Motivation

1. What is excitonic mass gap in graphene?
   - The spontaneous chiral symmetry broken phases in graphene can be realized through:
     - magnetic catalysis in the presence of external magnetic field,
     - dielectric substitutes like silicon carbide (SiC),
     - confining the motion of the charge carriers in graphene quantum dots or nano-ribbons,
     - interaction-induced localization of charge carriers in the presence of adatoms or vacancies,
     - applying structural changes (axial strain) - nanostructure engineering,
     - electron-electron interactions.

   Our goal is to understand the interplay between anisotropic non-interacting dispersion, due to applied uniaxial strain, and electron-electron interaction in graphene.

Theoretical model

We consider Dirac fermions interacting via long-range Coulomb interaction on a uniaxially strained two-dimensional biparticle honeycomb lattice whose low-energy effective non-interacting Hamiltonian is,

$$ H_0 = v_F p_x \sigma_x + v_F p_y \sigma_y $$

(2)

where $v_F$, $v_F$, $\sigma_x$, and $\sigma_y$ are velocities, Pauli matrices along $x$- and $y$-directions respectively. The hat over the symbol signifies two-dimensional matrices written in the basis of sub-lattices, $A$ and $B$, of the honeycomb structure. Following Ref. [1], we consider tensile strain along the $y$-direction and define an anisotropy parameter, $\delta$, proportional to the uniaxial strain such that,

$$ \delta = \frac{\alpha}{\alpha} = 1 + \alpha $$

(3)

In isotropic limit, $\delta = 0$, the Fermi velocity is given by $v_F = v_F = \approx 10^3\text{m/s}$ and in the extreme anisotropic limit, $\delta = 1$, the two dimensional graphene is reduced to decoupled chains of carbon atoms.

Diagonalizing the Hamiltonian in Eq. (2), we obtain the anisotropic non-interacting energy dispersion,

$$ E(p) = \sqrt{(\sqrt{v_F}p_x)^2 + (\sqrt{v_F}p_y)^2} $$

(4)

The interaction is modeled by a long-range Coulomb potential given by $V(p) = \frac{\alpha}{|p|}$, where $\alpha = 1$ is the dielectric constant for the case of free-standing graphene and $\alpha > 1$ for graphene on an insulating substrate.

The strength of interaction is varied by defining the dimensionless parameter, $\alpha = 1$, which is the ratio of interacting to that of non-interacting energy and for freely suspended ($\alpha = 1$) graphene, $\alpha = 2.2$.

Since the uniaxial strain is applied along the $y$-direction it is obvious that $v_F$ will decrease due to increasing bond length while $v_F$ will remain constant. Therefore we consider,

$$ \alpha = \frac{v_F}{v_F} $$

(5)

as the strength of interaction in free-standing graphene. We shall suppose $v_F$ and $v_F$, Eqs. (3) and (5) respectively, as model parameters in our calculations.

Methodology

We consider the interacting Green's function given as,

$$ \Sigma(p) = i \alpha \left( (\sqrt{v_F}p_x)^2 + (\sqrt{v_F}p_y)^2 \right) - \frac{1}{\epsilon} $$(6)

where $\omega$ is the external frequency, $\epsilon$ is two-dimensional identity matrix and the self-energy is,

$$ \Sigma(p) = M(p) \alpha \epsilon $$

(7)

with $M(p)$ being the chiral symmetry breaking order parameter, related to the generation of finite mass gap and $\delta$ is the Pauli matrix. Since $\sigma_z$, anti-commutes with the Hamiltonian given in Eq. (2), any non-zero value of $M(p)$ will result in opening a spectral gap in the dispersion relation indicating sub-lattice symmetry breaking i.e., spontaneous chiral symmetry due to electron-electron interaction. The anisotropic non-interacting gapless energy spectrum is given by Eq. (1).

The many-body self-energy in the perturbative zeroth order (without any vertex corrections) GW theory with random phase approximation (RPA) for the screened potential is,

$$ \Sigma(p) = \frac{\alpha}{2\epsilon^2} \left( \left( \frac{\alpha}{2\epsilon^2} \right) (p - q) \Sigma(q) \right) $$

(8)

where the effective interaction is given by

$$ V(q) = \frac{1}{|q|^2} \left( \frac{1}{1 - |q|^2/|p|^2} \right) $$

(9)

and in the static (zero external frequency) RPA the particle-hole bubble is,\n
$$ \Pi(p) = \frac{N_f}{2\epsilon^2} \sqrt{\left( \sqrt{v_F}p_x \right)^2 + \left( \sqrt{v_F}p_y \right)^2} $$

(10)

Conclusions and Outlook

- We perform large scale numerical calculations to obtain the excitonic mass gap equation as a self-consistent solution for the self-energy within Hartree-Fock mean-field ($N_f = 0$) and static RPA ($N_f = 4$) as a function of the dimensionless coupling constant ($\alpha$) and anisotropy parameter ($\delta$).
- The critical coupling, at which the gap becomes finite, is plotted against anisotropy and indicates that with an increase in anisotropy (uniaxial strain) in graphene, the strength of critical coupling decreases which suggests anisotropy supports formation of excitonic mass gap in graphene.
- Our final goal is to perform large scale numerical calculations combining nonperturbative methods like Dyson-Schwinger or functional renormalization group along with dynamic screening, velocity renormalization, vertex corrections and possibly renormalization effects.

References


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