SPATIALLY INHOMOGENEOUS STATES OF CHARGE CARRIERS IN GRAPHENE

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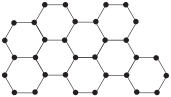
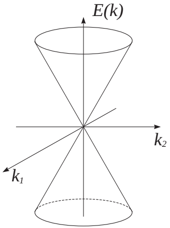
Basics

The effective massless Dirac Hamiltonian for graphene and conical dispersion relation near K-point

$$\widehat{\mathcal{H}} = u\boldsymbol{\sigma}\hat{\mathbf{p}} \quad \Rightarrow \quad E(\mathbf{p}) = \pm u|\mathbf{p}|, \quad u \sim 10^6 \mathrm{m/sec}$$

$\boldsymbol{\sigma} = (\sigma_1, \sigma_2) \rightarrow$ Pauli matrices, $\hat{\mathbf{p}} = -i\hbar\nabla$, $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y})$



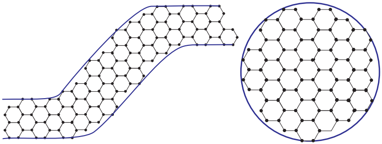


[*]K.S.Novoselov,A.K.Geim,et al.,*Science*,**306**,666(2004)
[*]V.V.Cheianov, V.I.Falko, Phys.Rev.B**74**,041403(2006)

Waveguides and quantum dots

The effective Hamiltonian

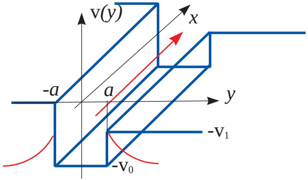
$$\widehat{\mathcal{H}} = u(\boldsymbol{\sigma}\hat{\mathbf{p}}) + v(x,y)$$



$v(x,y) \rightarrow$ the confinement potential, simulated "walls"

Straight quasi-1D waveguide with stepped potential

$$\widehat{\mathcal{H}} \begin{pmatrix} \chi_1^{\nu}(y) \\ \chi_2^{\nu}(y) \end{pmatrix} e^{ikx} = E^{\nu}(k) \begin{pmatrix} \chi_1^{\nu}(y) \\ \chi_2^{\nu}(y) \end{pmatrix} e^{ikx}$$



$k \rightarrow$ the longitudinal momentum

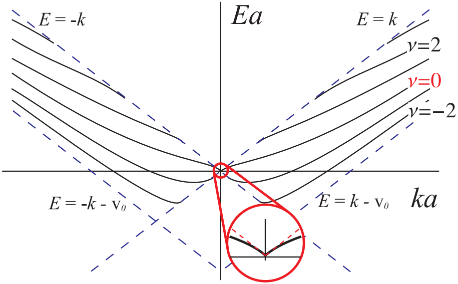
$\nu \rightarrow$ the number of the transversal subband

[*]J.Milton Pereira et al.,Phys.Rev.B **74**, 045424(2006)

The equation, determining the dispersion relations $\mathbf{E} = \mathbf{E}^{\nu}(\mathbf{k})$ for symmetric well:

$$[E(E+v_0)-k^2]\sin(2qa)-\varkappa q\cos(2qa)=0.$$

$$\varkappa=\sqrt{k^2-E^2},\ q=\sqrt{(E+v_0)^2-k^2}$$



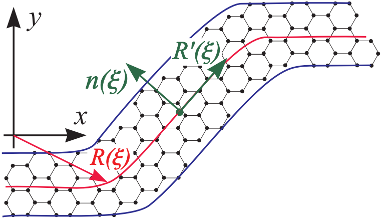
Linear dispersion for small k, $\cos(2v_0a)\neq 0$:

$$E^0(k)=|\mathbf{k}|\,\mathrm{sign}\{\sin(2v_0a)\}\cos(2v_0a).$$

1D-equation in curved stripe

$$(x, y) \to (\xi, \eta), \qquad \mathbf{r} = \mathbf{R}(\xi) + \eta \mathbf{n}(\xi), \qquad G = (1 - s(\xi)\eta)^2$$

$\xi \to$ longitudinal (length), $\eta \to$ transversal coordinate
$\mathbf{R}(\xi) \to$ the axis, $|\mathbf{R}'(\xi)| = 1$, $\mathbf{n}(\xi) \perp \mathbf{R}'(\xi)$, $|\mathbf{n}(\xi)| = 1$
$s(\xi) \to$ the curvature of the axis of the waveguide



$$\widehat{\mathcal{H}}_{curv} = \frac{1}{\sqrt[4]{G}} \widehat{\mathcal{H}} \sqrt[4]{G} = -\frac{(\boldsymbol{\sigma}\mathbf{R}')}{\sqrt[4]{G}} \frac{i\partial}{\partial \xi} \frac{1}{\sqrt[4]{G}} - (\boldsymbol{\sigma}\mathbf{n}) \frac{i\partial}{\partial \eta} - \frac{is(\xi)(\boldsymbol{\sigma}\mathbf{n})}{2\sqrt{G}} + v(\eta)$$

