Charged Impurities in Graphene

A little more about the Coulomb problem in graphene$^{(*)}$

Vitor M. Pereira

In collaboration with: Johan Nilsson, Valeri Kotov and A. H. Castro Neto

Workshop on Correlations and Coherence in Quantum Matter
November 10, 2008.

$^{(*)}$*PRL **99**, 166802 (2007) — PRB **78**, 075433 (2008) — PRB **78**, 085101 (2008)*

Long range scatterers

- Unscreened Coulomb impurities;
- Linear conductivity vs n_e: $\sigma = e\mu|n|$;
- Most parameters (n, n_i, ε) can be controlled.
- Is this Boltzmann-like behavior the final story?

Coulomb Center in undoped graphene

- Low energy Dirac effective Hamiltonian
- 2D Dirac Equation in a Coulomb Field:

Graphene Conductivity

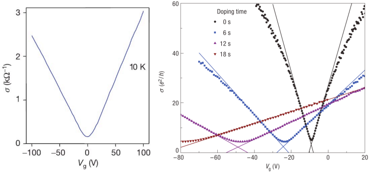


Fig. 1: Novoselov *et al.*, Nature 438; Chen *et al.* Nature Phys. 4.

Long range scatterers

- Unscreened Coulomb impurities;
- Linear conductivity vs n_e: $\sigma = e\mu|n|$;
- Most parameters (n, n_i, ε) can be controlled.
- Is this Boltzmann-like behavior the final story?

Coulomb Center in undoped graphene

- Low energy Dirac effective Hamiltonian
- 2D Dirac Equation in a Coulomb Field:

Graphene Conductivity

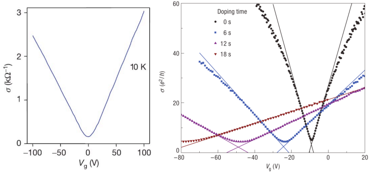


Fig. 1: Novoselov *et al.*, Nature 438; Chen *et al.* Nature Phys. 4.

Introduction – Graphene, Coulomb Impurities and Dirac Fermions

Long range scatterers

- Unscreened Coulomb impurities;
- Linear conductivity vs n_e: $\sigma = e\mu|n|$;
- Most parameters (n, n_i, ε) can be controlled.
- Is this Boltzmann-like behavior the final story?

Coulomb Center in undoped graphene

- Low energy Dirac effective Hamiltonian

$$H = -t \sum_{i \in A, \delta} a_i^\dagger b_{i+\delta} - t \sum_{i \in B, \delta} b_i^\dagger a_{i+\delta} \qquad (1)$$

$$\downarrow$$

$$\boxed{\mathcal{H} = \hbar v_F \, \tau_z \otimes \boldsymbol{\sigma} . \boldsymbol{p}} \qquad (2)$$

- 2D Dirac Equation in a Coulomb Field:

$$\left(\hbar v_F \, \boldsymbol{\sigma} . \boldsymbol{p} - \frac{Ze^2}{r} - E \right) \begin{pmatrix} \psi^A \\ \psi^B \end{pmatrix} = 0 \qquad (3)$$

Graphene Conductivity

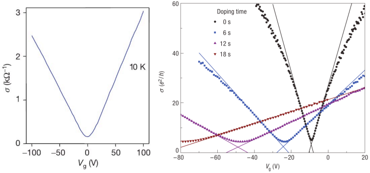
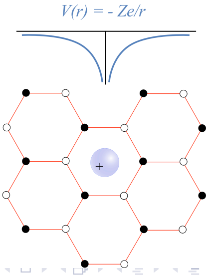


Fig. 1: Novoselov *et al.*, Nature 438; Chen *et al.* Nature Phys. 4.

Impurity Potential



Exact Solution of the Coulomb Problem in Graphene

$$\left(\boldsymbol{\sigma}.\boldsymbol{p} - \frac{\frac{Ze^2}{\hbar v_F}}{r} - \frac{E}{\hbar v_F}\right) = 0 \qquad \begin{pmatrix}\psi^A \\ \psi^B\end{pmatrix} = \frac{1}{\sqrt{r}}\begin{pmatrix} e^{i(j-\frac{1}{2})\varphi}\ \varphi_j^A(r) \\ ie^{i(j+\frac{1}{2})\varphi}\ \varphi_j^B(r)\end{pmatrix} \qquad \frac{\partial^2 f_\pm(r)}{\partial r^2} + \left[\epsilon^2 + \frac{2g\epsilon}{r} - \frac{\lambda(\lambda \mp 1)}{r^2}\right] f_\pm(r) = 0$$

$$g = \frac{Ze^2}{\hbar v_F} \qquad j = \pm\tfrac{1}{2},\ \pm\tfrac{3}{2},\ \ldots \qquad \lambda = \sqrt{j^2 - g^2}$$

The final solution is ($\tilde{g} = g\, s_\epsilon\,,\ \ \rho = |\epsilon| r$)

$$\varphi_j(r) = u_+ F_{\lambda-1}(-\tilde{g},\rho) + s_{g\epsilon} u_- F_\lambda(-\tilde{g},\rho), \qquad F_\lambda(\eta,\rho) = C_\lambda(\eta)\,\rho^{\lambda+1}\, e^{-i\rho}\,{}_1F_1(\lambda+1-i\eta;\ 2\lambda+2;\ 2i\rho) \qquad (5)$$

