

Induced charge generated by Coulomb Impurity in TMDs

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We investigate the charge density $\rho_{ind}(\mathbf{r})$ induced by an external field in two-dimensional Dirac materials. We calculate $\rho_{ind}(\mathbf{r})$ induced by the Coulomb impurity with potential $U(\mathbf{r}) = eQ/r$, where e is the electron charge, Q is the impurity charge. The induced charge is expressed through the Green's function of the electron in an external field as

$$\rho_{ind}(\mathbf{r}) = -ieN \int_C \frac{d\varepsilon}{2\pi} \text{Tr}\{G(\mathbf{r}, \mathbf{r}|\varepsilon)\}, \quad (1)$$

where $N = 4$, $G(\mathbf{r}, \mathbf{r}'|\varepsilon)$ is the electron Green's function in the Coulomb field [1], C is the integration contour. The integration contour depends on the position of the Fermi energy. In our case, the contour is chosen so that the Fermi energy is located at the center of the band gap. Using the representation (1), we analytically calculated the asymptotic behavior of the induced charge density at distances much less and much greater than the Compton wavelength λ of the electron in the material. At the distances $r \ll \lambda$ the induced charge density has the form:

$$\rho_{ind}(\mathbf{r}) = eN \left(A(\alpha)\delta(\mathbf{r}) + \frac{B(\alpha)}{\lambda^2} \left(\frac{r}{\lambda}\right)^{\gamma-1} + \frac{C(\alpha)}{\lambda^2} \right), \quad (2)$$

where $\alpha = eQ/(\hbar v_f)$ is the dimensionless coupling constant, $A(\alpha)$, $B(\alpha)$, $C(\alpha)$ are the calculated functions, $\gamma = \sqrt{1 - 4\alpha^2}$, v_f is the Fermi velocity in the material. One can see that the asymptotics contains an unusual contribution $r^{\gamma-1}$, which is related with the behavior of the Dirac wave function of the electron in the Coulomb field at small distances. The functions $A(\alpha)$, $B(\alpha)$, $C(\alpha)$ have a simple but cumbersome form, so they are not presented here. At distances $r \gg \lambda$ the induced charge density has a power-law asymptotic behavior $1/r^n$.

References

- [1] I. S. Terekhov, A. I. Milstein, V. N. Kotov, O. P. Sushkov, *Screening of Coulomb Impurities in Graphene*, Phys. Rev. Lett. **100**, 076803 (2008).