Adiabatically curved stripe, i.e. $s(\xi) \to 0$:

$$\widehat{\mathcal{H}}_{curv} \begin{pmatrix} \hat{\chi}_1 \\ \hat{\chi}_2 \end{pmatrix} \psi^\nu(\xi) = \varepsilon^\nu \begin{pmatrix} \hat{\chi}_1 \\ \hat{\chi}_2 \end{pmatrix} \psi^\nu(\xi)$$

$$[E^\nu(\hat{k}) + \hat{L}^\nu]\psi^\nu(\xi) = \varepsilon^\nu \psi^\nu(\xi), \qquad \hat{k} = -i\partial/\partial\xi$$

$E^\nu(\hat{k}) + \hat{L}^\nu \to$ the longitudinal Hamiltonian
$E^\nu(\hat{k}) \to$ "quantized" dispersion relation, $\hat{L}^\nu \to$ corrections
$\psi^\nu(\xi) \to$ the effective longitudinal wavefunction

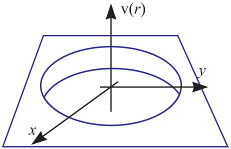
Effective equation for small momenta

$$\mathrm{sign}\{\sin(2v_0 a)\}\mathrm{sign}\{\hat{k}\} \left(-i\frac{\partial}{\partial\xi} + \frac{s(\xi)}{2}\right) \psi^0 = E^0 \psi^0$$

$v_{geom}(\xi) = s(\xi)/2 \to$ "geometric" potential, **no boundstates**
Quadratic dispersion: $v_{geom}(\xi) = -s^2(\xi)/4$, **boundstates**

Model of a quantum dot

$v(r) = -v_0$ if $r < a$, $v(r) = 0$ if $r \geq a$:



Cylindrical coordinates $x = r\cos\varphi$, $y = r\sin\varphi$

$$\widehat{\mathcal{H}} \begin{pmatrix} \chi_1(r)e^{in\varphi} \\ \chi_2(r)e^{i(n+1)\varphi} \end{pmatrix} = E \begin{pmatrix} \chi_1(r)e^{in\varphi} \\ \chi_2(r)e^{i(n+1)\varphi} \end{pmatrix}$$

$$\left\{ -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} + \frac{n^2}{r^2} - E^2 \right\} \chi_1 = 0, \quad r \geq a.$$

$\chi_1 = J_n(|\mathbf{E}|r), N_n(|\mathbf{E}|r) \Rightarrow$ **2D localization is impossible**

Scattering problem

Scattering state for the "particle" with positive energy

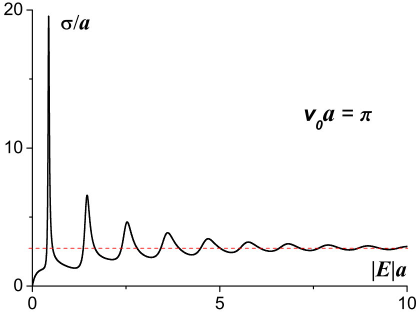
$$\Psi \to \frac{e^{i|E|r\cos\varphi}}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{e^{i|E|r}}{\sqrt{r}} \begin{pmatrix} f_1(\varphi) \\ f_2(\varphi) \end{pmatrix}, \quad r \to \infty.$$

Total cross section $\sigma(|E|)$

- demonstrates **resonance behavior**,
- **tends to a constant** when $|E|a \to \infty$.

Born approx. $(v_0 a \ll 1)$:

$$\sigma \to 16 v_0^2 a^3 / 3.$$



Quadratic dispersion: $\sigma \to 0$ when $|E|a \to \infty$

Conclusions

- **1D localization** in straight graphene waveguides **is possible**
- For the waveguide with symmetric stepped potential **the dispersion relation** at small longitudinal momenta **is linear**
- **The geometric potential** in the adiabatically curved graphene waveguide **cannot form boundstates**
- **2D localization** in a cylindrically symmetric quantum dot in graphene **is impossible**
- **The total crossection** of the scattering by the considered well demonstrates a **resonance behavior**

[*] T.Tudorovskiy, A.Chaplik, *JETP Lett.*, **84**, 11 (2006), 619–623

THANK YOU FOR YOUR ATTENTION!