THE RELATIVISTIC COULOMB PROBLEM

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Content

Coulomb interaction

Consider a Dirac electron interacting with a point charge Z through the Coulomb interaction:

$$V(r) = -\frac{Ze^2}{\varepsilon_{\text{ext}} r} = -\frac{\hbar v \beta}{r}$$

$$\beta := \frac{Ze^2}{\varepsilon_{\text{ext}} \hbar v}$$

- Connections to nuclear physics.
- Charge impurities limiting the electron mobility in graphene.
- Set the stage for the consideration of electron-electron interaction.

Radial potential $V(r)$

$$(-i\hbar v \sigma \cdot \boldsymbol{\nabla} + V(r)) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \tag{1}$$

let

$$x = r\cos\varphi \qquad r = \sqrt{x^2 + y^2}$$

$$y = r\sin\varphi \qquad \varphi = \tan^{-1}\left(\frac{y}{x}\right)$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \varphi}{\partial x}\frac{\partial}{\partial \varphi} = \cos\varphi \frac{\partial}{\partial r} - \frac{\sin\varphi}{r}\frac{\partial}{\partial \varphi}$$

$$\frac{\partial}{\partial y} = \ldots = \sin\varphi \frac{\partial}{\partial r} + \frac{\cos\varphi}{r}\frac{\partial}{\partial \varphi}$$

Eq. (1) becomes

$$\begin{pmatrix} V(r) & -i\hbar v e^{-i\varphi}\left(\frac{\partial}{\partial r} - \frac{i}{r}\frac{\partial}{\partial \varphi}\right) \\ -i\hbar v e^{i\varphi}\left(\frac{\partial}{\partial r} + \frac{i}{r}\frac{\partial}{\partial \varphi}\right) & V(r) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$$

Ansatz:

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} R_1(r)e^{i\ell\varphi} \\ R_2(r)e^{i(\ell+1)\varphi} \end{pmatrix} \qquad \ell \in \mathbb{Z} \quad (\Psi(\varphi + 2\pi) = \Psi(\varphi))$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix} \begin{pmatrix} R_1(r) \\ R_2(r) \end{pmatrix} e^{i\ell\varphi}$$

$$\frac{\partial}{\partial \varphi}\Psi = \begin{pmatrix} i\ell R_1(r)e^{i\ell\varphi} \\ i\left(\ell+1\right)R_2(r)e^{i(\ell+1)\varphi} \end{pmatrix} = i \begin{pmatrix} \ell & 0 \\ 0 & \ell+1 \end{pmatrix} \Psi$$

Solution to the Coulomb potential III

Eq. (1) becomes

$$\begin{pmatrix} V(r) & -i\hbar v e^{-i\varphi}\left(\frac{\partial}{\partial r}+\frac{\ell+1}{r}\right) \\ -i\hbar v e^{i\varphi}\left(\frac{\partial}{\partial r}-\frac{\ell}{r}\right) & V(r) \end{pmatrix}\Psi = E\Psi$$

multiply by $\begin{pmatrix} 1 & 0 \\ 0 & e^{-i\varphi} \end{pmatrix} e^{-i\ell\varphi}$ from the left

$$\begin{pmatrix} V(r) & -i\hbar v\left(\frac{\partial}{\partial r}+\frac{\ell+1}{r}\right) \\ -i\hbar v\left(\frac{\partial}{\partial r}-\frac{\ell}{r}\right) & V(r) \end{pmatrix}\begin{pmatrix} R_1 \\ R_2 \end{pmatrix} = E\begin{pmatrix} R_1 \\ R_2 \end{pmatrix}$$

and we have removed the φ dependence.

Next Ansatz:

$$\begin{pmatrix} R_1 \\ R_2 \end{pmatrix} = \begin{pmatrix} w_+(r) + w_-(r) \\ w_+(r) - w_-(r) \end{pmatrix} r^{s-\frac{1}{2}} e^{ikr}$$

where $k = -\frac{E}{\hbar v}$, $s = \sqrt{\Big(\underbrace{\ell + \tfrac{1}{2}}_{=:m}\Big)^2 - \beta^2}$ for the Coulomb potential.

