2: (color online). Critical magnetic field as a function of inverse square root of density (in units of 10^{-6} cm) for various gap energies.

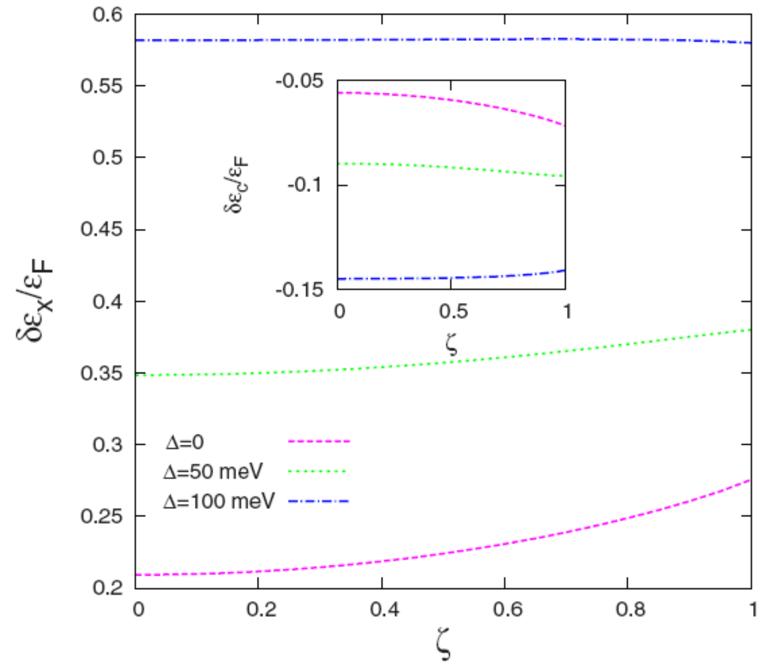


FIG. 1. (Color online). Exchange energy as a function of degree of spin polarization, ζ for various gap energies. In the inset: the correlation energy as a function of ζ for various gap energies.

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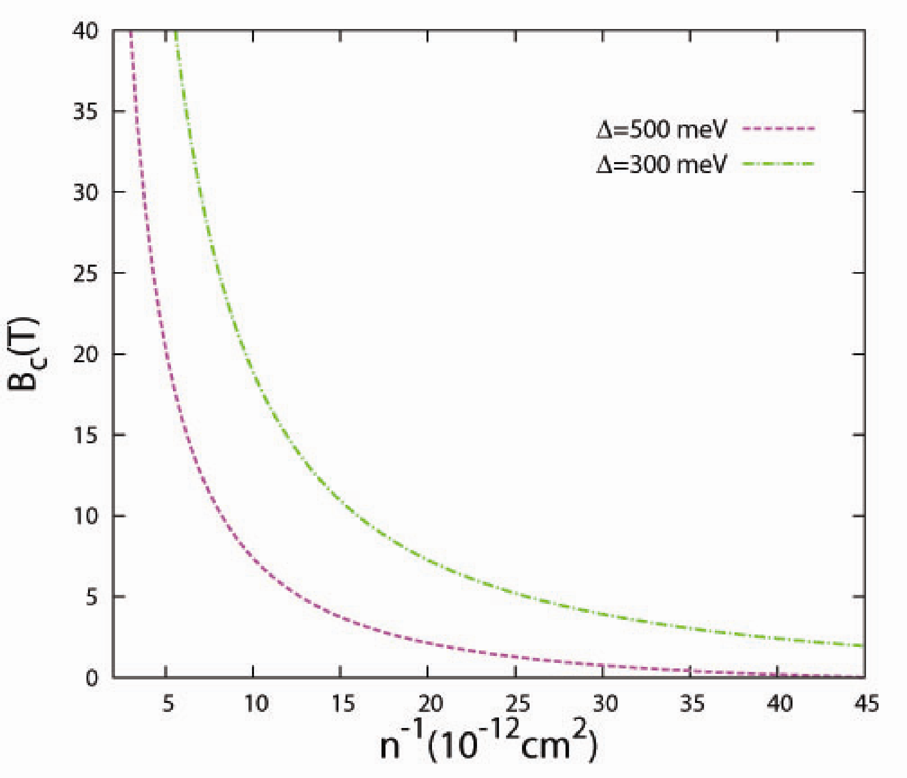
$$B_{c0} = \varepsilon_F / \sqrt{2}\mu_B$$

