

"ABC" of Relativistic QM

$$E = \frac{p^2}{2m} = \frac{1}{2}mv^2 \text{ (free particle)}$$

↑ Newtonian (non-relativistic)

$$\text{QM: } p \rightarrow \hat{p} \rightarrow \frac{\hbar}{i} \nabla ; E \rightarrow i\hbar \frac{\partial}{\partial t}$$

⇒ Schrödinger Equation ... (1925)

Non-relativistic QM

→ Triumph of 20th century physics!

↳ led to: Solid state physics
Semiconductor industry
Electronic devices

Computers

Atomic physics

Molecular physics / Quantum Chemistry

- Very early on, physicists (Klein, Gordon (1927)) (Dirac 1928) tried to formulate a Quantum Mechanics that is consistent with special relativity.

Klein-Gordon (1927) did the earliest attempt.

$$E^2 = c^2 p^2 + m^2 c^4$$

starting point is relativistic!

$$E \rightarrow i\hbar \frac{\partial}{\partial t}; \quad p_x \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x}, \text{ etc}$$

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = -\hbar^2 c^2 \nabla^2 \psi + m^2 c^4 \psi$$

$$\nabla^2 \psi - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \psi = \frac{m^2 c^2}{\hbar^2} \psi$$

Klein Gordon Equation

turned out to be

- applicable to bosons of mass m
- important in the development of Quantum field theory

(also written as $E^2 - p^2 = m^2$) ($c=1$ units)

$(\frac{E}{c}, \mathbf{p})$ or (E, \mathbf{p})

4 vector

$$p^\mu p_\mu = m^2$$

QM $\left\{ \begin{array}{l} \vec{p} \rightarrow \frac{\hbar}{i} \vec{\nabla} \rightarrow \frac{1}{i} \vec{\nabla} \quad (\hbar=1 \text{ units}) \\ E \rightarrow i\hbar \frac{\partial}{\partial t} \end{array} \right.$

But $\frac{\partial}{\partial x}, \frac{\partial}{\partial t}$ also form a 4-vector

$$(\partial^\mu \partial_\mu + m^2) \phi(x) = 0$$

OR

Klein Gordon Equation

$$(\square + m^2) \phi = 0$$

Dirac

- didn't like E^2 and preferred E
- So, he wanted to work on factorizing

$$E^2 - c^2 p_x^2 - c^2 p_y^2 - c^2 p_z^2 - m^2 c^4$$

5 terms
into something like $(E + \text{something})(E - \text{something})$,
want to see $(\not{\partial} + m)(\not{\partial} - m)$

then $(\not{\partial} - m)\psi = 0$ becomes his (Dirac) equation.

$$(i \gamma^\mu \partial_\mu - m)\psi = 0 \quad [\text{Dirac Equation}]$$

$$\gamma^0 = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & -\mathbf{I} \end{pmatrix}; \quad \gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix} \quad k=1,2,3$$

4x4 matrices

But massless ($m=0$) fermion case is simpler!

Massless Fermion

$$E^2 - c^2 p_x^2 - c^2 p_y^2 - c^2 p_z^2 = 0$$

"How to factorize this expression?"

Recall: Often some "new mathematics" is needed in factorization.

- $x^2 - y^2 = (x+y)(x-y)$

- $\underbrace{x^2 + y^2}_{2 \text{ terms}} = (x+iy)(x-iy)$ needs "i"

- $x^2 + y^2 + z^2$?
or $\underbrace{p_x^2 + p_y^2 + p_z^2}_{3 \text{ terms}}$?

Can factorize it if we extend consideration to 2×2 matrices

- Consider $\vec{\sigma}_x p_x + \vec{\sigma}_y p_y + \vec{\sigma}_z p_z = \vec{\sigma} \cdot \vec{p}$

where $\vec{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\vec{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\vec{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ Pauli matrices

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} p_x + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} p_y + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} p_z = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & p_z \end{pmatrix}$$

$$(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) = \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & p_z \end{pmatrix} \begin{pmatrix} p_z & p_x - ip_y \\ p_x + ip_y & p_z \end{pmatrix} = \begin{pmatrix} p_x^2 + p_y^2 + p_z^2 & 0 \\ 0 & p_x^2 + p_y^2 + p_z^2 \end{pmatrix}$$

$$\begin{aligned} \therefore E^2 - c^2(p_x^2 + p_y^2 + p_z^2) &= E^2 - c^2(\vec{\sigma} \cdot \vec{p})(\vec{\sigma} \cdot \vec{p}) \\ &= (E + c(\vec{\sigma} \cdot \vec{p}))(E - c(\vec{\sigma} \cdot \vec{p})) \end{aligned}$$

Thus, a relativistic equation for massless fermion is

$$(E + c(\vec{\sigma} \cdot \vec{p}))(E - c(\vec{\sigma} \cdot \vec{p}))\psi = 0$$

where ψ is a two-component wavefunction

OR simply $[E - c(\vec{\sigma} \cdot \vec{p})]\psi = 0$

OR $c(\vec{\sigma} \cdot \vec{p})\psi = E\psi$

for massless fermions

Band Structure of Graphene at K turns out to be describable by an equation of this form!