Index λ entails the existence of two strikingly different regimes $\left(\lambda = \sqrt{j^2 - g^2}, j = \pm\frac{1}{2}, \ldots\right)$

There is a critical coupling beyond which the particle "falls" onto the nucleus!!!

$$g_c = (Z\alpha)_c = \frac{1}{2}$$

Typically in graphene:

$$\alpha = \frac{e^2}{\varepsilon \hbar v_F} \sim 1 - 2 \quad \Rightarrow \quad Z_c \sim 1 \qquad (6)$$

Exact Solution of the Coulomb Problem in Graphene

$$\left(\boldsymbol{\sigma}.\boldsymbol{p} - \frac{\frac{Ze^2}{\hbar v_F}}{r} - \frac{E}{\hbar v_F}\right) = 0$$

$$g = \frac{Ze^2}{\hbar v_F}$$

$$\begin{pmatrix}\psi^A \\ \psi^B\end{pmatrix} = \frac{1}{\sqrt{r}}\begin{pmatrix} e^{i(j-\frac{1}{2})\varphi} & \varphi_j^A(r) \\ ie^{i(j+\frac{1}{2})\varphi} & \varphi_j^B(r)\end{pmatrix}$$

$$j = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots$$

$$\frac{\partial^2 f_\pm(r)}{\partial r^2} + \left[\epsilon^2 + \frac{2g\epsilon}{r} - \frac{\lambda(\lambda\mp 1)}{r^2}\right] f_\pm(r) = 0$$

$$\lambda = \sqrt{j^2 - g^2}$$

The final solution is ($\tilde{g} = g\, s_\epsilon\,,\ \ \rho = |\epsilon| r$)

$$\varphi_j(r) = u_+ F_{\lambda-1}(-\tilde{g},\rho) + s_{g\epsilon} u_- F_\lambda(-\tilde{g},\rho), \qquad F_\lambda(\eta,\rho) = C_\lambda(\eta)\,\rho^{\lambda+1}\,e^{-i\rho}\,{}_1F_1(\lambda+1-i\eta;\,2\lambda+2;\,2i\rho) \tag{5}$$

Index λ entails the existence of two strikingly different regimes $\left(\lambda = \sqrt{j^2-g^2}, j = \pm\frac{1}{2},\ldots\right)$

There is a critical coupling beyond which the particle "falls" onto the nucleus!!!

$$g_c = (Z\alpha)_c = \frac{1}{2}$$

Typically in graphene:

$$\alpha = \frac{e^2}{\varepsilon\hbar v_F} \sim 1-2 \quad\Rightarrow\quad Z_c \sim 1 \tag{6}$$

Exact Solution of the Coulomb Problem in Graphene

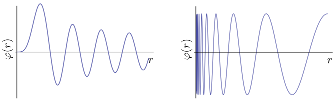
$$\left(\boldsymbol{\sigma}.\boldsymbol{p} - \frac{\frac{Ze^2}{\hbar v_F}}{r} - \frac{E}{\hbar v_F}\right) = 0 \qquad \begin{pmatrix}\psi^A \\ \psi^B\end{pmatrix} = \frac{1}{\sqrt{r}}\begin{pmatrix} e^{i(j-\frac{1}{2})\varphi}\ \varphi_j^A(r) \\ ie^{i(j+\frac{1}{2})\varphi}\ \varphi_j^B(r)\end{pmatrix} \qquad \frac{\partial^2 f_\pm(r)}{\partial r^2} + \left[\epsilon^2 + \frac{2g\epsilon}{r} - \frac{\lambda(\lambda\mp 1)}{r^2}\right] f_\pm(r) = 0$$

$$g = \frac{Ze^2}{\hbar v_F} \qquad j = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots \qquad \lambda = \sqrt{j^2 - g^2}$$

The final solution is ($\tilde{g} = g\, s_\epsilon\,,\ \ \rho = |\epsilon| r$)

$$\varphi_j(r) = u_+ F_{\lambda-1}(-\tilde{g}, \rho) + s_{g\epsilon} u_- F_\lambda(-\tilde{g}, \rho), \qquad F_\lambda(\eta, \rho) = C_\lambda(\eta)\, \rho^{\lambda+1}\, e^{-i\rho}\, {}_1F_1(\lambda + 1 - i\eta;\ 2\lambda + 2;\ 2i\rho) \tag{5}$$

Index λ entails the existence of two strikingly different regimes $\left(\lambda = \sqrt{j^2 - g^2}, j = \pm\frac{1}{2}, \ldots\right)$



$|g| < |j|$ $\qquad$ $|g| > |j|$

There is a critical coupling beyond which the particle "falls" onto the nucleus!!!

$$g_c = (Z\alpha)_c = \frac{1}{2}$$

Typically in graphene:

$$\alpha = \frac{e^2}{\varepsilon \hbar v_F} \sim 1 - 2 \quad \Rightarrow \quad Z_c \sim 1 \tag{6}$$

