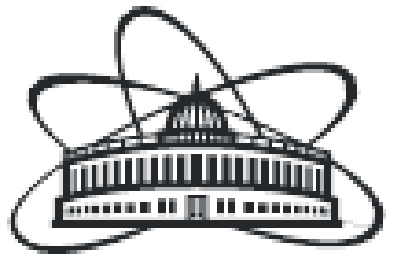

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"The Actual Problems of Microworld Physics"

Relativistic quantum-mechanical description and new properties of a graphene electron in external fields and free (2+1)-space

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OUTLINE

- Foldy-Wouthuysen transformation in (2+1)-space
- Foldy-Wouthuysen Hamiltonian for the planar graphene electron in electric and magnetic fields
- Pauli matrices vs Dirac matrices
- Exact solution for the planar graphene electron in a uniform magnetic field
- Multiwave Hermite-Gauss beams of graphene electrons in the free space
- Summary

Foldy-Wouthuysen transformation in (2+1)-space

$$\mathcal{H} = \beta\mathcal{M} + \mathcal{E} + \mathcal{O}, \quad \beta\mathcal{M} = \mathcal{M}\beta, \quad \beta\mathcal{E} = \mathcal{E}\beta, \quad \beta\mathcal{O} = -\mathcal{O}\beta$$

$$U = \frac{1 + \sqrt{1 + X^2} + \beta X}{\sqrt{2\sqrt{1 + X^2}(1 + \sqrt{1 + X^2})}} \qquad X = \left\{ \frac{1}{2\mathcal{M}}, \mathcal{O} \right\}.$$

$$\mathcal{H}_{FW} = \beta\epsilon + \mathcal{E} + \frac{1}{4}\left\{ \frac{1}{2\epsilon^2 + \{\epsilon, \mathcal{M}\}}, (\beta[\mathcal{O},[\mathcal{O},\mathcal{M}]] - [\mathcal{O},[\mathcal{O},\mathcal{F}]]) \right\}.$$

$$\mathcal{F} = \mathcal{E} - i\hbar\frac{\partial}{\partial t}$$

Relativistic Foldy-Wouthuysen (FW) transformation in (2+1)- and (3+1)-spaces is the same. *U* is the transformation operator. The method used is the only method giving an exact form of leading operators of the zero and first orders in $\hbar$. $\mathcal{M}$ and $\mathcal{E}$ are even terms and $\mathcal{O}$ is an odd term.

A.J. Silenko, J. Math. Phys. **44**, 2952 (2003); Phys. Rev. A **91**, 022103 (2015).

Foldy-Wouthuysen Hamiltonian for the planar graphene electron in electric and magnetic fields

Conventional choice:

$$\gamma^{\mu} = \left(\gamma^0, \gamma^1, \gamma^2\right) = \left(\sigma^3, i\sigma^1, i\sigma^2\right), \ \sigma^i \text{ are Pauli matrices}$$

$$\left\{\gamma^{\mu}, \gamma^{\nu}\right\} = 2\eta^{\mu\nu} = \text{diag}\left(1, -1, -1\right)$$

Dirac equation:

$$i\gamma^{\mu}\left(\partial_{\mu} + ieA_{\mu}\right)\psi = m\psi = 0, \qquad \mathbf{p} = -i\hbar\left(\frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}\right).$$

$$\left[\gamma^0\left(p_0 - eA_0\right) - \boldsymbol{\gamma}\cdot\left(\mathbf{p} - e\mathbf{A}\right) + m\right]\psi = 0, \ p_0 = \mathcal{H}, \ \boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}.$$

$$\mathcal{H}\psi = \left(\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + \beta m + eA_0\right)\psi, \ \beta = \gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3, \ \alpha^1 = -\sigma_2, \ \alpha^2 = \sigma_1.$$

In this equation:

$$\mathcal{M} = m, \ \mathcal{E} = eA_0, \ \mathcal{O} = \boldsymbol{\alpha}\cdot\boldsymbol{\pi}.$$

