Graphene in periodic deformation fields

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We present the results of calculation of the effect of scalar and vector potentials generated by periodic deformations of the graphene crystal lattice, on the electron energy spectrum. It is found that periodic fields do not create the gap in the Dirac point but they change substantially the velocity of electrons near the Dirac point, and the resulting electron energy spectrum can be strongly anisotropic. We discuss the effect of screening of the periodic scalar potential. For this purpose we calculate the dielectric function. This calculation shows that the periodic scalar field is strongly suppressed by the screening. The screening is relevant at nonzero chemical potential and is due to presence of free electrons and holes. Self-consisting consideration of the screening, which in its turn is depending on the electron spectrum (electron velocity), leads to renormalization of the electron velocity. We solved RG equations for velocity and found asymptotic isotropization and an increase of velocity with the renormalization parameter. Using the dependence of electron velocity on the periodic field we studied the variation of the plasmon spectra in graphene. We found that the spectrum of plasmons can be also effectively controlled by periodic field. Namely, the plasmon velocity in its linear part can be manipulated by the periodic strain.

Introduction

Electronic properties of graphene can be strongly affected by deformations generating certain scalar and vector gauge fields. Such fields act on electrons as effective pseudo-electric and pseudo-magnetic fields, which can have enormously high magnitude [1]. For example, the pseudo-magnetic field is estimated to reach up to 300 T. It gives us an additional tool for very effective manipulation of electrons in graphene by the strains (strain engineering). Especially important is using periodic deformations creating periodic pseudo-electric and magnetic fields, which do not necessarily break the periodicity of the lattice. As a result, we can obtain substantially modified electronic structure of graphene. One of the existing possibilities is related to creation of a standing strain wave in graphene.

Electron energy spectrum

Hamiltonian $\mathcal{H} = -iv\boldsymbol{\sigma}\cdot(\nabla - i\mathbf{A}) + V$

Schrödinger equation

$$\begin{pmatrix} \varepsilon - V & iv\partial_- + vA_- \\ iv\partial_+ + vA_+ & \varepsilon - V \end{pmatrix}\begin{pmatrix} \varphi \\ \chi \end{pmatrix} = 0$$

Scalar and vector potentials:

$$V(\mathbf{r}) = g\,(u_{xx} + u_{yy})$$
$$A_x(\mathbf{r}) = \frac{\beta t}{a_0}(u_{xx} - u_{yy})$$
$$A_y(\mathbf{r}) = -\frac{2\beta t}{a_0}u_{xy}$$

A. **Periodic scalar potential**

$$\tilde{\mathcal{H}} = \begin{bmatrix} -vk_x & v(\gamma_1 k_x - \gamma_2 k_y) \\ v(\gamma_1 k_x - \gamma_2 k_y) & vk_x, \end{bmatrix}$$

- effective Hamiltonian

$$\gamma_1 = \frac{1}{L}\int_0^L dx\,\cos\left[\frac{2}{v}\int_0^x V(x')\,dx'\right]$$
$$\gamma_2 = \frac{1}{L}\int_0^L dx\,\sin\left[\frac{2}{v}\int_0^x V(x')\,dx'\right]$$

Our method: kp -approximation

B. **Periodic vector potential**

$$V(x) = 0 \text{ and } \mathbf{A}(x) \neq 0$$

$$\tilde{\mathcal{H}} = \begin{pmatrix} 0 & \tilde{v}k_- \\ \tilde{v}^* k_+ & 0 \end{pmatrix}$$

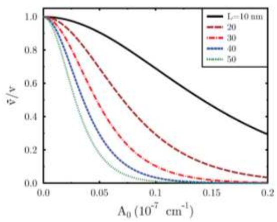
$$\varphi(x) = \exp\left[i\int_0^x A_+(x')\,dx'\right]$$
$$\chi(x) = \exp\left[i\int_0^x A_-(x')\,dx'\right]$$

Renormalized electron velocity:

$$\frac{\tilde{v}}{v} = \left\{\frac{1}{L^2}\int_0^L \exp\left[-2\int_0^{x_1} A_y(x')\,dx'\right]dx_1 \int_0^L \exp\left[2\int_0^{x_2} A_y(x')\,dx'\right]dx_2\right\}^{-1/2}.$$

