Screening of Coulomb Impurities in Graphene

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- Electron Green's function in a Coulomb field.
- Calculation of the induced charge.
- Results.

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- Introduction.
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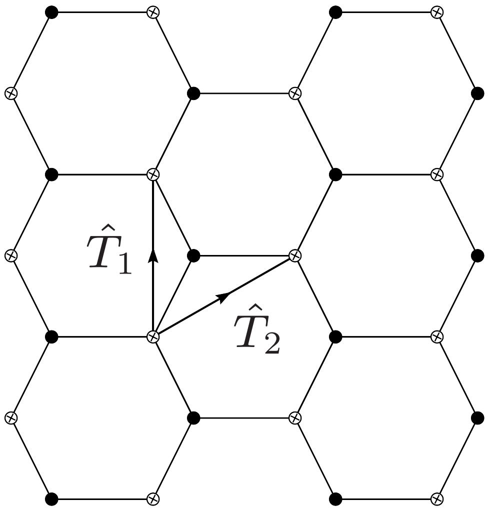
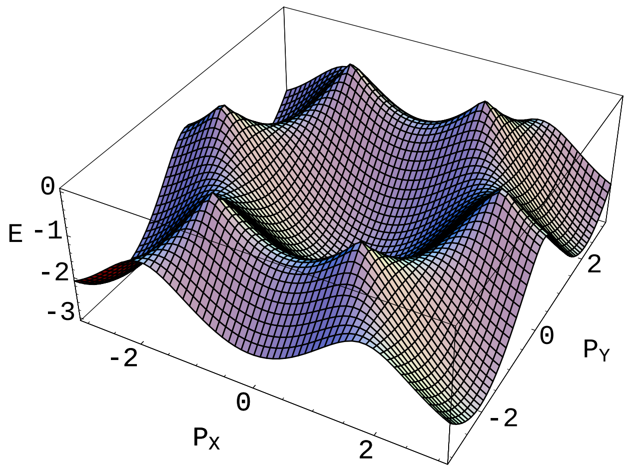
Introduction

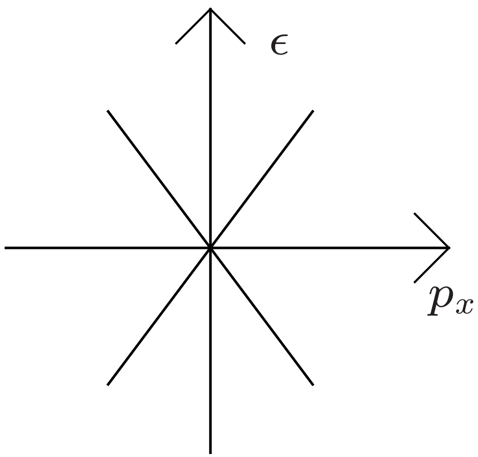
The equation for the electron wave function is

$$(\epsilon - (\boldsymbol{\sigma}\mathbf{p}))\,\psi(\mathbf{r},\epsilon) = 0\,,$$

where $\mathbf{p} = (p_x, p_y)$, $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$.