Eq. (1) becomes

$$r\frac{\mathrm{d}w_-}{\mathrm{d}r} + (s + i\beta)\, w_- - m w_+ = 0,$$
$$r\frac{\mathrm{d}w_+}{\mathrm{d}r} + \big(s - i\beta + \underbrace{2ikr}_{=:\,-z}\big) w_+ - m w_- = 0.$$

Combine into a confluent hypergeometric equation

$$z\frac{\mathrm{d}^2 w_-}{\mathrm{d}z^2} + \big(\underbrace{2s+1}_{=:c} - z\big)\frac{\mathrm{d}w_-}{\mathrm{d}z} - \underbrace{(s + i\beta)}_{=:a} w_- = 0$$

SOLUTION TO THE COULOMB POTENTIAL V

General solution:

$$w_-(z) = A\,{}_1F_1(a,c;z) + Bz^{1-c}\,{}_1F_1(a-c+1,2-c;z)$$

- Case $|\beta| < |m|$, asymptotic expression for $kr \gg 1$:

$$w_-(r) = \frac{\lambda \exp\left(-i\beta \ln\left(2kr\right)\right)}{(2kr)^s}, \qquad \textit{scattered wave}$$

$$w_+(r) = \frac{\lambda^* \exp\left(i\beta \ln\left(2kr\right)\right)}{(2kr)^s} e^{-2ikr}. \qquad \textit{incident wave}$$

$$\frac{w_-(r)}{w_+(r)} = \exp\left(2i\delta_m(k) + 2ikr\right), \qquad \delta_m(k) = -\beta \ln\left(2kr\right) + \arg\lambda.$$

- Case $|\beta| > |m|$

solution is ill defined

Relativistic collapse

Using the Heisenberg uncertainty principle we have $p \approx \hbar/R$.

- For a nonrelativistic particle:

$$E(R) \approx \frac{\hbar^2}{2mR^2} - \frac{Ze^2}{R} \qquad \Rightarrow \qquad R_0 = \frac{\hbar^2}{mZe^2}$$

- For a relativistic particle:

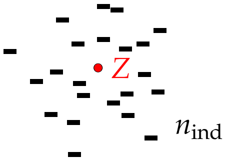
$$E(R) \approx \sqrt{\left(\frac{\hbar c}{R}\right)^2 + (mc^2)^2} - \frac{Ze^2}{R} \qquad \Rightarrow \qquad R_0 = \frac{\hbar}{mc}\underbrace{\sqrt{\left(\frac{\hbar c}{Ze^2}\right)^2 - 1}}_{\sqrt{(Z_c/Z)^2 - 1}}$$

There is a real R_0 only for

$$Z < Z_c = \frac{\hbar c}{e^2} = \frac{1}{\alpha} \approx 137. \qquad \left(\text{graphene: } Z_c = \frac{1}{\alpha_{\text{eff}}} = \frac{\hbar v}{e^2} \approx 1\right)$$

For $Z > Z_c$: *relativistic collapse*.

$$V_{\text{ind}}(\boldsymbol{r}) = \underbrace{\frac{e^2}{\varepsilon_{\text{ext}}} \int \mathrm{d}\boldsymbol{r}' \, \frac{n_{\text{ind}}(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}}_{\text{Hartree}} + \underbrace{V_{\text{xc}}(\boldsymbol{r})}_{\substack{\text{exchange}\\ \text{correlation}}}$$



Approximations:

- $V_{\text{xc}}(\boldsymbol{r})$ neglected
- $\mu = 0$

Dimensional analysis:

$$n_{\text{ind}}(r) = A(\beta)\delta(\boldsymbol{r}) + \frac{B(\beta)}{r^2}$$

Screening of charge impurities II

- $A(\beta)$: charge renormalization

$$Q^A_{\text{ind}} = \int \mathrm{d}\boldsymbol{r}'\, A(\beta)\delta(\boldsymbol{r}') = A(\beta)$$

$$-\frac{Z}{\varepsilon_{\text{ext}}} \to -\frac{Z}{\varepsilon_{\text{ext}}} + A(\beta) \qquad \left(= -\frac{Z}{\varepsilon}, \text{ phenomenologically}\right)$$

Thus

$$A(\beta) = Z\left(\frac{1}{\varepsilon} - \frac{1}{\varepsilon_{\text{ext}}}\right)$$