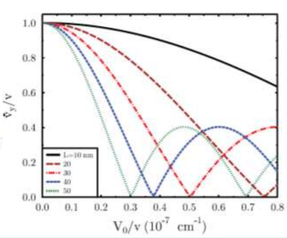
Renormalized velocity as a function of the amplitude of periodic field

$$A_y(x) = A_0 \sin(2\pi x/L)$$



C. **Longitudinal standing wave**

$$u_x = u_x(x) \text{ and } u_y = 0$$
$$\tilde{v}_x = v$$
$$\tilde{v}_y/v = 2|\zeta|$$
$$\zeta = \frac{1}{2L}\int_0^L \exp\left[-\frac{i}{v}\int_0^x V(x')\,dx'\right]dx$$

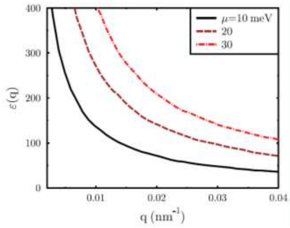


The energy spectrum is anisotropic

Screening

RPA approximation

$$\Pi_0(\mathbf{q}) = -i\,\mathrm{Tr}\int\frac{d^2\mathbf{k}\,d\varepsilon}{(2\pi)^3}\,G(\mathbf{k}+\mathbf{q},\varepsilon)\,G(\mathbf{k},\varepsilon)$$
$$G(\mathbf{k},\varepsilon) = \frac{\varepsilon + \mu + v\sigma\cdot\mathbf{k}}{(\varepsilon + \mu + i\delta\,\mathrm{sgn}\,\varepsilon)^2 - \varepsilon_k^2}$$
$$\epsilon(q) = 1 - u_0(q)\,\Pi_0(q)$$



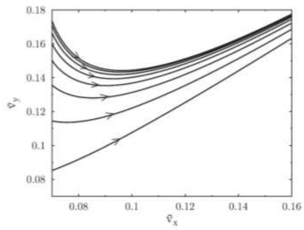
e-e interaction

Electron self energy due to Coulomb interaction:

$$\Sigma(\mathbf{k}) = \frac{e^2}{4\pi}\int_{|\mathbf{k}-\mathbf{q}|>k_F}\frac{d^2\mathbf{q}}{q}\,\frac{\tilde{v}_x\sigma_x(k_x - q_x) + \tilde{v}_y\sigma_y(k_y - q_y)}{\tilde{\varepsilon}_{\mathbf{k}-\mathbf{q}}}$$

RG equations:

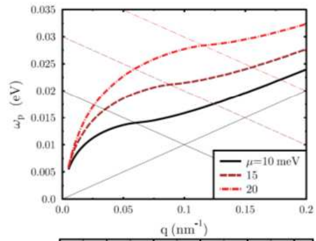
$$\frac{\partial\tilde{v}_x}{\partial\xi} = \frac{e^2\tilde{v}_x\xi}{\pi\tilde{v}_y}\left[\mathsf{K}(m) - \frac{\tilde{v}_x^2}{\tilde{v}_y^2}\mathsf{R}(m)\right]$$
$$\frac{\partial\tilde{v}_y}{\partial\xi} = \frac{e^2\xi}{\pi}[\mathsf{K}(m) - \mathsf{P}(m)].$$
$$m = 1 - \tilde{v}_x^2/\tilde{v}_y^2$$
$$\xi = \log(1/k_F L)$$
$$\xi_0 = \log(L/a_0)$$



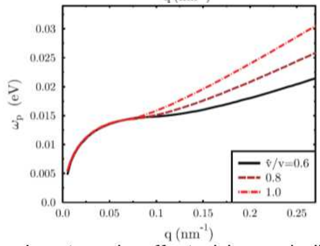
Characteristics of RG equations

Plasmons in graphene

$$\epsilon(\mathbf{q},\omega) = 1 - \frac{2\pi e^2}{q}\,\mathrm{Re}\,\Pi_0(\mathbf{q},\omega)$$
$$\epsilon(\mathbf{q},\omega_p) = 0$$



Plasmon spectrum for graphene for different values of chemical potential



Plasmon spectrum for graphene under periodic perturbation

Conclusion

The electronic spectrum in graphene can be strongly affected by periodic perturbation related to the deformations. In the vicinity of of Dirac points the electron velocity is renormalized and the spectrum is anisotropic. Screeing strongly suppresses the scalar potential. The linear sp[ectrum of plasmons in graphene is also affected by the periodic fields.

References

1. M.I. Katsnelson. Graphene: Carbon in Two Dimensions (Cambridge Univ. Press, 2012)
2. V.K. Dugaev, M.I. Katsnelson, Phys. Rev. B 86, 115405 (2012)

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