Dirac equation in the Foldy-Wouthuysen representation:

$$\mathcal{H}_{FW} = \beta\varepsilon + eA_0 + \frac{e}{8}\left\{\frac{1}{\varepsilon\left(\varepsilon + m\right)}, \sigma_3\left(\boldsymbol{\pi}\times\mathbf{E} - \mathbf{E}\times\boldsymbol{\pi}\right)_3\right\}, \ \varepsilon = \sqrt{m^2 + \boldsymbol{\pi}^2 - \sigma_3 B}.$$

Alternative choice:

The original Dirac matrices can be used

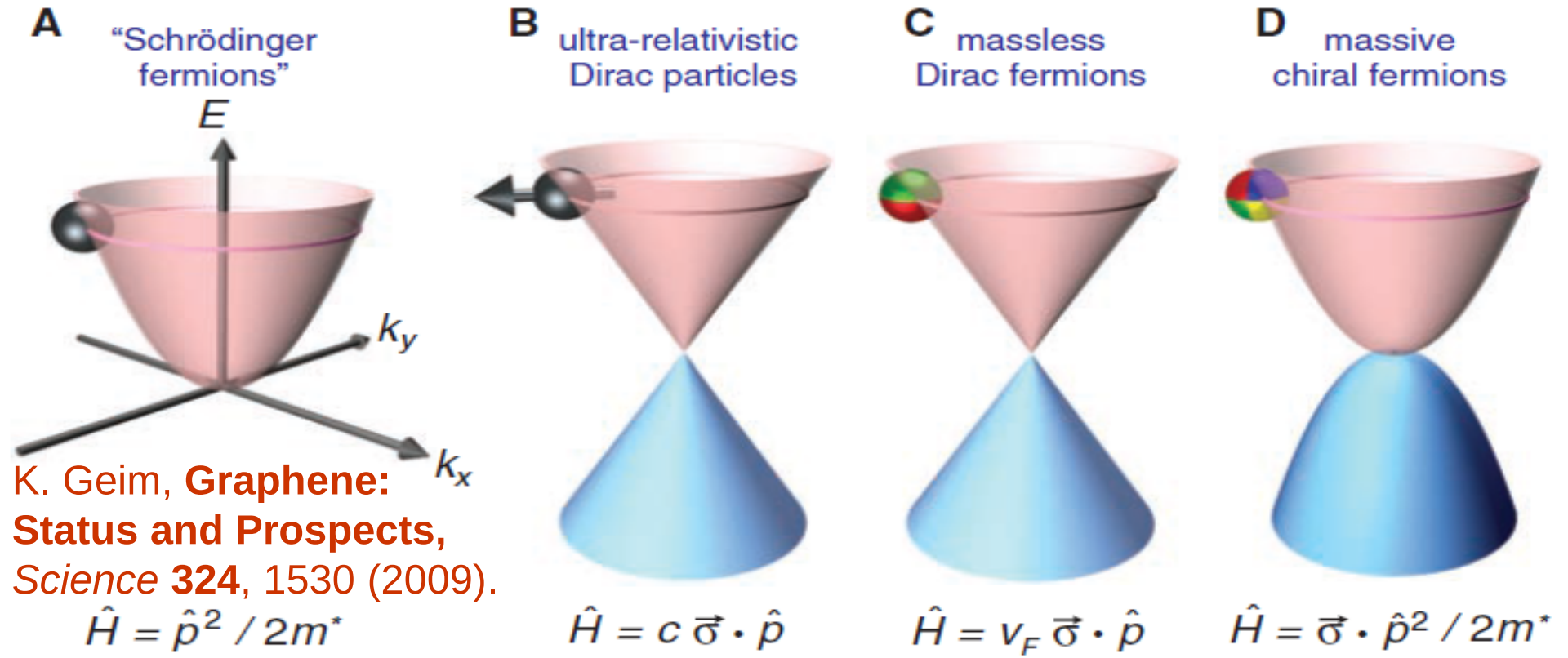
Y. E. Lozovik, S. P. Merkulova and A. A. Sokolik, Collective electron phenomena in graphene, Phys.-Usp. 51, 727 (2008).