Can the critical magnetic field be accessed experimentally?



$$\begin{cases}\Delta = 300\ meV \\ n = 4\times 10^{10}\ cm^{-2}\end{cases} \rightarrow B_c = 5\,T$$

$$\begin{cases}\Delta = 500\ meV \\ n \approx 1\times 10^{11}\ cm^{-2}\end{cases} \rightarrow B_c = 5\,T$$

Compressibility

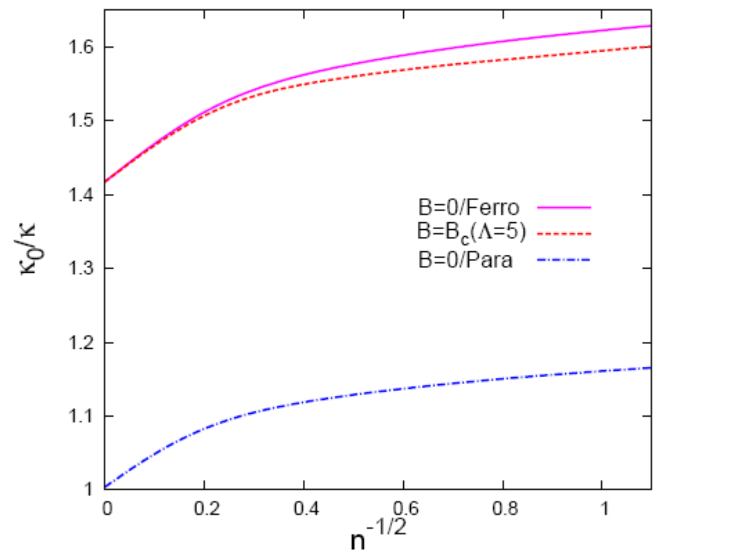


FIG. 5: (color online). Compressibility of gapless graphene as a function of inverse square root of density (in units of 10^{-6} cm) for both fully spin polarized and unpolarized states.

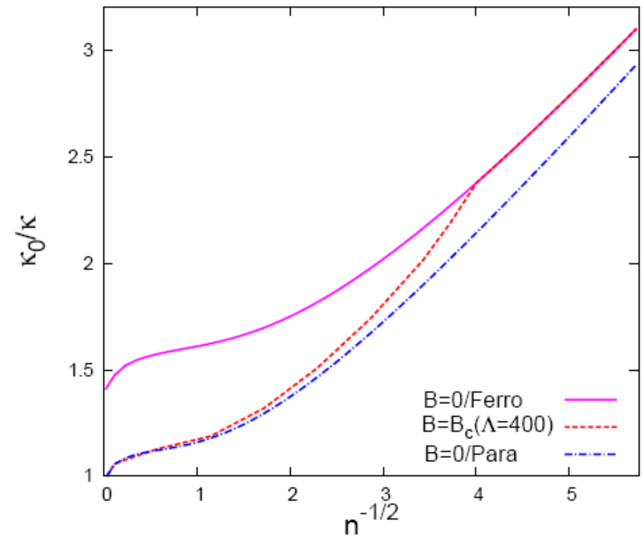
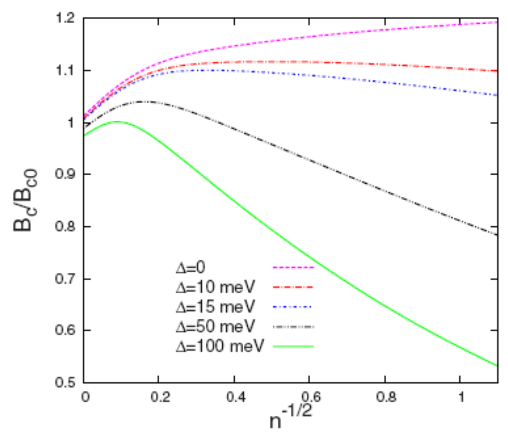


FIG. 6: (color online). Compressibility of gapped graphene with $\Delta = 100$meV as a function of inverse square root of density (in units of 10^{-6} cm) for both fully spin polarized and unpolarized states.



$$\boxed{\begin{cases} \Delta = 100\,meV \\ n = 10^{8}\,cm^{-2} \end{cases} \rightarrow B_c = 0}$$

A. Qaiumzadeh and R. Asgari, *Phys. Rev. B* ***80,*** 035429(2009)

Thank you for your attention

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