PY411 / 506
Computational Physics 2

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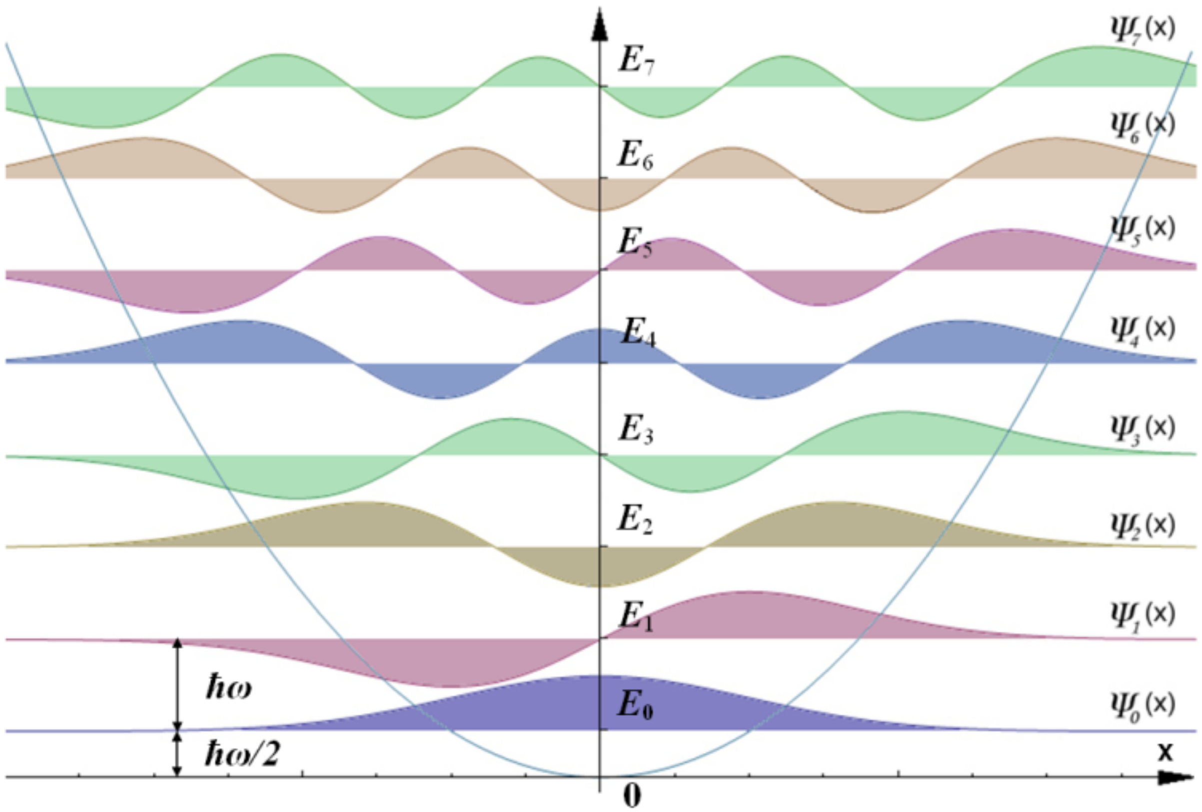
Quantum Mechanics

- Quantum mechanics: Describes motion of small things
  - Hydrogen atom
  - Quantum harmonic oscillator



- Quantize:

$$H = \frac{p^2}{2m} + V(x)$$

$$\vec{p} \to -i\hbar\vec{\nabla} \qquad E \to i\hbar\frac{\partial}{\partial t}$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$$

$$H\psi = E\psi \qquad i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

Quantum Mechanics

- Probability density:

$$\rho = \psi^* \psi = |\psi|^2$$

- Evolves according to the probability “current” vector:

$$J = -\frac{i\hbar}{2m} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right)$$

- Conservation equation:

$$\nabla \cdot J + \frac{\partial \rho}{\partial t} = 0$$

Relativity

- Relativity:
  - Describes motion of fast things

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

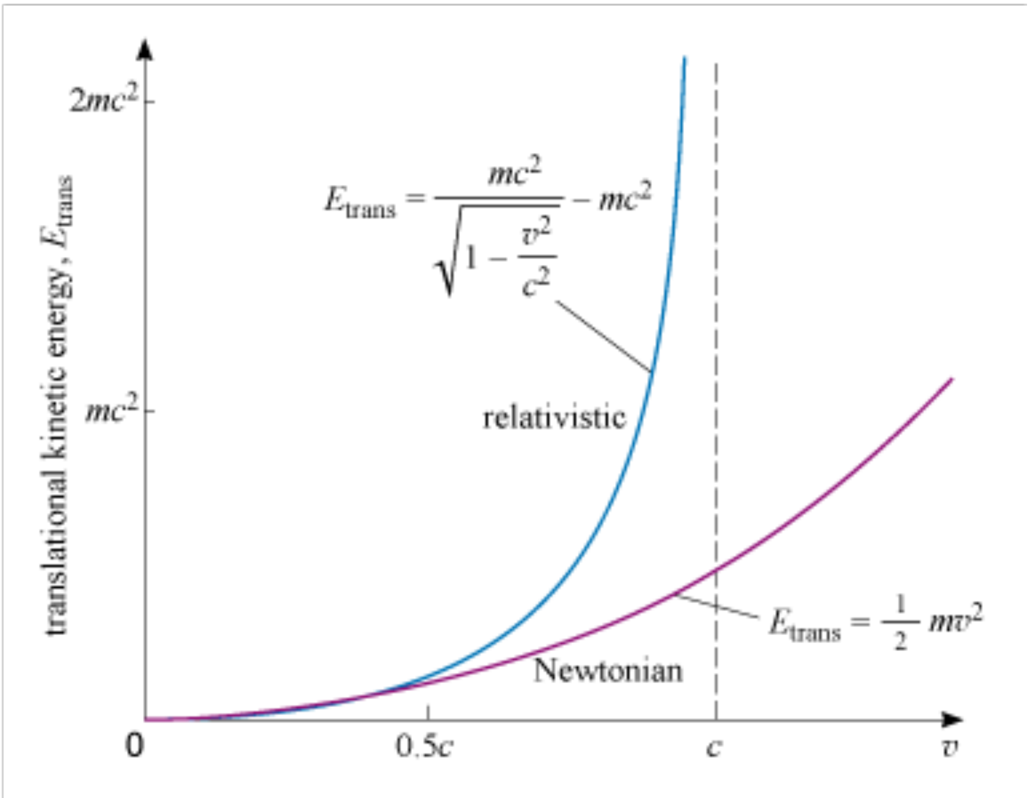
$$c = 1$$

$$E = \pm m\left(1 + \frac{p^2}{m^2}\right)^{1/2}$$

$$E \approx \pm m\left(1 + \frac{1}{2}\frac{p^2}{m^2}\right)$$

$$KE = \frac{p^2}{2m}$$

- Describes all particles:
  - Photons
  - Electrons
  - Protons
  - Etc



Relativistic Quantum Mechanics

- Try Schroedinger's trick:

$$\vec{p} \rightarrow -i\hbar\vec{\nabla} \qquad E \rightarrow i\hbar\frac{\partial}{\partial t}$$