When the original Dirac matrices are utilized, the relativistic FW Hamiltonian has the form

$$\mathcal{H}_{FW} = \beta\epsilon + eA_0 + \frac{e}{8}\left\{\frac{1}{\epsilon(\epsilon+m)}, \Sigma_3(\boldsymbol{\pi}\times\boldsymbol{E} - \boldsymbol{E}\times\boldsymbol{\pi})_3\right\}, \qquad \epsilon = \sqrt{m^2+\boldsymbol{\pi}^2 - e\Sigma_3 B}.$$

In this case, the spin can have two values for any (positive and negative) energy.

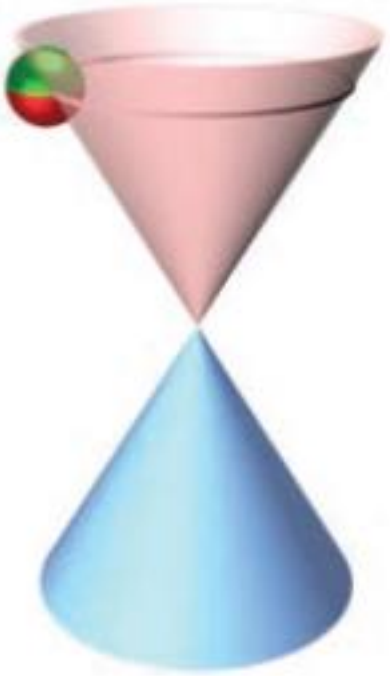
Pauli matrices vs Dirac matrices



K. Geim, **Graphene: Status and Prospects,** *Science* **324**, 1530 (2009).

Fig. 2. Quasi-particle zoo. (**A**) Charge carriers in condensed matter physics are normally described by the Schrödinger equation with an effective mass m^* different from the free electron mass ($\hat{p}$ is the momentum operator). (**B**) Relativistic particles in the limit of zero rest mass follow the Dirac equation, where c is the speed of light and $\vec{\sigma}$ is the Pauli matrix. (**C**) Charge carriers in graphene are called massless Dirac fermions and are described by a 2D analog of the Dirac equation, with the Fermi velocity $v_F \approx 1 \times 10^6$ m/s playing the role of the speed of light and a 2D pseudospin matrix $\vec{\sigma}$ describing two sublattices of the honeycomb lattice (*3*). Similar to the real spin that can change its direction between, say, left and right, the pseudospin is an index that indicates on which of the two sublattices a quasi-particle is located. The pseudospin can be indicated by color (e.g., red and green). (**D**) Bilayer graphene provides us with yet another type of quasi-particles that have no analogies. They are massive Dirac fermions described by a rather bizarre Hamiltonian that combines features of both Dirac and Schrödinger equations. The pseudospin changes its color index four times as it moves among four carbon sublattices (*2*–*4*).

C massless Dirac fermions



$$\hat{H} = v_F \vec{\sigma} \cdot \hat{p}$$

K. Geim, **Graphene: Status and Prospects,** *Science* **324**, 1530 (2009).

(**C**) Charge carriers in graphene are called massless Dirac fermions and are described by a 2D analog of the Dirac equation, with the Fermi velocity $v_F \approx 1 \times 10^6$ m/s playing the role of the speed of light and a 2D pseudospin matrix $\vec{\sigma}$ describing two sublattices of the honeycomb lattice (*3*). Similar to the real spin that can change its direction between, say, left and right, the pseudospin is an index that indicates on which of the two sublattices a quasi-particle is located. The pseudospin can be indicated by color (e.g., red and green).