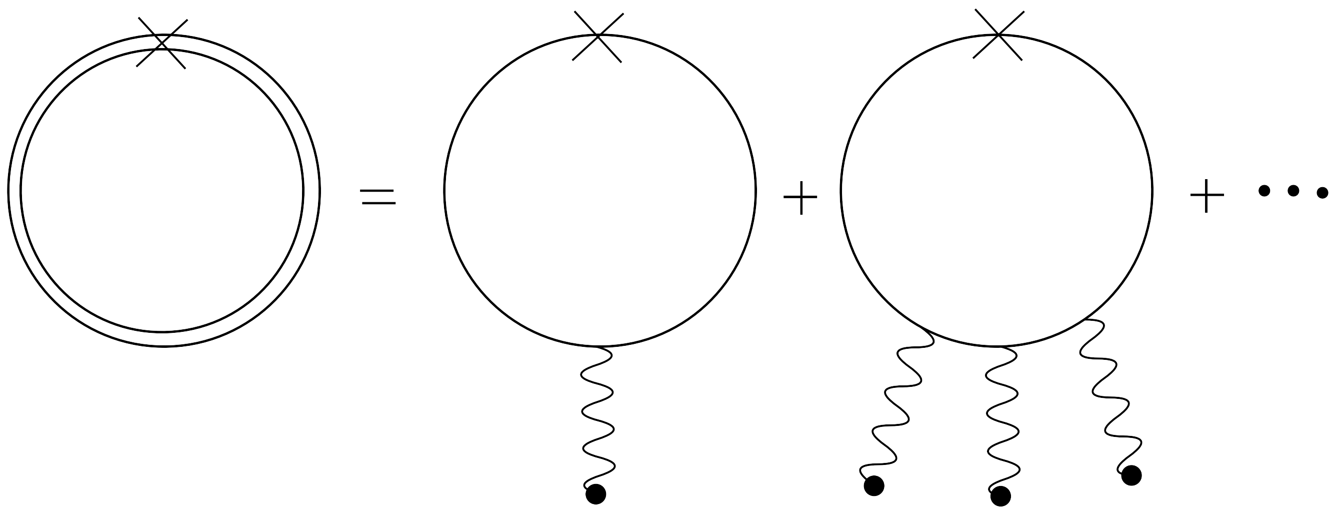




$$\left(\epsilon + \frac{Z\alpha}{r} - (\boldsymbol{\sigma}\mathbf{p})\right)\psi(\mathbf{r},\epsilon) = 0\,, \quad Z\alpha \sim 1\,.$$

Induced charge.

$\rho_{ind} =$



Critical $Z\alpha > 1/2$, and Subcritical $Z\alpha < 1/2$ Regimes

Using the dimension considerations we can write the expression for induced charge in the form:

$$\rho_{ind}(\boldsymbol{r}) = e\,A(Z\alpha)\delta(\boldsymbol{r}) + \frac{e\,B(Z\alpha)}{r^2} + e\,C(Z\alpha)\frac{r_0}{r^3}.$$

For $Z\alpha < 1/2$:

$$\rho_{ind}(\boldsymbol{r}) = e\,A(Z\alpha)\delta(\boldsymbol{r}).$$

A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, arXiv:0705.4663v2, R. R. Biswas, S. Sachdev, and D. T. Son, arXiv:0706.3907.

For $Z\alpha > 1/2$:

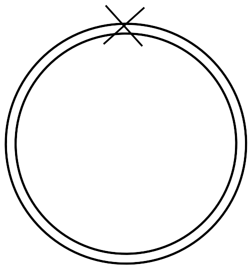
$$\rho_{ind}(\boldsymbol{r}) = e\,A(Z\alpha)\delta(\boldsymbol{r}) + \frac{e\,B(Z\alpha)}{r^2}.$$

A. V. Shytov, M. I. Katsnelson, and L. S. Levitov, arXiv:0705.4663v2.

For $Z\alpha \gg 1/2$. M. I. Katsnelson(2006). Fogler et al.(2007).

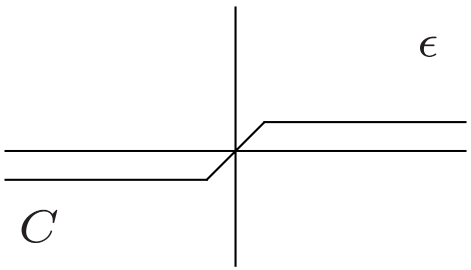
Explanation of the calculation method

We consider the case $Z\alpha < 1/2$



$$\rho_{ind}(\mathbf{r}) = -ieN\int_C \frac{d\epsilon}{2\pi}\mathrm{Tr}\{\hat{G}(\mathbf{r},\mathbf{r}|\epsilon)\}\,,$$

where $N = 4$, and $\hat{G}(\mathbf{r},\mathbf{r}'|\epsilon)$ is the electron Green's function in a Coulomb field. (A.I. Milstein, V.M. Strahovenko (1983))