- We get the Klein-Gordon equation

$$\left(-\frac{1}{c^2}\frac{\partial^2}{\partial t^2} + \nabla^2\right)\phi = \frac{m^2c^2}{\hbar^2}\phi$$

- Problem: Cannot interpret phi as a simple probability density anymore
  - Hyperbolic equation can arbitrarily specify ϕ and $\partial\phi/\partial t$
- This describes motion of spin-zero fields

Relativistic Quantum Mechanics

- What about probability density?

$$\rho = \phi^* \phi = |\phi|^2$$

- Doesn't work, because can now arbitrarily specify ϕ and $\partial\phi/\partial t$
- Need a density symmetric in space and time
  - Makes sense! Special relativity is!
- Adjust (purposely changing phi to psi):

$$\rho = \frac{i\hbar}{2mc^2}\left(\psi^* \partial_t \psi - \psi \partial_t \psi^*\right)$$

- Make that zeroth component of 4-vector:

$$J^\mu = \frac{i\hbar}{2m}\left(\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^*\right)$$

Relativistic Quantum Mechanics

- Does it work?

- Still no. If we specify the time derivative arbitrarily, can get negative values (i.e. unphysical for a probability density)

- This means : cannot simply generalize Schroedinger equation assuming SCALAR fields

Relativistic Quantum Mechanics

- Dirac came up with solution:
  - Expand:

$$\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} = \left(A\partial_x + B\partial_y + C\partial_z + \frac{i}{c}D\partial_t\right)^2$$

  - Cross terms like $\partial_x\partial_y$ cancel if $\{A, B\} = 0$ but $A^2 = B^2 = \ldots = 1$

- This works if A, B, C, and D are MATRICES, not numbers!
- Arrive at Dirac equation:

$$i\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0$$

where γ^μ are special matrices:

$$\gamma^0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \gamma^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \gamma^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \gamma^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}$$

- These are 4x4 matrices:

$$\gamma^0 = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \gamma^1 = \begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}, \gamma^2 = \begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix}, \gamma^3 = \begin{pmatrix} 0 & \sigma_z \\ -\sigma_z & 0 \end{pmatrix}$$

- Where I is the identity matrix and the sigmas are the Pauli matrices:

$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Relativistic Quantum Mechanics

- What does this MEAN, though?
- There are 4 components of ψ!
  - Relativistic spin-1/2 field
  - Includes antimatter!

(Geek out about that for a second)

- Define "slash" notation as a sum over these matrices times the components :

$$\not{v} = \sum_i \gamma_i v_i$$

- Set c = 1, and we get the Dirac equation:

$$(i\not{\partial} - m)\,\psi = 0$$

Relativistic Quantum Mechanics

- Now define the adjoint spinor:

$$\bar{\psi} = \psi^\dagger \gamma^0$$

- And Now the current density equation becomes:

$$\partial_\mu \left(\bar{\psi} \gamma^\mu \psi \right) = 0$$

- The probability density is:

$$J^0 = \bar{\psi} \gamma^0 \psi = \psi^\dagger \psi$$

Quantum Field Theory

- If you remember E+M, it is the relationship between CURRENTS and FIELDS
  - We have the currents
  - What about the fields?
- Recall Maxwell's equations, but now in 4-vector notation:
  - Electric and magnetic potentials put to 4-vector:

$$A^\mu = \left(\phi, \vec{A}\right)$$

  - Then the field strength tensor is:

$$F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu$$

  - Maxwell's equations become:

$$\partial_\mu F^{\mu\nu} = 4\pi J^\mu$$

Quantum Field Theory

- But remember from elementary E+M: the potentials are not physical quantities, the fields are
- So we can perform an operation on the potentials:

$$A^\mu \rightarrow A^\mu + \partial^\mu \lambda$$

and if lambda does not change Maxwell's equations, it is equally fine as a potential

- This is a "Gauge Transformation"

VEGAS Algorithm

- Paper by LePage: J. Comput. Phys. 17, 192-203 (1978)
  - Originally in FORTRAN
  - PYTHON Github page:
    - https://github.com/gplepage/vegas
  - C++ Implementations around, for instance in Numerical Recipes

VEGAS Algorithm

- Simplest MC integration: Throw “pseudo-experiments”, count the total:

$$I = \int_a^b dx\, f(x) \simeq (b-a)\left[\frac{1}{N}\sum_{n=1}^{N} f(x_i) \pm \frac{\sigma_f}{\sqrt{N}}\right]$$

- Where:

$$\sigma_f^2 = \left(\frac{1}{b-a}\int_a^b f^2(x)\,\mathrm{d}x\right) - \left(\frac{1}{b-a}\int_a^b f(x)\,\mathrm{d}x\right)^2 \simeq \left(\frac{1}{N}\sum_{i=1}^{N} f^2(x_i)\right) - \left(\frac{1}{N}\sum_{i=1}^{N} f(x_i)\right)^2 .$$