Electromagnetic field and angular momentum tensors in (2+1)-space

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 \\ -E_1 & 0 & -B \\ -E_2 & B & 0 \end{pmatrix} = (\mathbf{E}, B), \quad F_{\mu\nu} = \frac{\partial A_\mu}{\partial x^\nu} - \frac{\partial A_\nu}{\partial x^\mu}.$$

$$L^{\mu\nu} = \sum \begin{pmatrix} 0 & -K_1 & -K_2 \\ K_1 & 0 & L \\ K_2 & -L & 0 \end{pmatrix} = (-\mathbf{K}, -L) = \left(\sum \left(ct\mathbf{p} - \frac{\mathscr{E}\mathbf{r}}{c} \right), -L \right),$$

$$L^{\mu\nu} = x^\mu p^\nu - x^\nu p^\mu.$$

***B* and *L* (and, therefore, the spin) are numbers, positive and negative. As a result, the spin should have two components, +1/2 and -1/2.**

As a result, the use of the Pauli matrices is unsatisfactory!

Exact solution for the planar graphene electron in a uniform magnetic field

For the reduced spin matrices, the relativistic FW Hamiltonian takes the form

$$\mathcal{H}_{FW} = \sigma_3 \sqrt{m^2 + \boldsymbol{\pi}^2 - e\sigma_3 B}.$$

This equation can be presented as follows:

$$\mathcal{H}_{FW} = \begin{pmatrix} \sqrt{m^2 + \boldsymbol{\pi}^2 - eB} & 0 \\ 0 & -\sqrt{m^2 + \boldsymbol{\pi}^2 + eB} \end{pmatrix}.$$

The Dirac equation with the reduced matrices does not describe the true spin. It follows from these equations that, in particular, a spin-1/2 particle in positive-energy states has only one spin value. Such a spin is not an additional degree of freedom.

Quantum mechanics with the Dirac matrices

In the magnetic field only

$$\mathcal{H}_{FW} = \beta\sqrt{m^2 + \boldsymbol{\pi}^2 - \Sigma_3 B}.$$

In this case, the spin has two values for any (positive and negative) energy.

In the FW representation (positive energies), the exact equation in any static uniform or nonuniform magnetic field reads

$$\mathcal{H}_{FW} = \sqrt{m^2 + \boldsymbol{\pi}^2 - \sigma_3 B}.$$

For the uniform magnetic field, m=0, **and symmetric gauge** $A_\phi = Br/2$, $A_r = 0$,

$$-\nabla_\perp^2 + ieB\frac{\partial}{\partial\phi} + \frac{e^2B^2r^2}{4} - 2esB = \mathcal{E}^2, \quad \nabla_\perp^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}.$$

The exact wave eigenfunctions are the well-known eigenfunctions of the operator $\boldsymbol{\pi}^2$ with the symmetric gauge. They are based on the Laguerre polynomials:

$$\Phi_{FW} = \mathcal{A}\exp(i\ell\phi) \qquad \int \Phi_{FW}^\dagger \Phi_{FW} r\,dr\,d\phi = 1,$$

$$\mathcal{A} = \frac{C_{n\ell}}{w_m}\left(\frac{\sqrt{2}\,r}{w_m}\right)^{|\ell|} L_n^{|\ell|}\left(\frac{2r^2}{w_m^2}\right)\exp\left(-\frac{r^2}{w_m^2}\right)\eta, \qquad C_{n\ell} = \sqrt{\frac{2n!}{\pi(n+|\ell|)!}}, \qquad w_m = \frac{2}{\sqrt{|e|B}}$$

The energy spectrum for the zero mass is given by

$$\mathcal{E} = \sqrt{(2n + 1 + |l| + l + 2s)|e|B}, \quad s = \pm 1/2.$$

For the uniform magnetic field, m=0, **and the formed Landau gauge** A_x=-By, A_y=0,

$$-\nabla_\perp^2 + 2ieBy\frac{\partial}{\partial x} + e^2B^2y^2 - 2esB = \mathcal{E}^2, \quad \nabla_\perp^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