- $B(\beta)$: nonlinear screening

$$Q^B_{\text{ind}} = \int \mathrm{d}\boldsymbol{r}'\, \frac{B(\beta)}{(r')^2} \approx 2\pi B(\beta) \ln\left(\frac{r_{\max}}{r_{\min}}\right)$$

where

$$r_{\min} \approx a, \qquad r_{\max} \approx L$$

Thomas-Fermi approximation I

Approach: write

$$V(\boldsymbol{r}) = -\frac{Ze^2}{\varepsilon_{\text{ext}} r} + V_{\text{ind}}(\boldsymbol{r}) = -\frac{e^2}{\varepsilon_{\text{ext}}}\tilde{F}(\ln r)$$

$$n_{\text{ind}}(\boldsymbol{r}) = n\left[\mu - V(\boldsymbol{r})\right] - n\left[\mu\right]$$

$$n\left[\mu\right] = \int_0^{\mu} \mathrm{d}E\, N(E) = \frac{\mu\,|\mu|}{\pi\hbar^2 v^2}$$

and try to determine $V(\boldsymbol{r})$ self-consistently.

$$\tilde{F}(x) \to Z - q\int_{\ln a}^{x} \mathrm{d}t\, \tilde{F}(t)\left|\tilde{F}(t)\right| \quad \text{for large } x, \text{ where } q := 2\left(\frac{e^2}{\varepsilon_{\text{ext}}\hbar v}\right)^2$$

$$\Leftrightarrow$$

$$\frac{\mathrm{d}\tilde{F}(x)}{\mathrm{d}x} = -q\tilde{F}(x)\left|\tilde{F}(x)\right|, \qquad \tilde{F}(0) = Z$$

Thomas-Fermi approximation II

$$\tilde{F}(x) = \frac{Z}{1 + |Z| \, qx}$$

$$F(r) = \tilde{F}(\ln r) = \frac{Z}{1 + |Z| \, q \ln\left(\frac{r}{a}\right)} \to \frac{\mathrm{sgn}(Z)}{q \ln\left(\frac{r}{a}\right)}$$

$$V(\boldsymbol{r}) = -\frac{e^2 Z}{\varepsilon_{\mathrm{ext}} \left(1 + |Z| \, q \ln\left(\frac{r}{a}\right)\right)} \to -\frac{e^2 \mathrm{sgn}(Z)}{\varepsilon_{\mathrm{ext}} q \ln\left(\frac{r}{a}\right)}$$

$$B(\beta) = -\frac{q}{2\pi} \frac{Z \, |Z|}{\left(1 + |Z| \, q \ln\left(\frac{r}{a}\right)\right)^2}$$

Renormalization group approach I

Starting from the Friedel sum rule

$$Q_{\mathrm{ind}} = -\frac{4}{\pi}\sum_m \delta_m(k_F)$$

we take

$$\delta_m(k \sim \frac{1}{r}) = \sqrt{\beta^2 - m^2}\ln\left(\frac{r}{a}\right)$$

to obtain

$$B(\beta) = -\frac{2}{\pi^2}\beta\sum_m \sqrt{\beta^2 - m^2}$$

We see that $B(|\beta| < \beta_c = \frac{1}{2}) = 0$. Additionally, a flow of effective charge is dictated by

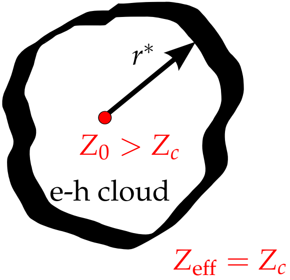
$$\frac{\mathrm{d}\beta}{\mathrm{d}\ln r} = 2\pi\beta_0 B(\beta), \qquad \text{where } \beta_0 = \frac{Z_0 e^2}{\varepsilon_{\mathrm{ext}}\hbar\nu}$$

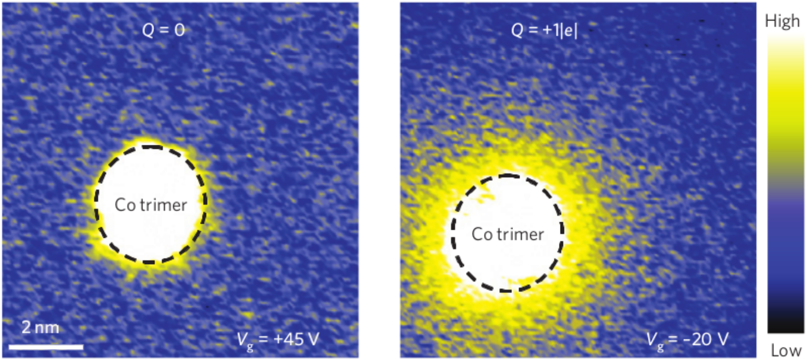
The flow stops when $|\beta(r)|$ reaches

$$\beta_c = \frac{\nu}{\alpha c} \approx \frac{1}{2}.$$

Further calculations show that this happens on a length scale

$$r^* = a \exp\left(\frac{\pi \varepsilon_{\mathrm{ext}} \hbar \nu}{4e^2} \cosh^{-1}(2\beta_0)\right)$$
$$= a \exp\left(\frac{\pi Z}{4\beta_0} \cosh^{-1}(2\beta_0)\right)$$