Exact Solution of the Coulomb Problem in Graphene

$$\left(\boldsymbol{\sigma}.\boldsymbol{p} - \frac{\frac{Ze^2}{\hbar v_F}}{r} - \frac{E}{\hbar v_F}\right) = 0$$

$$g = \frac{Ze^2}{\hbar v_F}$$

$$\begin{pmatrix}\psi^A\\ \psi^B\end{pmatrix} = \frac{1}{\sqrt{r}}\begin{pmatrix} e^{i(j-\frac{1}{2})\varphi}\,\varphi_j^A(r)\\ ie^{i(j+\frac{1}{2})\varphi}\,\varphi_j^B(r)\end{pmatrix}$$

$$j = \pm\tfrac{1}{2}, \pm\tfrac{3}{2}, \ldots$$

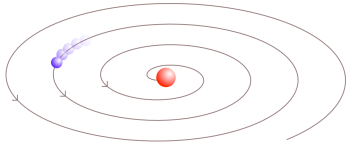
$$\frac{\partial^2 f_\pm(r)}{\partial r^2} + \left[\epsilon^2 + \frac{2g\epsilon}{r} - \frac{\lambda(\lambda\mp 1)}{r^2}\right] f_\pm(r) = 0$$

$$\lambda = \sqrt{j^2 - g^2}$$

The final solution is ($\tilde{g} = g\, s_\epsilon\,,\ \ \rho = |\epsilon| r$)

$$\varphi_j(r) = u_+ F_{\lambda-1}(-\tilde{g},\rho) + s_{g\epsilon} u_- F_\lambda(-\tilde{g},\rho), \qquad F_\lambda(\eta,\rho) = C_\lambda(\eta)\,\rho^{\lambda+1}\, e^{-i\rho}\, {}_1F_1(\lambda+1-i\eta;\, 2\lambda+2;\, 2i\rho) \tag{5}$$

Index λ entails the existence of two strikingly different regimes $\left(\lambda = \sqrt{j^2-g^2}, j = \pm\frac{1}{2}, \ldots\right)$



There is a critical coupling beyond which the particle "falls" onto the nucleus!!!

$$\mathbf{g_c} = (\mathbf{Z}\alpha)_\mathbf{c} = \frac{\mathbf{1}}{\mathbf{2}}$$

Typically in graphene:

$$\alpha = \frac{e^2}{\varepsilon\hbar v_F} \sim 1 - 2 \quad\Rightarrow\quad \boldsymbol{Z_c} \sim \mathbf{1} \tag{6}$$

Undercritical and Supercritical Regimes – LDOS

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon, \mathbf{r}) = \Psi^\dagger(\epsilon, \mathbf{r})\Psi(\epsilon, \mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon, \mathbf{r})$$

$$n_j(\epsilon, r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

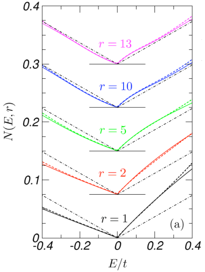


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

Profound spectrum rearrangement.

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon, \mathbf{r}) = \Psi^\dagger(\epsilon, \mathbf{r})\Psi(\epsilon, \mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon, \mathbf{r})$$

$$n_j(\epsilon, r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

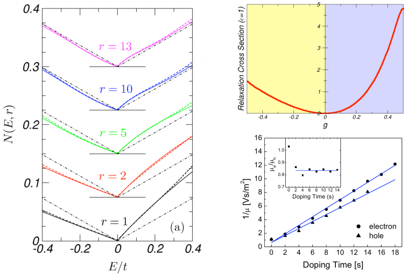


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

Profound spectrum rearrangement.

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon, \mathbf{r}) = \Psi^\dagger(\epsilon, \mathbf{r})\Psi(\epsilon, \mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon, \mathbf{r})$$

$$n_j(\epsilon, r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

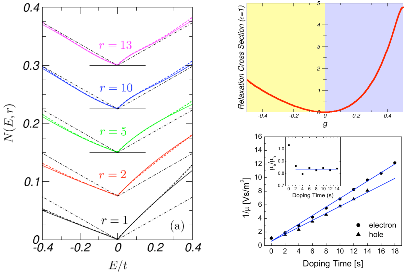


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

$$N(\epsilon, \mathbf{r}) = \sum_{|j|<|g|} \bar{n}_j(\epsilon, r) + \sum_{|j|>|g|} n_j(\epsilon, r)$$

Profound spectrum rearrangement.

Undercritical and Supercritical Regimes – LDOS

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon, \mathbf{r}) = \Psi^\dagger(\epsilon, \mathbf{r})\Psi(\epsilon, \mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon, \mathbf{r})$$

$$n_j(\epsilon, r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

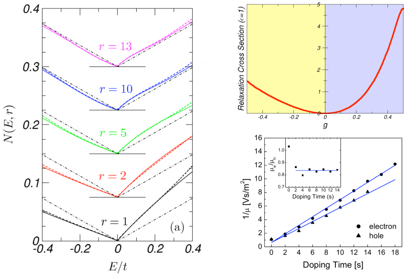


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

$$N(\epsilon, \mathbf{r}) = \qquad + \sum_{|j|>|g|} n_j(\epsilon, r)$$

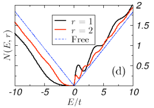


Fig. 4: **VM Pereira** *et al.*, PRL 07.