VEGAS Algorithm

- VEGAS has “importance sampling” : samples the space where integrand is largest more often
  - Similar to the Metropolis algorithm
- Consider f(x) and its integral: $I = \int_0^1 dx\; f(x)$
- If we have PDF p(x):

$$p(x) > 0\,, \qquad \int_0^1 dx\; p(x) = 1$$

- Optimal variance arrived when: $p(x) = \frac{|f(x)|}{\int_0^1 dx |f(x)|}$

VEGAS Algorithm

- Approximates p(x) with step functions:
  - Starts with uniform probability p(x) = 1
  - Adapts p(x) as:

$$p(x) = \frac{1}{N\Delta x_i}\ , \quad x_i - \Delta x_i \le x \le x_i\ , \quad i = 1, \ldots, N\ , \qquad \sum_{i=1}^{N} \Delta x_i = 1\ ,$$

    where Δx_i is the width of each step
- Then subdivide each step into further steps:
  - Similar to adaptive methods for our PDF evaluation, or adaptive RK

$$m_i = K \frac{\bar{f}_i \Delta x_i}{\sum_j \bar{f}_j \Delta x_j}\ , \quad \bar{f}_i = \sum_{x \in \Delta x_i} |f(x)| \propto \frac{1}{\Delta x_i} \int_{\Delta x_i} dx\ |f(x)|\ ,$$

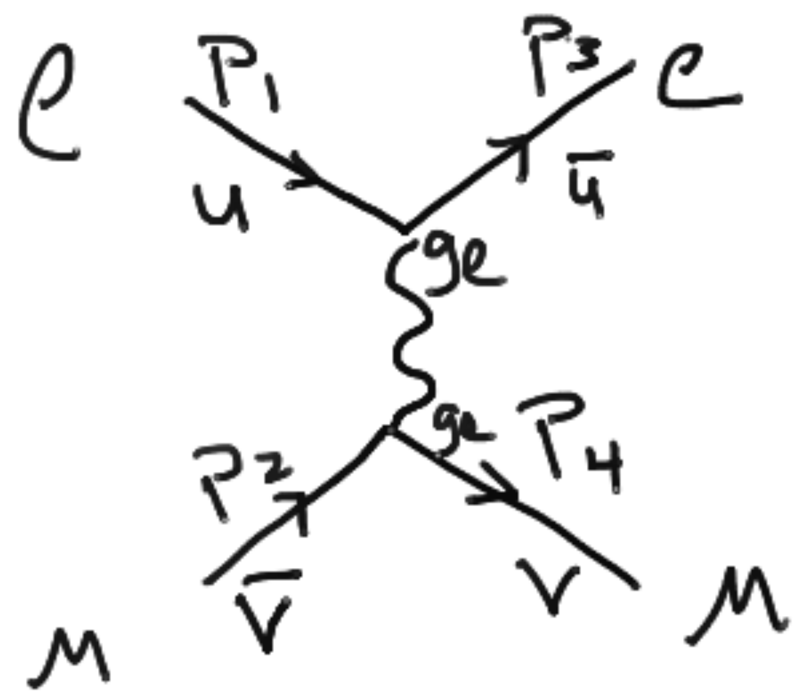
  - Finer binning where the function is largest

VEGAS Algorithm

- Examples :
  - Trivial 1-d integral
  - Path integral integral for QHO

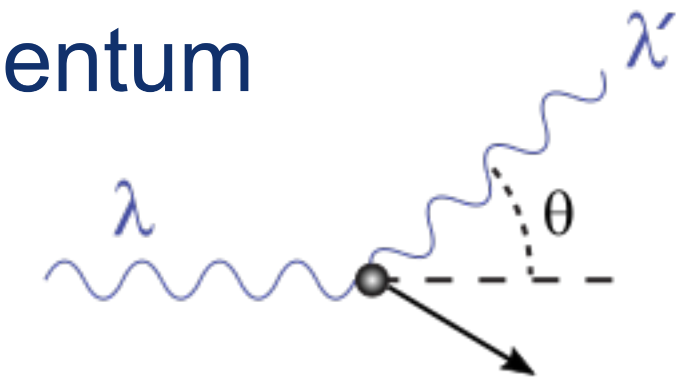
Quantum Field Theory

- Similar currents exist for matter (electrons, etc)
- Interactions are then specified in terms of interactions of the currents and the fields
- See Peskin + Schroeder, for instance



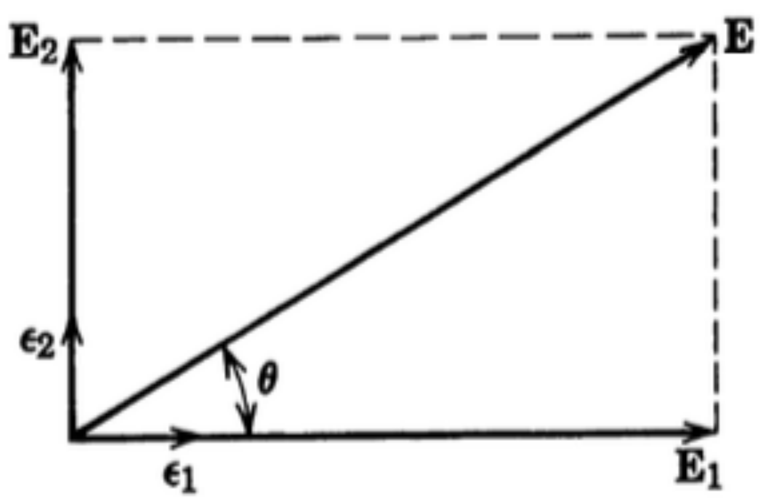
Compton Scattering

- Scattering of light off of electrons at rest
  - Must be near nucleus to conserve momentum

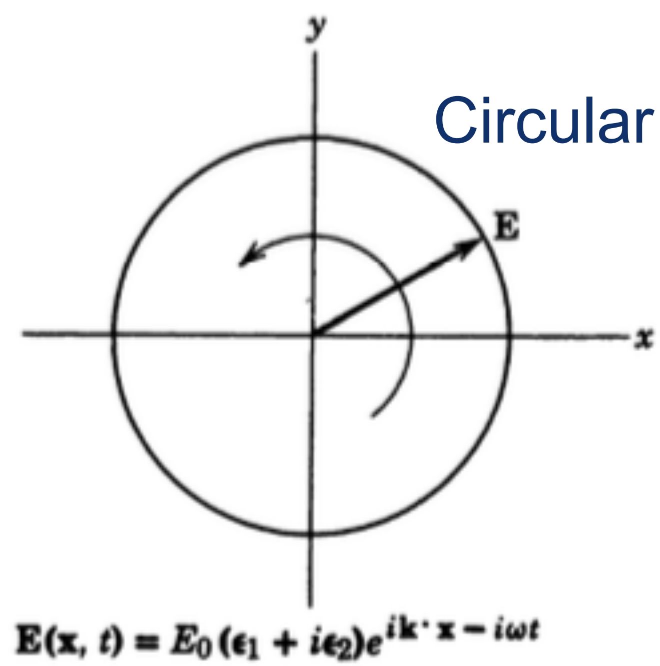


- Specify polarization of incoming light beams:

Linear polarization



Circular polarization

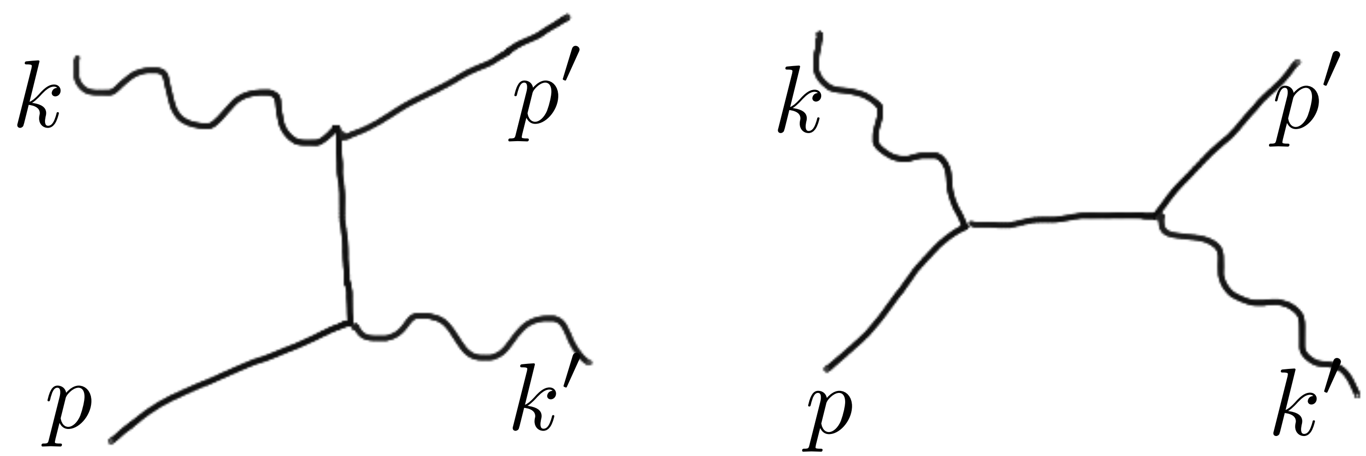


$$\mathbf{E}(\mathbf{x},t) = (\boldsymbol{\epsilon}_1 E_1 + \boldsymbol{\epsilon}_2 E_2) e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t}\,, \quad \mathbf{E}(\mathbf{x},t) = (\boldsymbol{\epsilon}_+ E_+ + \boldsymbol{\epsilon}_- E_-) e^{i\mathbf{k}\cdot\mathbf{x} - i\omega t}\,, \quad \boldsymbol{\epsilon}_\pm = \frac{1}{\sqrt{2}}(\boldsymbol{\epsilon}_1 \pm i\boldsymbol{\epsilon}_2)\,,$$

E+ and E- are + and - helicity states

Compton Scattering

- Calculation of matrix element:



- Initial conditions:

$$p^\mu = (mc, 0, 0, 0)\ , \quad k^\mu = (1, 0, 0, 1)\frac{\hbar\omega}{c}\ , \quad k'^\mu = (1, \sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\frac{\hbar\omega'}{c}$$

- Kinematics and conservation of 4-momentum gives:

$$\begin{aligned} p' \cdot p' = m^2c^2 &= (p + k - k') \cdot (p + k - k') = p^2 + 2p \cdot (k - k') + (k - k')^2 \\ &= m^2c^2 + 2m\hbar(\omega - \omega') - 2\hbar^2\omega\omega'(1 - \cos\theta) \end{aligned}$$

$$i\mathcal{M} = -ie^2\epsilon^*_\mu(k')\epsilon_\nu(k)\bar{u}(p')\left[\frac{\gamma^\mu \not{k}\gamma^\nu + 2\gamma^\mu p^\nu}{2p \cdot k} + \frac{-\gamma^\nu \not{k}\gamma^\mu + 2\gamma^\nu p^\mu}{-2p \cdot k'}\right]u(p)$$

Compton Scattering

- Differential cross section:

$$\frac{d\sigma}{d\Omega} = \frac{\text{Energy radiated/unit time/unit solid angle}}{\text{Incident energy flux/unit area/second}}$$
$$= \frac{\text{Number of photons detected/unit time/unit solid angle}}{\text{Number of photons incident/unit area/unit time}}$$

$$\frac{d\sigma}{d\Omega} = \left(\frac{e^2}{mc^2}\right)^2 \left(\frac{\omega'}{\omega}\right)^2 \left[|\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0|^2 + \frac{(\omega-\omega')^2}{4\omega\omega'}\{1 + (\boldsymbol{\epsilon}^* \times \boldsymbol{\epsilon}) \cdot (\boldsymbol{\epsilon}_0 \times \boldsymbol{\epsilon}_0^*)\}\right]$$

$$(\boldsymbol{\epsilon}^* \times \boldsymbol{\epsilon}) \cdot (\boldsymbol{\epsilon}_0 \times \boldsymbol{\epsilon}_0^*) = (\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0)(\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}_0^*) - (\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0^*)(\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}_0) = |\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0|^2 - |\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}_0|^2$$

Compton Scattering

- With some convenient units, can work in dimensionless units:

$$r_e = \frac{e^2}{mc^2} = 2.81794033 \times 10^{-13}\ \mathrm{cm}\ , \qquad r_e^2 = 0.07940787703\ \mathrm{b} \simeq 79.4\ \mathrm{mb}\ .$$

$$\frac{1}{r_e^2}\sigma_T = \int_{-1}^{+1} d(\cos\theta) \int_0^{2\pi} d\phi\, \frac{1}{r_e^2}\frac{d\sigma}{d\Omega}$$

$$\frac{1}{r_e^2}\frac{d\sigma}{d\theta} = \sin\theta \int_0^{2\pi} d\phi\, \frac{1}{r_e^2}\frac{d\sigma}{d\Omega}$$