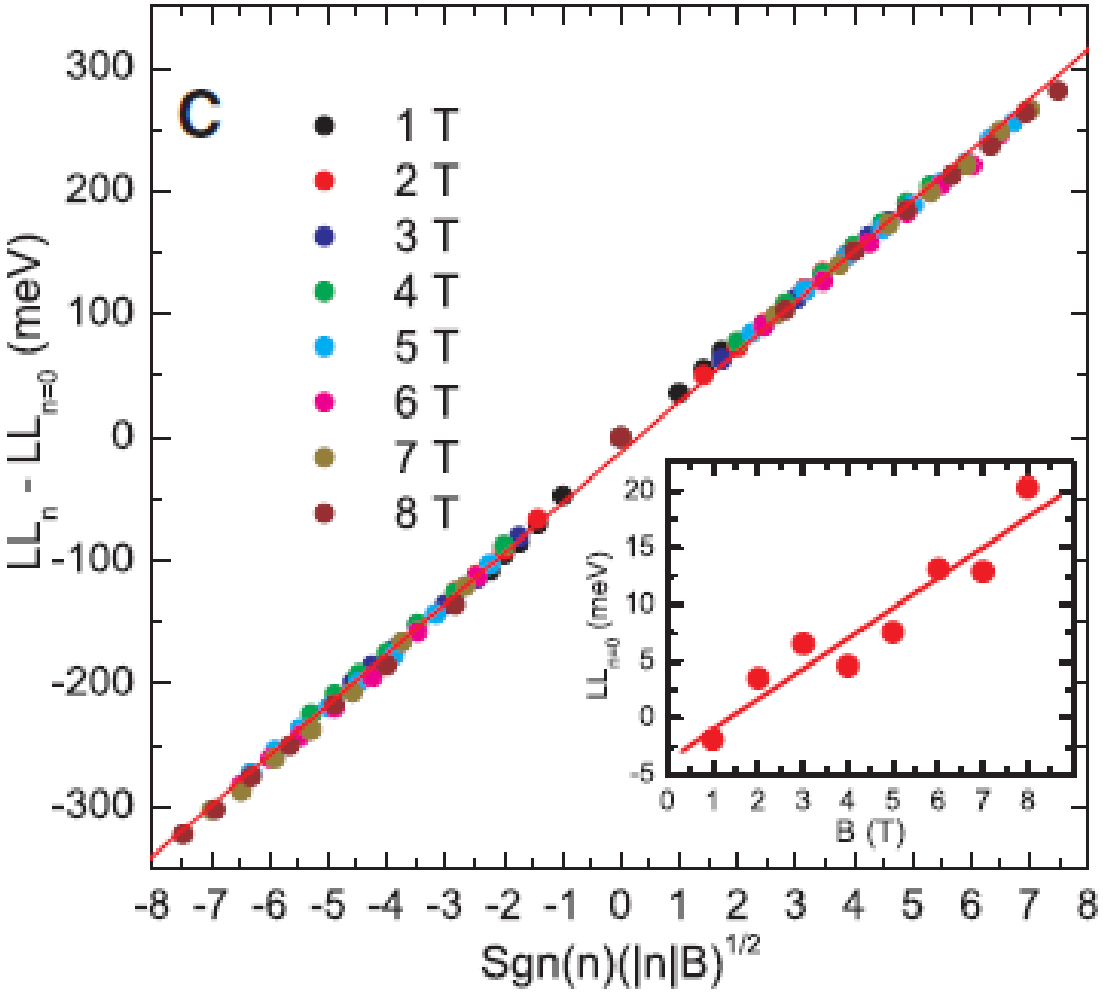
The exact wave eigenfunctions are the well-known eigenfunctions of the operator $\boldsymbol{\pi}^2$ with the former Landau gauge. They are based on the Hermite polynomials:

$$\chi_n(y) = \frac{1}{\pi^{1/4}a_H^{1/2}\sqrt{(2^n n!)}} \exp\left[-\frac{(y-y_0)^2}{2a_H^2}\right] H_n\left(\frac{y-y_0}{a_H}\right),$$

$$\psi = \exp(ip_x x)\chi(y), \quad y_0 = -\frac{p_x}{eB}, \quad \nabla_\perp^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

The energy spectrum for the zero mass is the same:

$$\mathcal{E} = \sqrt{(2n+1+2s)|e|B}, \quad s = \pm 1/2.$$



(**C**) LL peak energies for applied fields of 1 to 8 T, showing a collapse of the data when plotted versus square root of LL index and applied field. The solid line shows a linear fit yielding a characteristic velocity of $c^* = (1.128 \pm 0.004) \times 10^6$ ms^{-1} (*20*). (Inset) The shift in the LL_0 peak position as a function of applied field (symbols). The error is smaller than the symbol size. The solid line is a linear fit to the data points.