Profound spectrum rearrangement.

Undercritical and Supercritical Regimes – LDOS

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon,\mathbf{r}) = \Psi^\dagger(\epsilon,\mathbf{r})\Psi(\epsilon,\mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon,\mathbf{r})$$

$$n_j(\epsilon,r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

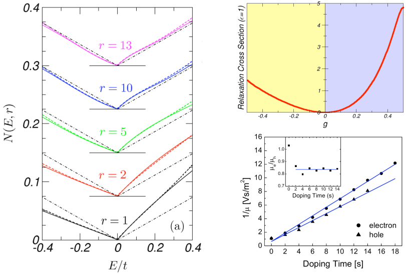


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

$$N(\epsilon,\mathbf{r}) = \sum_{|j|<|g|} \bar{n}_j(\epsilon,r)$$

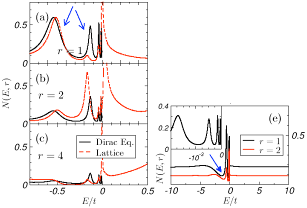


Fig. 4: **VM Pereira** *et al.*, PRL 07.

Profound spectrum rearrangement.

Undercritical and Supercritical Regimes – LDOS

Undercritical LDOS ($g < 1/2$)

$$N(\epsilon, \mathbf{r}) = \Psi^\dagger(\epsilon, \mathbf{r})\Psi(\epsilon, \mathbf{r}) = \sum_{j=-\infty}^{\infty} n_j(\epsilon, \mathbf{r})$$

$$n_j(\epsilon, r) = \frac{j^2}{2\pi^2\lambda^2 r}\left[F_{\lambda-1}^2 + F_\lambda^2 + 2\tilde{g}F_\lambda F_{\lambda-1}/|j|\right]$$

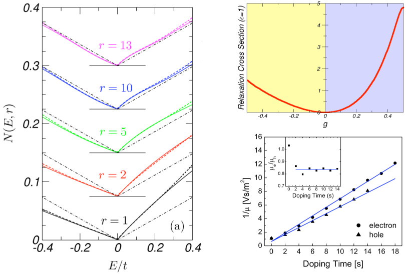


Fig. 3: **VM Pereira** PRL 07; Chen *et al.* Nature 08, Novikov PRB 07.

Weak particle-hole asymmetry.

Supercritical LDOS ($g > 1/2$)

$$N(\epsilon, \mathbf{r}) = \sum_{|j|<|g|} \bar{n}_j(\epsilon, r) + \sum_{|j|>|g|} n_j(\epsilon, r)$$

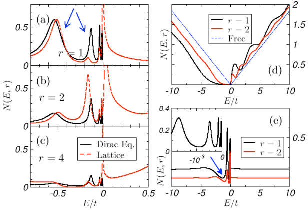
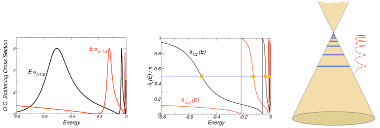


Fig. 4: **VM Pereira** *et al.*, PRL 07.



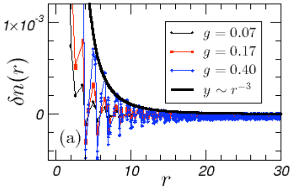
Profound spectrum rearrangement.

$$\delta\rho(\mathbf{r}) = \int_{-\Lambda}^{E_F}\left[N(\epsilon,\mathbf{r}) - N^0(\epsilon,\mathbf{r})\right]d\epsilon = \sum_{j=-\infty}^{\infty}\int_{-\Lambda}^{E_F}\left[n_j(\epsilon,\mathbf{r}) - n_j^0(\epsilon,\mathbf{r})\right]d\epsilon = \sum_{j=-\infty}^{\infty}\left[n_j(\mathbf{r}) - n_j^0(\mathbf{r})\right]d\epsilon \quad (7)$$

Undercritical ($g < g_c$)

$$\delta\rho(\mathbf{r}) = \frac{h_{\rm osc}(\Lambda r)}{r^3} \xrightarrow{a\to 0} \boxed{\delta\rho(\mathbf{r}) = Q\,\delta(\mathbf{r})}$$

Coulomb's law prevails: $Z_{\rm eff} = Z - Q$.



$$\delta\rho(q) =$$

$$= \frac{q}{4}\frac{2\pi Z\alpha}{q} = \frac{\pi}{2}Z\alpha \equiv Q$$

Supercritical ($g > g_c$)

$$\delta\rho(\mathbf{r}) = \frac{B}{r^2}$$

Coulomb's law changes.

† See also Shytov *et al.*, PRL 99, 236801 (2007), Kolezhuk *et al.*, PRB 74, 165114 (2006).