A cobalt trimmer impurity on graphene is tuned by the back gate voltage (V_g) into a charge-neutral state (left) or a $Q = +1\,|e|$ state (right). The long-range radially symmetric charge cloud forming around the Co trimmer is observed by differential conductance ($\mathrm{d}I/\mathrm{d}V$, color scale) mapping.

Wang et al. 2012

Content

Part I: Point charges

Part II: Electron-electron interaction

Content

Single- versus many-particle picture

- Up to now, electrons in graphene treated in the independent-particle approximation.

- Theoretically, the effective coupling constant

$$\alpha_{\text{eff}} = \frac{e^2}{\hbar v} \approx 2.2$$

  indicate that many-body interactions should play an important role.

- Experimentally, very few evidences of many-body effects.

Many-particle Hamiltonian

Consists of the kinetic term

$$H_0 = -i\hbar v \boldsymbol{\sigma} \cdot \boldsymbol{\nabla}$$

and the electron-electron interaction

$$H_C = \frac{e^2}{2} \sum_{\alpha,\beta} \iint \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}' \, \frac{\hat{\psi}^\dagger_\alpha(\boldsymbol{r}) \hat{\psi}_\alpha(\boldsymbol{r}) \hat{\psi}^\dagger_\beta(\boldsymbol{r}') \hat{\psi}_\beta(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}$$

MEAN-FIELD APPROXIMATION I

Hartree-Fock approximation (mean field approx.):

$$\psi_\alpha^\dagger \psi_\alpha \psi_\beta^\dagger \psi_\beta \simeq \underbrace{\left\langle \psi_\alpha^\dagger \psi_\alpha \right\rangle \psi_\beta^\dagger \psi_\beta}_{\text{Hartree}} + \underbrace{\left\langle \psi_\alpha^\dagger \psi_\beta \right\rangle \psi_\beta^\dagger \psi_\alpha}_{\text{Fock}}$$

- Hartree:

$\sum_\alpha \left\langle \psi_\alpha^\dagger \psi_\alpha \right\rangle = n(\boldsymbol{r})$ compensated by interactions with ions for electrostatic, homogeneous, electroneutral systems

- Fock:

$$\left\langle \psi_\alpha^\dagger(\boldsymbol{r}) \psi_\beta(\boldsymbol{r}') \right\rangle = \left\langle \left(\sum_{\boldsymbol{k}} \psi_{\alpha \boldsymbol{k}}^\dagger e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \right) \left(\sum_{\boldsymbol{k}'} \psi_{\beta \boldsymbol{k}'} e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \right) \right\rangle$$

$$\left\langle \psi_\alpha^\dagger(\boldsymbol{r}+\boldsymbol{t}) \psi_\beta(\boldsymbol{r}'+\boldsymbol{t}) \right\rangle \stackrel{!}{=} \left\langle \psi_\alpha^\dagger(\boldsymbol{r}) \psi_\beta(\boldsymbol{r}') \right\rangle$$

$$\Rightarrow \boldsymbol{k} = \boldsymbol{k}' \qquad \text{(neglecting Umklapp)}$$

$$\Rightarrow \left\langle \psi_\alpha^\dagger(\boldsymbol{r}) \psi_\beta(\boldsymbol{r}') \right\rangle = \sum_{\boldsymbol{k}} \underbrace{\left\langle \psi_{\alpha \boldsymbol{k}}^\dagger \psi_{\beta \boldsymbol{k}} \right\rangle}_{=: \rho_{\beta\alpha}(\boldsymbol{k})} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}$$