D. L. Miller *et al.,* Observing the Quantization of Zero Mass Carriers in Graphene**,** Science **324**, 924 (2009).
F. D. M. Haldane, Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly”, Phys. Rev. Lett. **61,** 2015 (1988).
R. Jackiw, Fractional charge and zero modes for planar systems in a magnetic field, Phys. Rev. D **29**, 2375 (1984).

Multiwave Hermite-Gauss beams of graphene electrons in the free space

Multiwave Hermite-Gauss beam in the free space are well-known (in the paraxial approximation) for photons and electrons:

Hermite–Gaussian Modes, PR Photonics Encyclopedia, https://www.rp-photonics.com/hermite_gaussian_modes.html

F. Pampaloni, J. Enderlein, Gaussian, Hermite-Gaussian, and Laguerre-Gaussian beams: A primer, arXiv:physics/0410021 (2004).

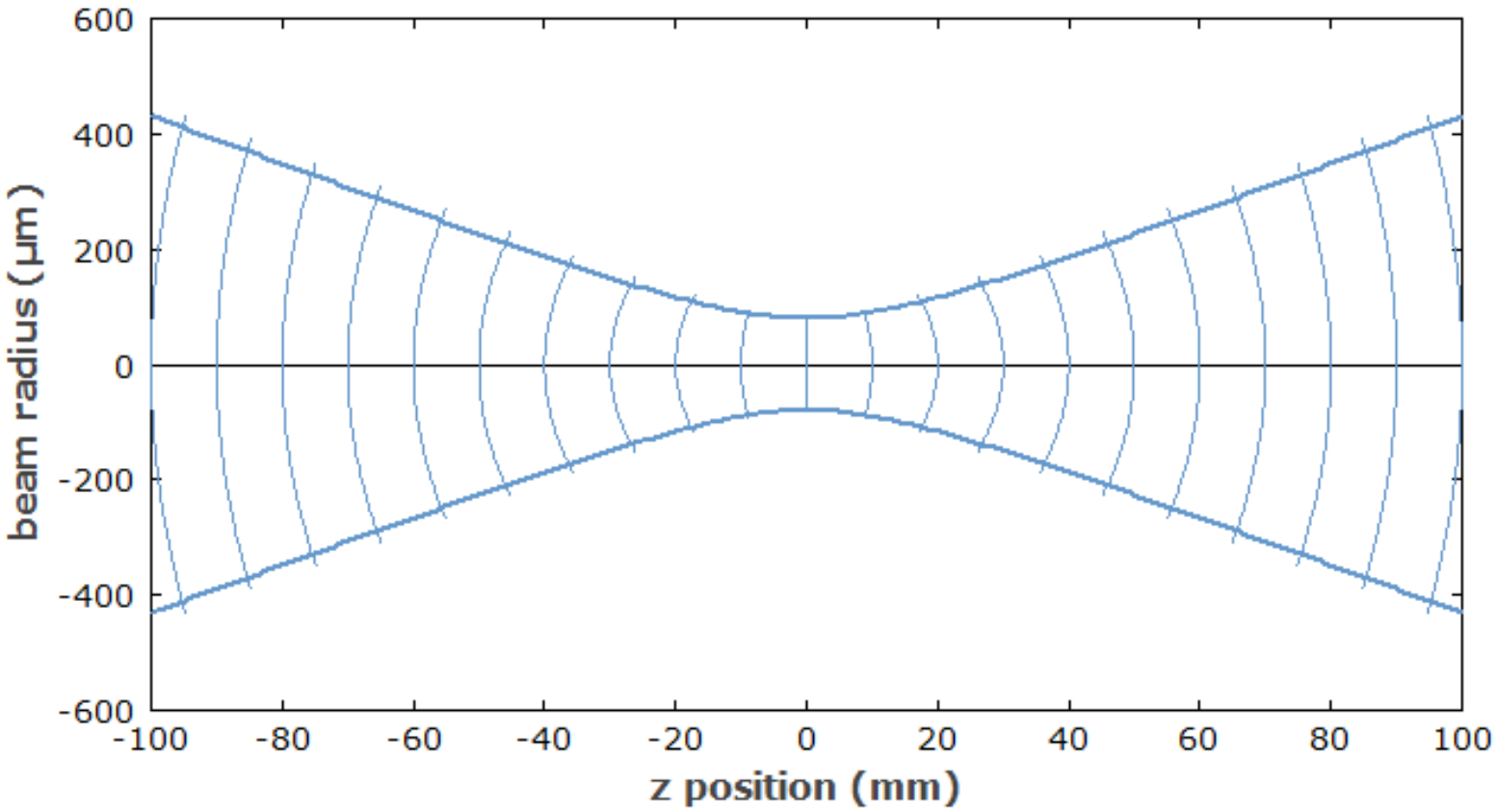
$$E_{nm}(x,y,z) = E_0 \frac{w_0}{w(z)} \cdot H_n\left(\sqrt{2}\frac{x}{w(z)}\right)\exp\left(-\frac{x^2}{w(z)^2}\right)\cdot H_m\left(\sqrt{2}\frac{y}{w(z)}\right)\exp\left(-\frac{y^2}{w(z)^2}\right) \cdot \exp\left(-i\left[kz-(1+n+m)\arctan\frac{z}{z_R}+\frac{k\left(x^2+y^2\right)}{2R(z)}\right]\right)$$