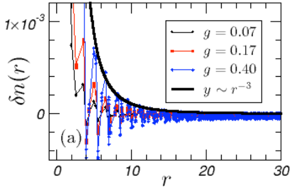
Induced Charge and Impurity Shielding†

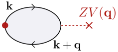
$$\delta\rho(\mathbf{r}) = \int_{-\Lambda}^{E_F} \left[N(\epsilon,\mathbf{r}) - N^0(\epsilon,\mathbf{r})\right] d\epsilon = \sum_{j=-\infty}^{\infty} \int_{-\Lambda}^{E_F} \left[n_j(\epsilon,\mathbf{r}) - n_j^0(\epsilon,\mathbf{r})\right] d\epsilon = \sum_{j=-\infty}^{\infty} \left[n_j(\mathbf{r}) - n_j^0(\mathbf{r})\right] d\epsilon \tag{7}$$

Undercritical ($g < g_c$)

$$\delta\rho(\mathbf{r}) = \frac{h_{\rm osc}(\Lambda r)}{r^3} \xrightarrow{a\to 0} \boxed{\delta\rho(\mathbf{r}) = Q\,\delta(\mathbf{r})}$$

Coulomb's law prevails: $Z_{\rm eff} = Z - Q$.



$\delta\rho(q) =$ 

$$= \frac{q}{4}\frac{2\pi Z\alpha}{q} = \frac{\pi}{2} Z\alpha \equiv Q$$

Supercritical ($g > g_c$)

$$\delta\rho(\mathbf{r}) = \frac{B}{r^2}$$

Coulomb's law changes.

† See also Shytov *et al.*, PRL 99, 236801 (2007), Kolezhuk *et al.*, PRB 74, 165114 (2006).

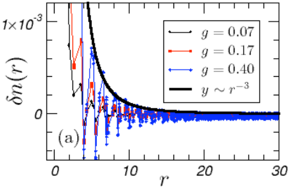
Induced Charge and Impurity Shielding†

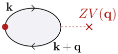
$$\delta\rho(\mathbf{r}) = \int_{-\Lambda}^{E_F} \left[N(\epsilon,\mathbf{r}) - N^0(\epsilon,\mathbf{r})\right] d\epsilon = \sum_{j=-\infty}^{\infty} \int_{-\Lambda}^{E_F} \left[n_j(\epsilon,\mathbf{r}) - n_j^0(\epsilon,\mathbf{r})\right] d\epsilon = \sum_{j=-\infty}^{\infty} \left[n_j(\mathbf{r}) - n_j^0(\mathbf{r})\right] d\epsilon \quad (7)$$

Undercritical ($g < g_c$)

$$\delta\rho(\mathbf{r}) = \frac{h_{osc}(\Lambda r)}{r^3} \xrightarrow{a\to 0} \boxed{\delta\rho(\mathbf{r}) = Q\,\delta(\mathbf{r})}$$

Coulomb's law prevails: $Z_{eff} = Z - Q$.



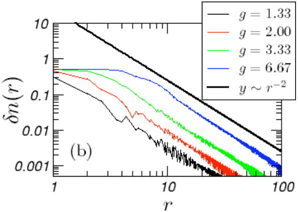
$$\delta\rho(q) =$$ 

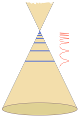
$$= \frac{q}{4}\frac{2\pi Z\alpha}{q} = \frac{\pi}{2} Z\alpha \equiv Q$$

Supercritical ($g > g_c$)

$$\delta\rho(\mathbf{r}) = \frac{B}{r^2}$$

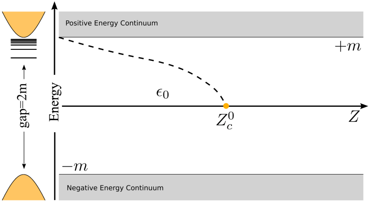
Coulomb's law changes.





† See also Shytov *et al.*, PRL 99, 236801 (2007), Kolezhuk *et al.*, PRB 74, 165114 (2006).

I. Diving states (Hydrogen atom in QED)

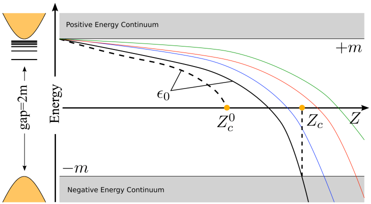


$$E_{nj} = mc^2 \left\{ 1 + \left[\frac{Z\alpha}{n + \sqrt{\kappa^2 - (Z\alpha)^2}} \right]^2 \right\}^{-1/2}$$

$$E_0 = mc^2 \sqrt{1 - (Z\alpha)^2}, \qquad (n = 0, \kappa = -1)$$

$$Z_C^0 = \frac{1}{\alpha} \approx 137$$

I. Diving states (Hydrogen atom in QED)



$$E_{nj} = mc^2 \left\{ 1 + \left[\frac{Z\alpha}{n + \sqrt{\kappa^2 - (Z\alpha)^2}} \right]^2 \right\}^{-1/2}$$