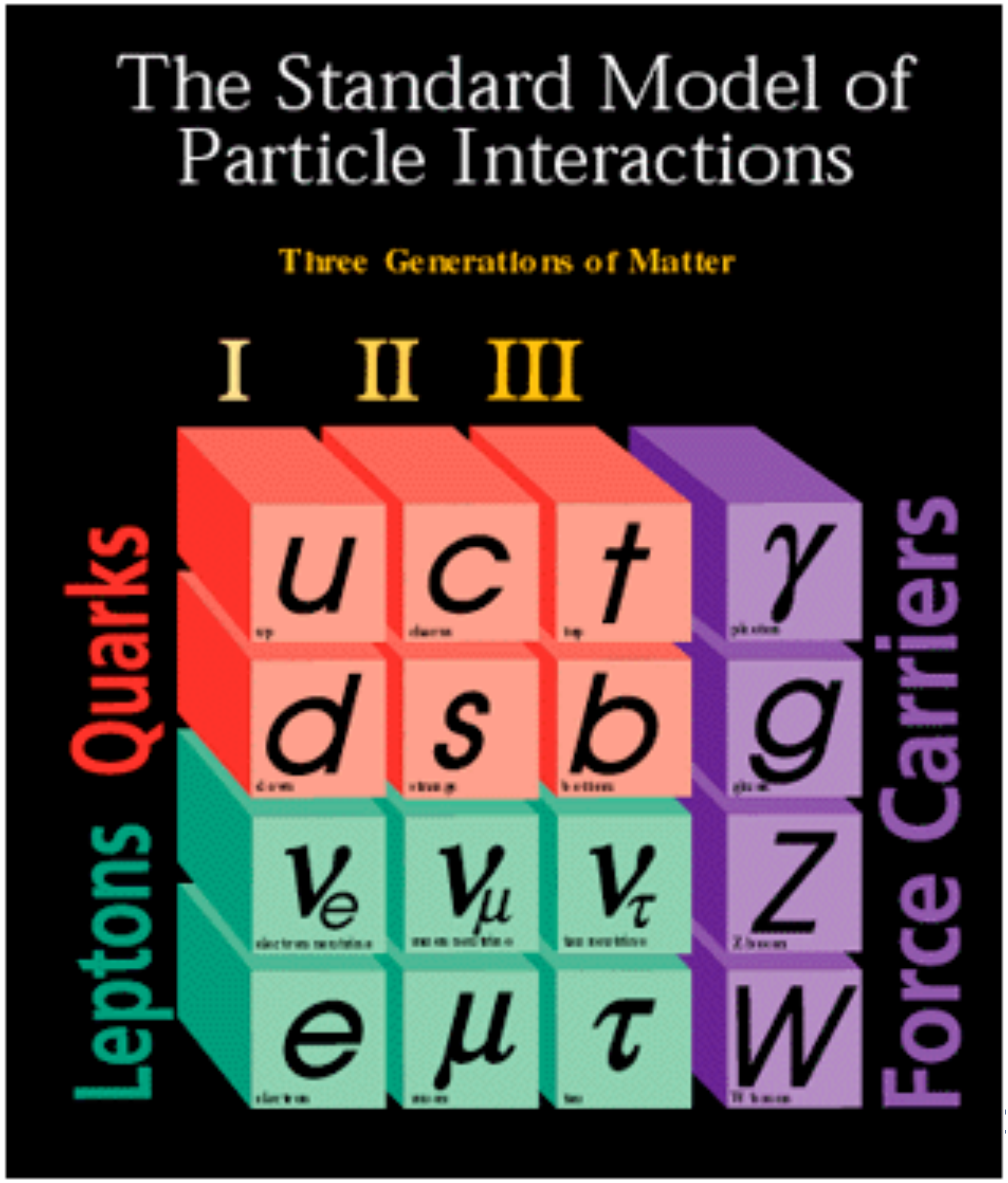
$$\frac{1}{r_e^2}\frac{d\sigma}{d\Omega} = \left(\frac{\omega'}{\omega}\right)^2 \left[|\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0|^2 + \frac{(\omega - \omega')^2}{4\omega\omega'} \left(1 + |\boldsymbol{\epsilon}^* \cdot \boldsymbol{\epsilon}_0|^2 - |\boldsymbol{\epsilon} \cdot \boldsymbol{\epsilon}_0|^2\right) \right]$$

Note: Averaged over initial electron spin states, summed over final electron spin states

Quantum Field Theory

- Last time: computed Compton scattering cross section

- Now: Compute Z production cross section
  - e+e- —> Z —> e+e-
  - pp —> Z —> e+e-