Electron Green's function

$$\left(\epsilon + \frac{Z\alpha}{r} - (\boldsymbol{\sigma}\mathbf{p})\right)\psi(\mathbf{r},\epsilon) = 0\,,$$

$$\left(\epsilon + \frac{Z\alpha}{r} - (\boldsymbol{\sigma}\cdot\mathbf{p}) - \sigma_3 M\right)\hat{G}(\mathbf{r},\mathbf{r}'|\epsilon) = \delta(\mathbf{r}-\mathbf{r}').$$

For $Z = 0$ we have $\epsilon = \pm\sqrt{p^2 + M^2}$. (A.I. Milstein, V.M. Strahovenko (1982))

$$\hat{G}(\mathbf{r},\mathbf{r}'|\epsilon) = -\left(\epsilon + \frac{Z\alpha}{r} + (\boldsymbol{\sigma}\cdot\mathbf{p}) + \sigma_3 M\right)\sum_{\lambda} P_{\lambda}(\phi,\phi')\int_0^{\infty}\frac{k\,ds}{\sin(ks)}e^{2is\epsilon Z\alpha}$$

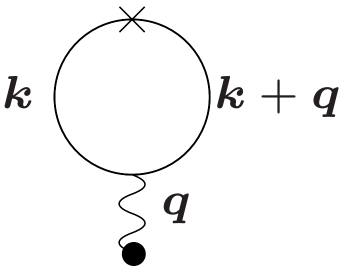
$$\times \exp\left[ik(r+r')\cot(ks) - i\pi\lambda\right] J_{2\lambda}\left(\frac{2k\sqrt{rr'}}{\sin(ks)}\right) .$$

$$\lambda = \gamma \mp \frac{1}{2},\quad \gamma = \sqrt{(m+1/2)^2 - (Z\alpha)^2},\quad m = 0, 1, 2...$$

Induced Charge

$$\rho_{ind}(r) = -\frac{eN}{\pi^2 r}\sum_{m=0}^{\infty}\int\limits_0^{\infty}\int\limits_0^{\infty} d\epsilon\, ds\, e^{-y\cosh s}\left(2Z\alpha\cos(\mu s)\coth s I_{2\gamma}(y) - \sin(\mu s)\frac{\epsilon}{k} y I'_{2\gamma}(y)\right)$$

Here $k = \sqrt{\epsilon^2 + M^2}$, $y = 2rk/\sinh s$, $\mu = 2Z\alpha\epsilon/k$, $\gamma = \sqrt{(m+1/2)^2 - (Z\alpha)^2}$, $m = 0, 1, 2..$

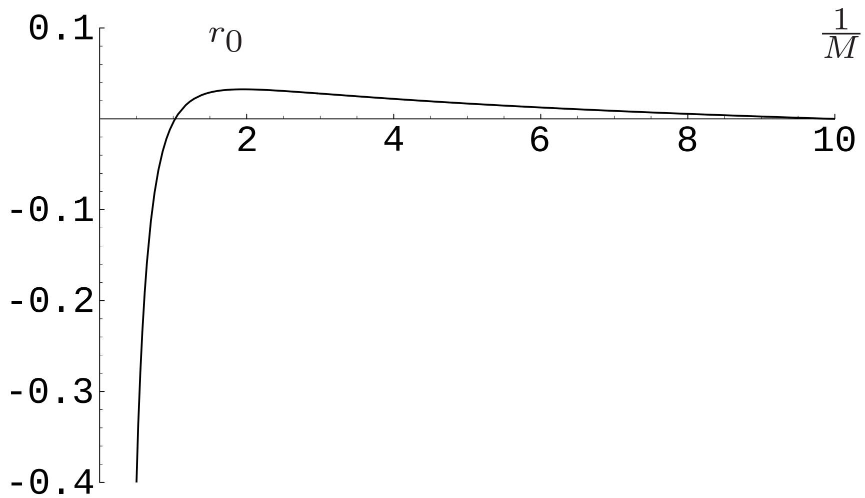


$$\int \frac{d^2k}{(2\pi)^2}\int\frac{d\epsilon}{2\pi}\frac{1}{(\epsilon - (\boldsymbol{\sigma k}) + i0)(\epsilon - (\boldsymbol{\sigma}(\boldsymbol{k}+\boldsymbol{q})) + i0)}$$