$$E_0 = mc^2 \sqrt{1 - (Z\alpha)^2}, \qquad (n = 0, \kappa = -1)$$

$$Z_C^0 = \frac{1}{\alpha} \approx 137$$

1971 г. Ноябрь Том 105, вып. 3

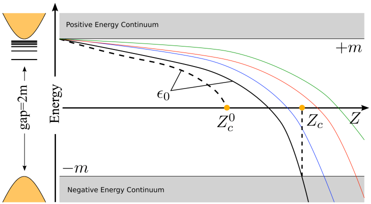
УСПЕХИ ФИЗИЧЕСКИХ НАУК

ЭЛЕКТРОННАЯ СТРУКТУРА СВЕРХТЯЖЕЛЫХ АТОМОВ

Я. Б. Зельдович, В. С. Попов

Gershtein, Popov, Zeldovich, Perolomov, Greiner, *et al.*
Electronic Structure Of Superheavy Atoms
Ya. B. Zeldovich *et al.*, Sov. Phys. Usp. 14 673 (1972)

I. Diving states (Hydrogen atom in QED)



$$E_{nj} = mc^2 \left\{ 1 + \left[\frac{Z\alpha}{n + \sqrt{\kappa^2 - (Z\alpha)^2}} \right]^2 \right\}^{-1/2}$$

$$E_0 = mc^2 \sqrt{1 - (Z\alpha)^2}, \qquad (n = 0, \kappa = -1)$$

$$Z_C^0 = \frac{1}{\alpha} \approx 137$$

1971 г. Ноябрь — Том 105, вып. 3

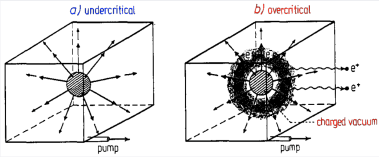
УСПЕХИ ФИЗИЧЕСКИХ НАУК

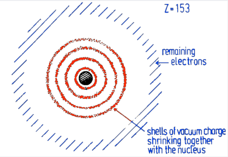
ЭЛЕКТРОННАЯ СТРУКТУРА СВЕРХТЯЖЕЛЫХ АТОМОВ

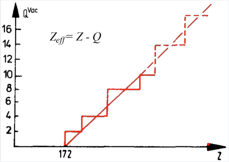
Я. Б. Зельдович, В. С. Попов

Gershtein, Popov, Zeldovich, Perolomov, Greiner, *et al.*
Electronic Structure Of Superheavy Atoms
Ya. B. Zeldovich *et al.*, Sov. Phys. Usp. 14 673 (1972)

II. Charged Vacuum — An yet untested prediction of QED under strong fields







Gapped Graphene and Critical Coupling Renormalization

Massive Dirac fermions in 2D

$$\hbar v_F \left(-i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} - \frac{g}{r} + \frac{m v_F}{\hbar} \sigma_z \right) \Psi(\mathbf{r}) = E\, \Psi(\mathbf{r})$$

$$E_0 = m\sqrt{1 - (2g)^2}\,, \quad \lambda_C = \hbar / m v_F$$

Diving State in Regularized Potential ($E \approx -m$)

$$|\psi_c^\dagger \psi_c| \propto r^{-1/2} \exp\left(-2\sqrt{8\tilde{g}_c\, r / \lambda_C} \right) \qquad (8)$$

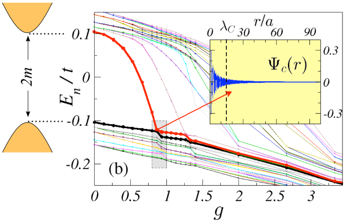
!! Localized State in the Continuum !!

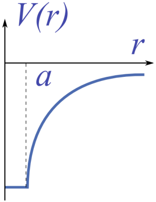
Critical Coupling Renormalization

- Extra diving from $E = 0$ to $E = -m$ delays the critical point.

$$\tilde{g}_c(ma) = g_c + \delta g_c(ma)$$

Diving Levels in the Lattice vs Dirac Eq.





Gapped Graphene and Critical Coupling Renormalization

Massive Dirac fermions in 2D

$$\hbar v_F \left(-i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} - \frac{g}{r} + \frac{m v_F}{\hbar} \sigma_z \right) \Psi(\mathbf{r}) = E \, \Psi(\mathbf{r})$$

$$E_0 = m\sqrt{1 - (2g)^2} \, , \quad \lambda_C = \hbar / m v_F$$

Diving State in Regularized Potential ($E \approx -m$)

$$|\psi_c^\dagger \psi_c| \propto r^{-1/2} \exp\left(-2\sqrt{8\tilde{g}_c \, r / \lambda_C} \right) \qquad (8)$$

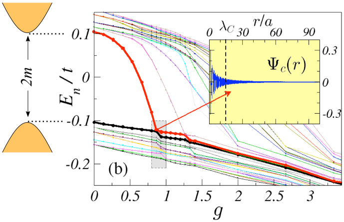
!! Localized State in the Continuum !!

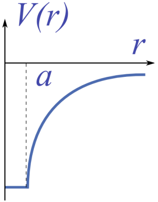
Critical Coupling Renormalization

- Extra diving from $E = 0$ to $E = -m$ delays the critical point.

$$\tilde{g}_c(ma) = g_c + \delta g_c(ma)$$

Diving Levels in the Lattice vs Dirac Eq.