$$w(z) = w_0\sqrt{1+(z/z_R)^2} \qquad z_R = \frac{\pi w_0^2}{\lambda} \qquad R(z) = z\left[1+(z_R/z)^2\right]$$

The beam radius — Rayleigh length — The radius of curvature *R* of the wave front

Paraxial Hermite-Gauss beam in the free (2+1)-space

$$\chi(y) = \left(\frac{2}{\pi}\right)^{1/4} \sqrt{\frac{1}{2^n n! w(z)}} e^{i(n+1/2)\psi} H_n\left(\frac{\sqrt{2}x}{w(z)}\right) e^{-ik\frac{x^2}{2R(z)}} e^{-\frac{x^2}{w^2(z)}}$$



$$w(z) = w_0\sqrt{1+(z/z_R)^2}$$

The beam radius

$$z_R = \frac{\pi w_0^2}{\lambda}$$

Rayleigh length

$$R(z) = z\left[1+(z_R/z)^2\right]$$

The radius of curvature *R* of the wave front

$$\mathbf{v} = \frac{c\mathbf{p}}{\sqrt{\mathbf{p}^2}}, \quad \left|\langle \mathbf{v} \rangle\right| < c.$$

Due to the hidden transversal motion, the beam is subluminal.

$$\mathscr{E} = \sqrt{p_z^2 + p_x^2}, \quad M = \sqrt{\mathscr{E}^2 - p_z^2}.$$

Quanta of graphene electrons in multiwave states have effective quantized masses (<p_x^2> is quantized).

Summary

- Foldy-Wouthuysen transformation in (2+1)-space has been fulfilled in the ``relativistic'' case
- Foldy-Wouthuysen Hamiltonian for the planar graphene electron in electric and magnetic fields has been derived
- Initial Dirac equation in (2+1)-space should utilize usual Dirac matrices but not Pauli ones
- Exact solution for the planar graphene electron in a uniform magnetic field has been obtained
- Multiwave Hermite-Gauss beams of graphene electrons in the free (2+1)-space have been considered


Thank you for your attention