$$\int \frac{d^2k}{(2\pi)^2}\int\frac{d\epsilon}{2\pi} \neq \int\frac{d\epsilon}{2\pi}\int\frac{d^2k}{(2\pi)^2}$$

$$\int \rho_{ind}(\boldsymbol{r}) d^2r = 0\,.$$

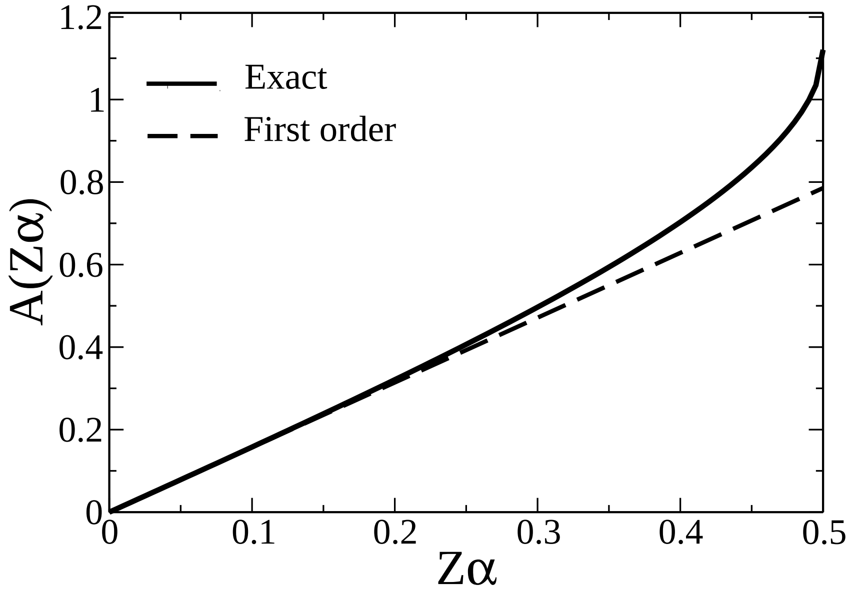
$$\rho^{(1)}(\boldsymbol{r}) = -|e|Z\alpha\left(\frac{\pi}{8}\delta(\boldsymbol{r}) + \frac{M^2}{4}\ln(Mr)\right), \quad \text{for } r_0 \ll r \ll \frac{1}{M} .$$



$$\rho_{ind}(\mathbf{r}) = Q_{ind}\delta(\mathbf{r}) + \rho_{distr} \; .$$

$$Q_{ind} = eN\left[\frac{\pi}{8}Z\alpha + \Lambda(Z\alpha)\right] \equiv -|e|A(Z\alpha) \; .$$

$$\Lambda(Z\alpha) = \frac{2}{\pi}\sum_{m=0}^{\infty} \mathrm{Im}\left[\ln\Gamma(\gamma - iZ\alpha) + \frac{1}{2}\ln(\gamma - iZ\alpha) - (\gamma - iZ\alpha)\psi(\gamma - iZ\alpha) + \frac{iZ\alpha}{2\varkappa} - iZ\alpha\varkappa\psi'(\varkappa)\right] \; .$$



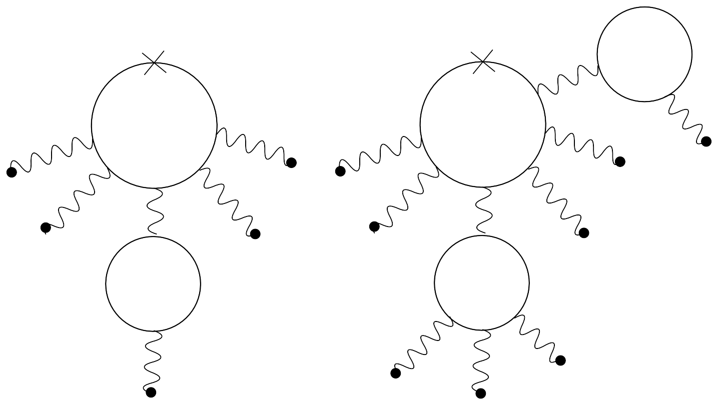
$$A(Z\alpha) = \frac{\pi}{2}(Z\alpha) + 0.783(Z\alpha)^3 + 1.398(Z\alpha)^5 + \ldots$$