Massive Dirac fermions in 2D

$$\hbar v_F \left(-i\boldsymbol{\sigma} \cdot \boldsymbol{\nabla} - \frac{g}{r} + \frac{m v_F}{\hbar} \sigma_z \right) \Psi(\mathbf{r}) = E\, \Psi(\mathbf{r})$$

$$E_0 = m\sqrt{1 - (2g)^2}\,, \quad \lambda_C = \hbar / m v_F$$

Diving State in Regularized Potential ($E \approx -m$)

$$|\psi_c^\dagger \psi_c| \propto r^{-1/2} \exp\left(-2\sqrt{8\tilde{g}_c\, r/\lambda_C} \right) \quad (8)$$

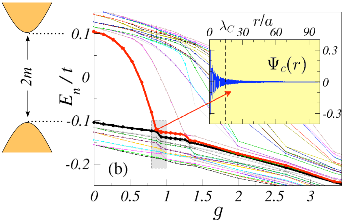
!! Localized State in the Continuum !!

Critical Coupling Renormalization

- Extra diving from $E = 0$ to $E = -m$ delays the critical point.

$$\tilde{g}_c(ma) = g_c + \delta g_c(ma)$$

Diving Levels in the Lattice vs Dirac Eq.



Critical Coupling Renormalization

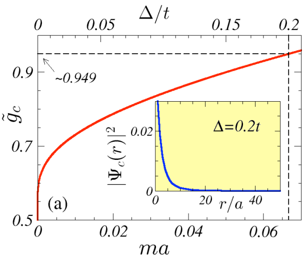


Fig. 5: **VM Pereira** *et al.* PRB 78, 085101 (2008).

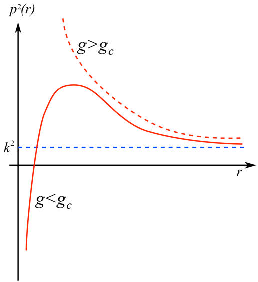
Semiclassical action and momentum ("WKB")

$$E^2 = p^2 + m^2 \quad \rightarrow \quad (E - V)^2 = p^2 + m^2 \tag{9}$$

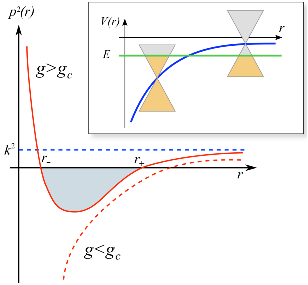
$$p^2 = p_r^2 + \frac{l^2}{r^2} = (E - V)^2 - m^2 \tag{10}$$

$$\boxed{p_r^2 = k^2 + \frac{2gE}{r} + \frac{g^2 - l^2}{r^2}} \tag{11}$$

Particle States ($E > 0$)



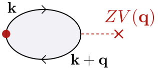
Hole States ($E < 0$)



Induced Charge and Vacuum Polarization

As before, we compute the induced charge:

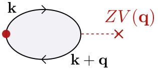
$$\delta\rho(\mathbf{r}) = \sum_{E \le E_F} |\Psi_E(\mathbf{r})|^2 - \sum_{E \le -m} |\Psi_E^0(\mathbf{r})|^2 \simeq \boxed{|\Psi^c(\mathbf{r})|^2 + \delta\rho_{\text{pol}}(\mathbf{r})}, \qquad \delta\rho_{\text{pol}}(\mathbf{r}) = \tag{12}$$



where $\delta\rho_{\text{pol}}(\mathbf{r})$ represents the polarization charge caused by the deformation of the continuum wavefunctions.

As before, we compute the induced charge:

$$\delta\rho(\mathbf{r}) = \sum_{E\leq E_F} |\Psi_E(\mathbf{r})|^2 - \sum_{E\leq -m} |\Psi_E^0(\mathbf{r})|^2 \simeq \boxed{|\Psi^c(\mathbf{r})|^2 + \delta\rho_{\mathrm{pol}}(\mathbf{r})}, \qquad \delta\rho_{\mathrm{pol}}(\mathbf{r}) = \tag{12}$$



where $\delta\rho_{\mathrm{pol}}(\mathbf{r})$ represents the polarization charge caused by the deformation of the continuum wavefunctions.

Gapped System ($\Delta = 0.2t$)

Polarization charge inside R:

$$Q(R) = N \int_{|\mathbf{r}|<R} \delta\rho(\mathbf{r}) d\mathbf{r} \, .$$

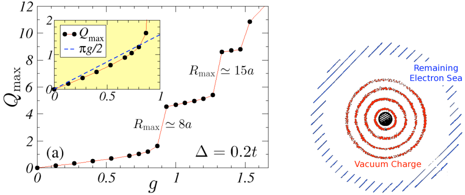
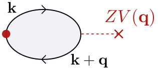


Fig. 6: **VM Pereira** *et al.* PRB 78, 085101 (2008).