Mean-field approximation II

$$
\begin{aligned}
H_F &= -e^2 \sum_{\alpha,\beta} \iint \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}' \, \frac{\left\langle \psi^\dagger_\alpha(\boldsymbol{r}) \psi_\beta(\boldsymbol{r}') \right\rangle \hat{\psi}^\dagger_\beta(\boldsymbol{r}') \hat{\psi}_\alpha(\boldsymbol{r})}{|\boldsymbol{r} - \boldsymbol{r}'|} \\
&= -e^2 \sum_{\alpha,\beta} \sum_{\boldsymbol{k},\boldsymbol{k}'} \iint \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}' \, \frac{\rho_{\beta\alpha}(\boldsymbol{k}') \psi^\dagger_{\beta\boldsymbol{k}} \psi_{\alpha\boldsymbol{k}} e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{|\boldsymbol{r} - \boldsymbol{r}'|} \\
&= -e^2 \sum_{\alpha,\beta} \sum_{\boldsymbol{k},\boldsymbol{k}'} \psi^\dagger_{\beta\boldsymbol{k}} \psi_{\alpha\boldsymbol{k}} \rho_{\beta\alpha}(\boldsymbol{k}') \underbrace{\iint \mathrm{d}\boldsymbol{r}\, \mathrm{d}\boldsymbol{r}' \, \frac{e^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{|\boldsymbol{r} - \boldsymbol{r}'|}}_{=: I(\boldsymbol{k},\boldsymbol{k}')} \\
&= \sum_{\boldsymbol{k}} \sum_{\alpha,\beta} \psi^\dagger_{\beta\boldsymbol{k}} \psi_{\alpha\boldsymbol{k}} \underbrace{\sum_{\boldsymbol{k}'} \rho_{\beta\alpha}(\boldsymbol{k}') I(\boldsymbol{k},\boldsymbol{k}') \left(-e^2\right)}_{=: h_{\beta\alpha}(\boldsymbol{k})}
\end{aligned}
$$

Renormalization of the Fermi velocity I

Using standard perturbation theory

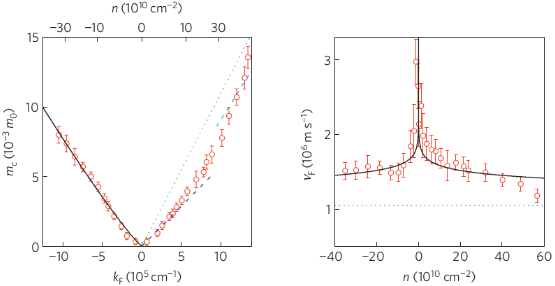
$$
\begin{aligned}
E_{\pm}^{(0)}(\boldsymbol{k}) &= \pm\hbar v k \\
E_{\pm}^{(1)}(\boldsymbol{k}) &= \pm \sum_{\boldsymbol{k}'} \frac{2\pi e^2}{|\boldsymbol{k}-\boldsymbol{k}'|} \frac{1}{2}\left(1 \pm \frac{\boldsymbol{k}\cdot\boldsymbol{k}'}{kk'}\right) \\
&= \pm \int_0^{k_c \approx \frac{1}{a}} \mathrm{d}\boldsymbol{k}' \, \frac{2\pi e^2}{|\boldsymbol{k}-\boldsymbol{k}'|} \frac{1}{2}\left(1 \pm \frac{\boldsymbol{k}\cdot\boldsymbol{k}'}{kk'}\right) \\
&= \pm \hbar \underbrace{\frac{e^2}{4\hbar} \ln\left(\frac{1}{ka}\right)}_{=:\,\delta v} k
\end{aligned}
$$

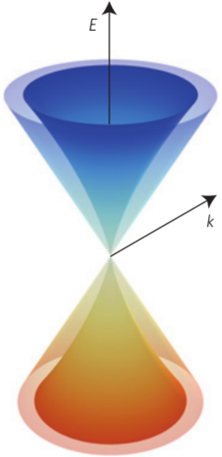
Doped graphene:

$$
\delta v_F \approx \frac{e^2}{4\hbar} \ln\left(\frac{1}{k_F a}\right)
$$

Account for virtual electron-hole transition:

$$\delta v_F \approx \frac{e^2}{4\hbar\varepsilon} \ln\left(\frac{1}{k_F a}\right)$$





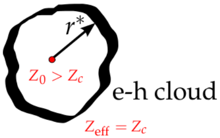
Measurement of the cyclotron mass in graphene as a function of doping (left) and corresponding Fermi velocity (right) showing the logarithmic correction.

Elias et al. 2011

Summary

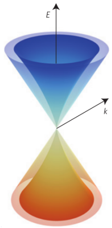
Part I: Point charges

- Solved the case of a point charge Z interacting with Dirac electrons.
- Supercritical charges are screened by an electron-hole cloud of size r^*.



Part II: Electron-electron interaction

- Many-body effects in graphene are predicted but only a few are observed.
- Electron-electron interaction leads to a renormalization of the Fermi velocity.



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