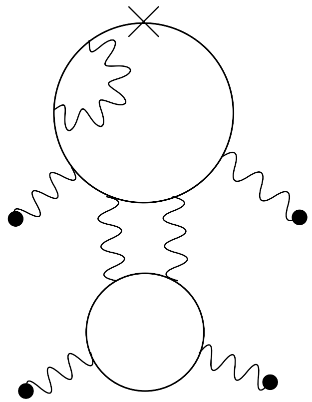
Shytov et al., Biswas et al.

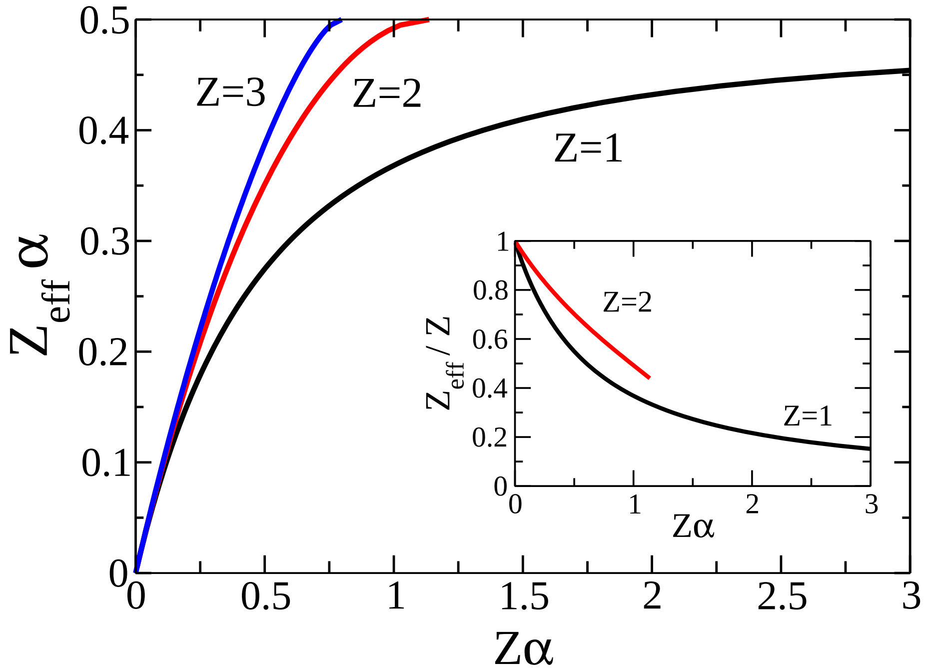
$$A(Z\alpha) = 1.12 - 1.19\sqrt{\frac{1}{2} - Z\alpha} - 0.29\left(\frac{1}{2} - Z\alpha\right) + \ldots$$

$$Z_{\text{eff}} = Z - A(Z\alpha)$$

$$Z_{\rm eff}\alpha = Z\alpha - \alpha A(Z_{\rm eff}\alpha)$$






0.5
0.4
0.3
0.2
0.1
0
Z=3
Z=2
Z=1
$Z_{eff}\alpha$
0
0.5
1
1.5
2
2.5
3
$Z\alpha$
1
0.8
0.6
0.4
0.2
0
Z_{eff} / Z
Z=2
Z=1
0
1
2
3
$Z\alpha$

Results

- Using the operator method we have found useful integral representation for Green's function of electron in a Coulomb field .

- Using this Green's function we obtain distribution of induced charge in all orders in $Z\alpha$ for $Z\alpha < 1/2$.

- We have found the effective charge number Z_{eff} for Coulomb impurity in the self-consistent way.