As before, we compute the induced charge:

$$\delta\rho(\mathbf{r}) = \sum_{E\le E_F} |\Psi_E(\mathbf{r})|^2 - \sum_{E\le -m} |\Psi_E^0(\mathbf{r})|^2 \simeq \boxed{|\Psi^c(\mathbf{r})|^2 + \delta\rho_{\text{pol}}(\mathbf{r})}\,, \qquad \delta\rho_{\text{pol}}(\mathbf{r}) = \tag{12}$$

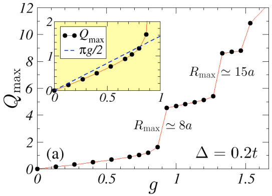


where $\delta\rho_{\text{pol}}(\mathbf{r})$ represents the polarization charge caused by the deformation of the continuum wavefunctions.

Gapped System ($\Delta = 0.2t$)

Polarization charge inside R:

$$Q(R) = N \int_{|\mathbf{r}|<R} \delta\rho(\mathbf{r}) d\mathbf{r}\,.$$



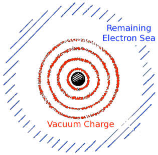
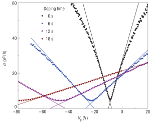


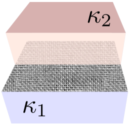
Fig. 6: **VM Pereira** *et al.* PRB 78, 085101 (2008).

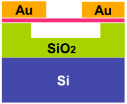
Massless graphene constitutes a nontrivial limit: an *ultra* critical situation where ∞ bound levels have penetrate the continuum at once beyond g_c.

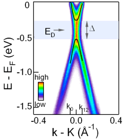
One needs to address/control several physical parameters, namely

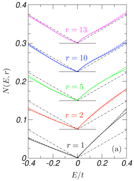
- Coulomb impurities in a controlled way:
  - ✓ Chen *et al.* Nature Phys. 4 (08).
- Tune impurity valence ($Z\alpha > g_c$):
  - ✓ Jang *et al.* arXiv:0805.3780.
  - ✓ Mohiuddin *et al.* arXiv:0809.1162.
  - ✓ X. Du *et al.* arXiv:0802.2933.
  - ✓ Bolotin *et al.* PRL 101, 096802 (2008)
- Generate a gap:
  - ✓ Zhou *et al.* Nature Mat. 6, 770 (07).
  - ✓ Gruneis *et al.* PRB 77, 193401 (08).
  - ✓ Li *et al.* arXiv:0803.4016.

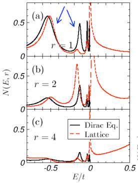


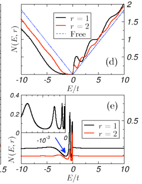


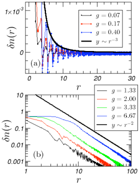


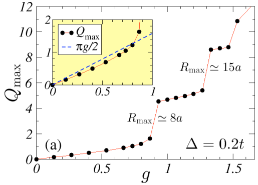












PRL ***99****, 166802 (2007); PRB* ***78****, 075433 (2008); PRB* ***78****, 085101 (2008)*

The Role of Interactions

Radiative corrections in QED

1. Vacuum polarization
   Negative Lamb shift: $\Delta Z_c \sim -\alpha Z_c$
2. Self-energy
   Positive Lamb shift: $\Delta Z_c \sim +\alpha Z_c$

The Role of Interactions

Radiative corrections in QED

1. Vacuum polarization
   Negative Lamb shift: $\Delta Z_c \sim -\alpha Z_c$
2. Self-energy
   Positive Lamb shift: $\Delta Z_c \sim +\alpha Z_c$

Key issues

1. Unlike QED, $\alpha \sim 1$ (cfr. $\alpha \sim 0.007$);
2. Unlike QED, $Q \approx Z_{\text{cr}} \sim 1$ (cfr. $Q \ll Z_{\text{cr}}$);

There is a strong tendency for over-screening

...and therefore one might need to investigate the role of interactions.

The Role of Interactions

Radiative corrections in QED

1. Vacuum polarization
   Negative Lamb shift: $\Delta Z_c \sim -\alpha Z_c$
2. Self-energy
   Positive Lamb shift: $\Delta Z_c \sim +\alpha Z_c$

Key issues

1. Unlike QED, $\alpha \sim 1$ (cfr. $\alpha \sim 0.007$);
2. Unlike QED, $Q \approx Z_{cr} \sim 1$ (cfr. $Q \ll Z_{cr}$);

There is a strong tendency for over-screening

...and therefore one might need to investigate the role of interactions.

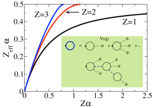
1. Non-linear screening [A. Shytov *et al.*, PRL 99 236801 (2007)].

$$g(r) \to g_c \,, \quad \left[\; r > r^* \sim a(1 + \sqrt{g - g_c}) \;\right]$$

"supercritical protection".

2. Self consistent effective valence – Hartree correction, [Terekhov *et al.*, PRL 100,76803 (2008)].

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



3. Other non-linear, non-perturbative effects
   M. Katsnelson, PRB 74 201401 (2006), M. Fogler *et al.*, PRB 76 233402 (2007).