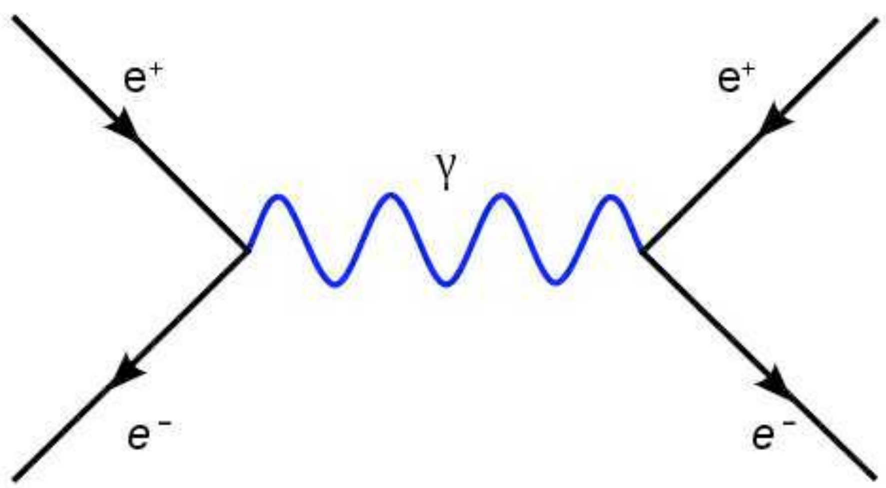
$$
\begin{aligned}
\mathcal{L} = & -\frac{1}{4}B_{\mu\nu}B^{\mu\nu} - \frac{1}{8}tr(\mathbf{W}_{\mu\nu}\mathbf{W}^{\mu\nu}) - \frac{1}{2}tr(\mathbf{G}_{\mu\nu}\mathbf{G}^{\mu\nu}) && \text{(U(1), SU(2) and SU(3) gauge terms)} \\
& +(\bar{\nu}_L, \bar{e}_L)\,\tilde{\sigma}^{\mu} iD_{\mu} \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} + \bar{e}_R \sigma^{\mu} iD_{\mu} e_R + \bar{\nu}_R \sigma^{\mu} iD_{\mu} \nu_R + \text{(h.c.)} && \text{(lepton dynamical term)} \\
& -\frac{\sqrt{2}}{v}\left[(\bar{\nu}_L, \bar{e}_L)\,\phi M^{e} e_R + \bar{e}_R \bar{M}^{e} \bar{\phi} \begin{pmatrix} \nu_L \\ e_L \end{pmatrix} \right] && \text{(electron, muon, tauon mass term)} \\
& -\frac{\sqrt{2}}{v}\left[(-\bar{e}_L, \bar{\nu}_L)\,\phi^{*} M^{\nu} \nu_R + \bar{\nu}_R \bar{M}^{\nu} \phi^{T} \begin{pmatrix} -e_L \\ \nu_L \end{pmatrix} \right] && \text{(neutrino mass term)} \\
& +(\bar{u}_L, \bar{d}_L)\,\tilde{\sigma}^{\mu} iD_{\mu} \begin{pmatrix} u_L \\ d_L \end{pmatrix} + \bar{u}_R \sigma^{\mu} iD_{\mu} u_R + \bar{d}_R \sigma^{\mu} iD_{\mu} d_R + \text{(h.c.)} && \text{(quark dynamical term)} \\
& -\frac{\sqrt{2}}{v}\left[(\bar{u}_L, \bar{d}_L)\,\phi M^{d} d_R + \bar{d}_R \bar{M}^{d} \bar{\phi} \begin{pmatrix} u_L \\ d_L \end{pmatrix} \right] && \text{(down, strange, bottom mass term)} \\
& -\frac{\sqrt{2}}{v}\left[(-\bar{d}_L, \bar{u}_L)\,\phi^{*} M^{u} u_R + \bar{u}_R \bar{M}^{u} \phi^{T} \begin{pmatrix} -d_L \\ u_L \end{pmatrix} \right] && \text{(up, charmed, top mass term)} \\
& +\overline{(D_{\mu}\phi)} D^{\mu}\phi - m_h^2[\bar{\phi}\phi - v^2/2]^2/2v^2. && \text{(Higgs dynamical and mass term)} \quad (1)
\end{aligned}
$$

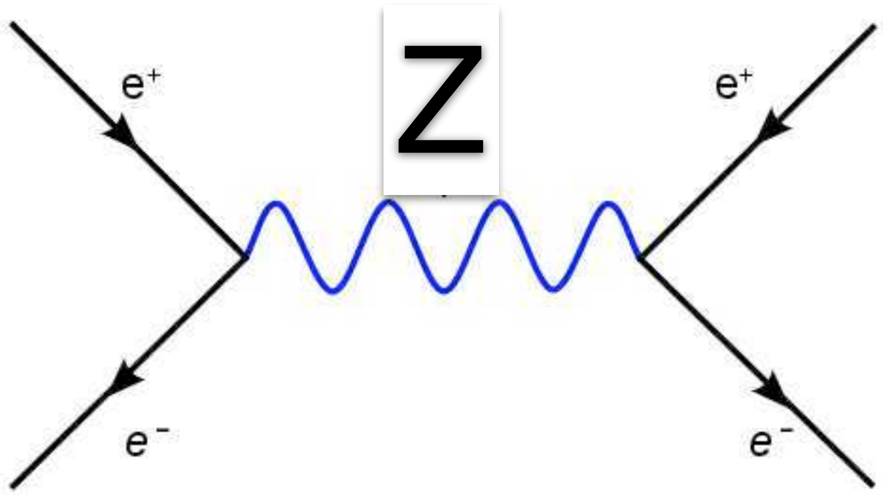
Quantum Field Theory

- Electroweak interaction: follows SU(2) x U(1) symmetry

3 bosons → SU(2)

1 boson → U(1)





Quantum Field Theory

- Group theory representations:

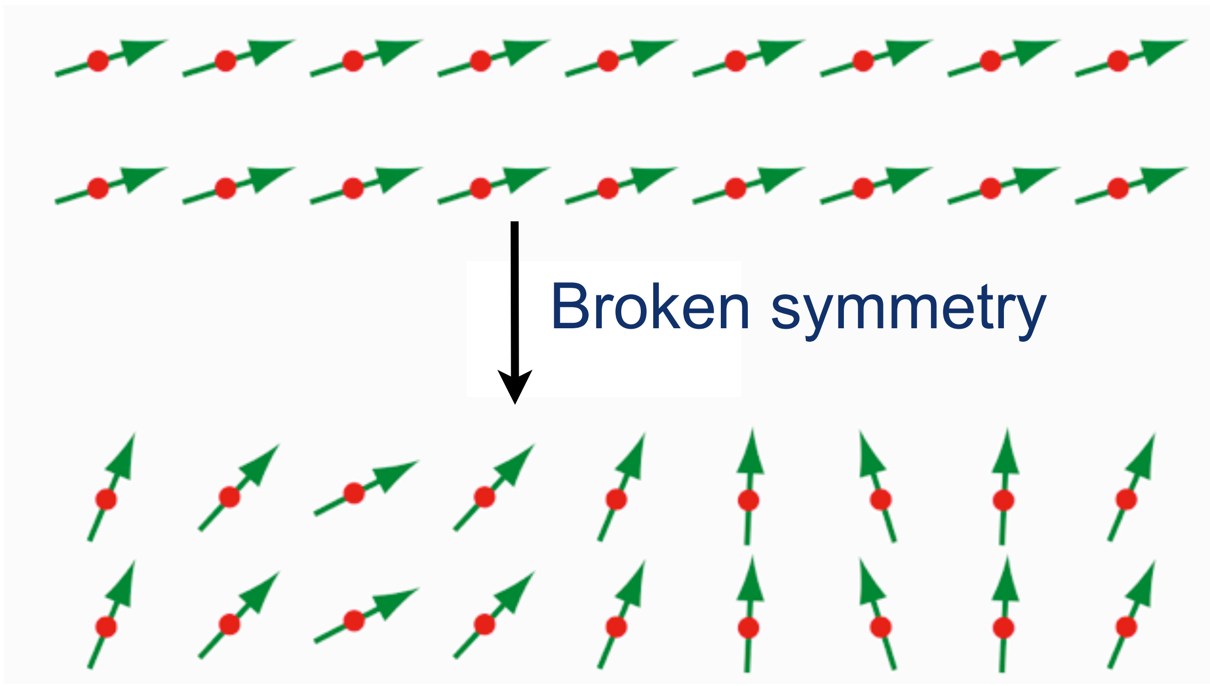
"SU(1)" = U(1): 1 vector field — photon

SU(2): 3 vector fields — W/Z

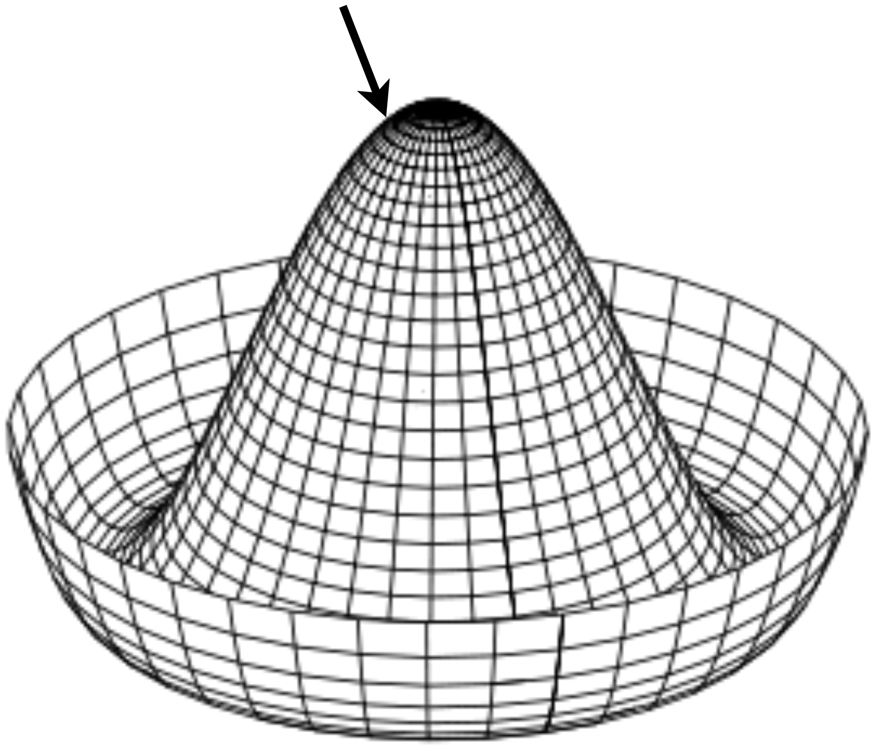
SU(3): 8 vector fields — gluons

Quantum Field Theory

- Simplest explanation for EWSB is the “Higgs mechanism”
- Nambu-Goldstone boson for the spontaneously broken symmetry of SU(2)XU(1)
- Similar to superconductor or ferromagnet!
- Simplest field to do this is a “Sombrero” potential



Nambu-Goldstone boson “generated” by the broken symmetry



Ground state breaks the EW symmetry!

Quantum Field Theory

- Bit of a wrinkle: The eigenbasis of SU(2) x U(1) is not the “mass” eigenbasis of the actual particles
- There is a mixing angle:

$$\begin{pmatrix} \gamma \\ Z^0 \end{pmatrix} = \begin{pmatrix} \cos\theta_\mathrm{W} & \sin\theta_\mathrm{W} \\ -\sin\theta_\mathrm{W} & \cos\theta_\mathrm{W} \end{pmatrix} \begin{pmatrix} B^0 \\ W^0 \end{pmatrix}$$

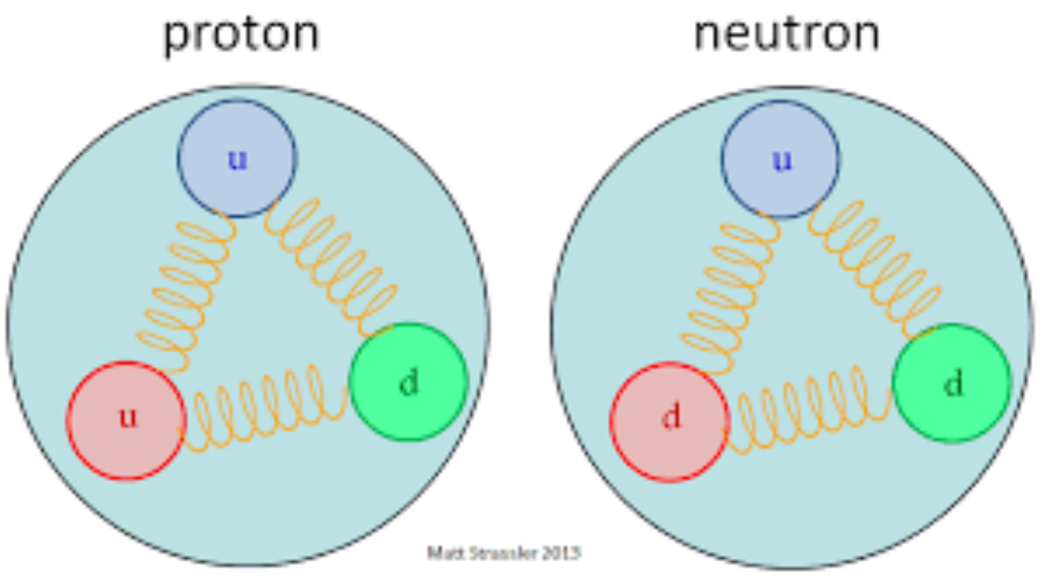
- “Weinberg angle”:

$$\cos\theta_\mathrm{W} = \frac{g}{\sqrt{g^2 + g'^2}}$$

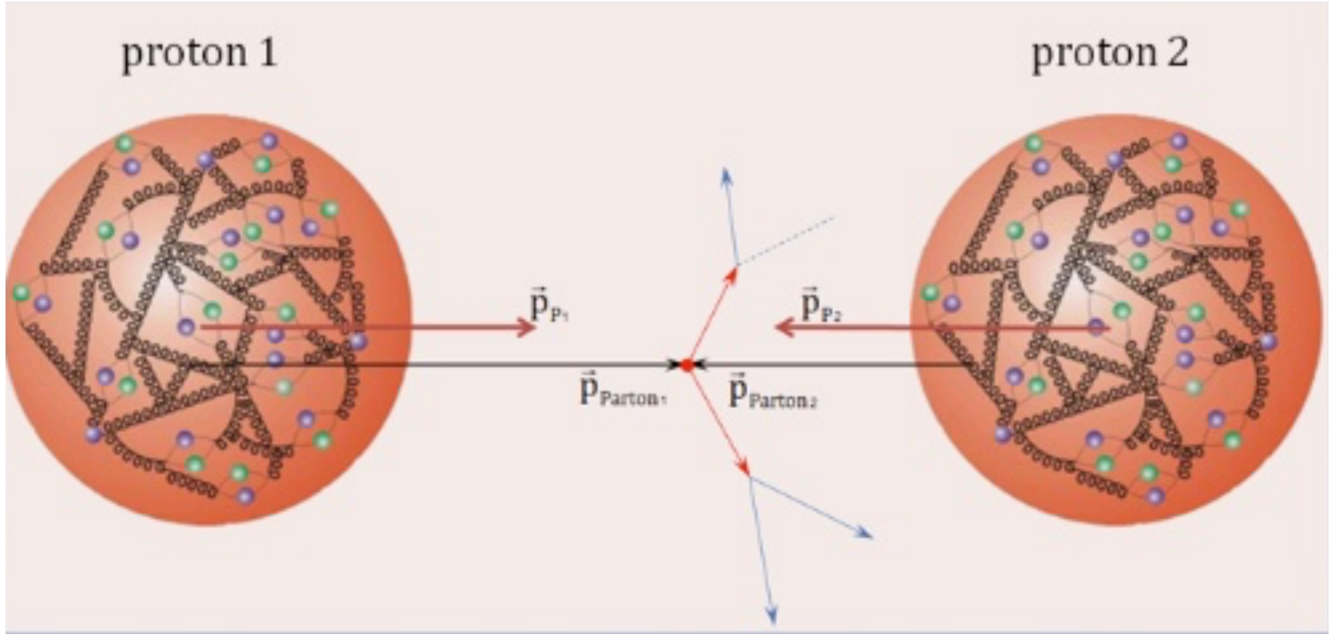
$$\sin^2\theta_W = 0.23126$$

Quantum Field Theory

- You've been told proton looks like this:



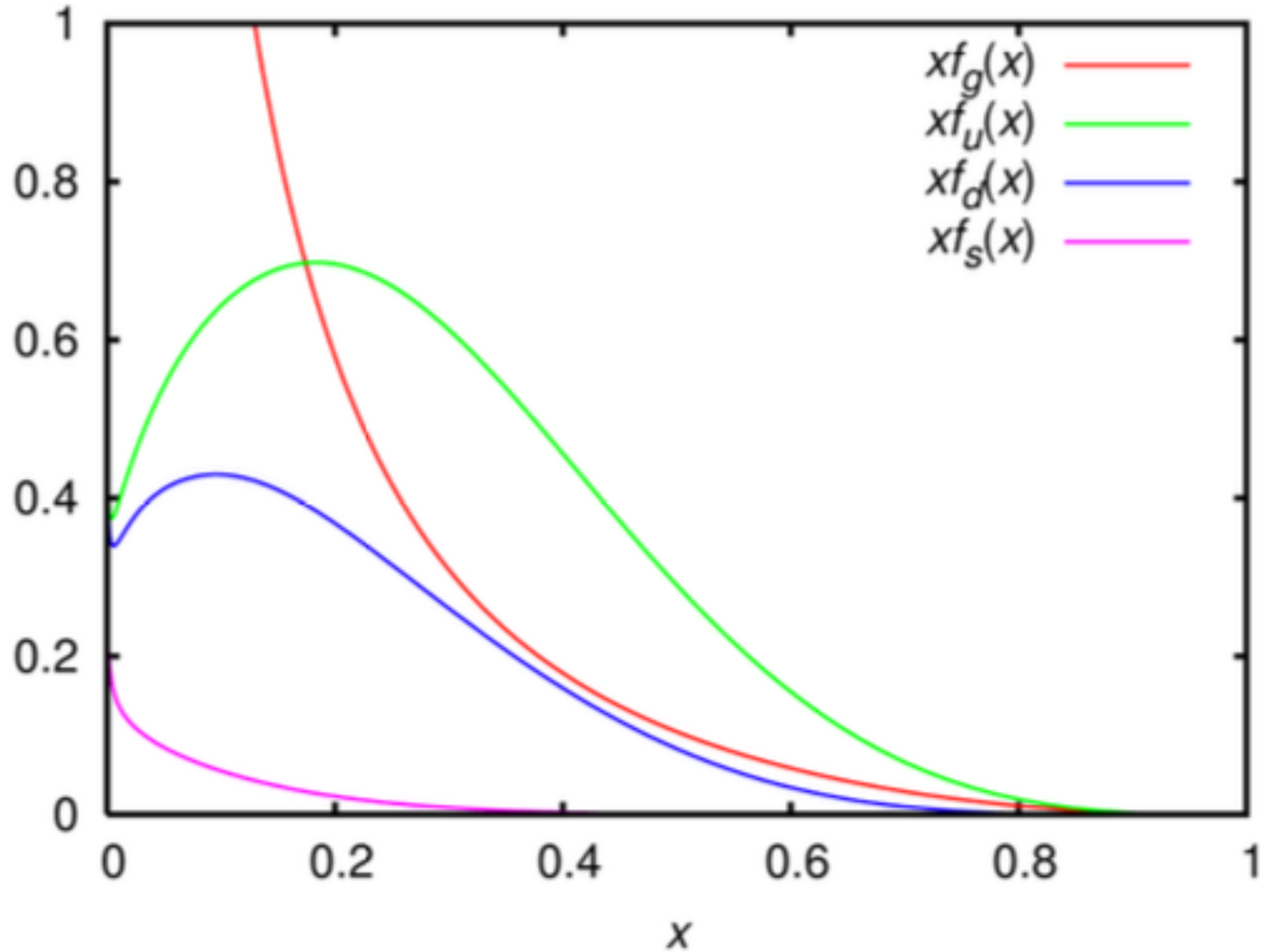
- Really looks like this:



Distributions of stuff INSIDE the proton!

Quantum Field Theory

- Parton distribution functions (PDFs):



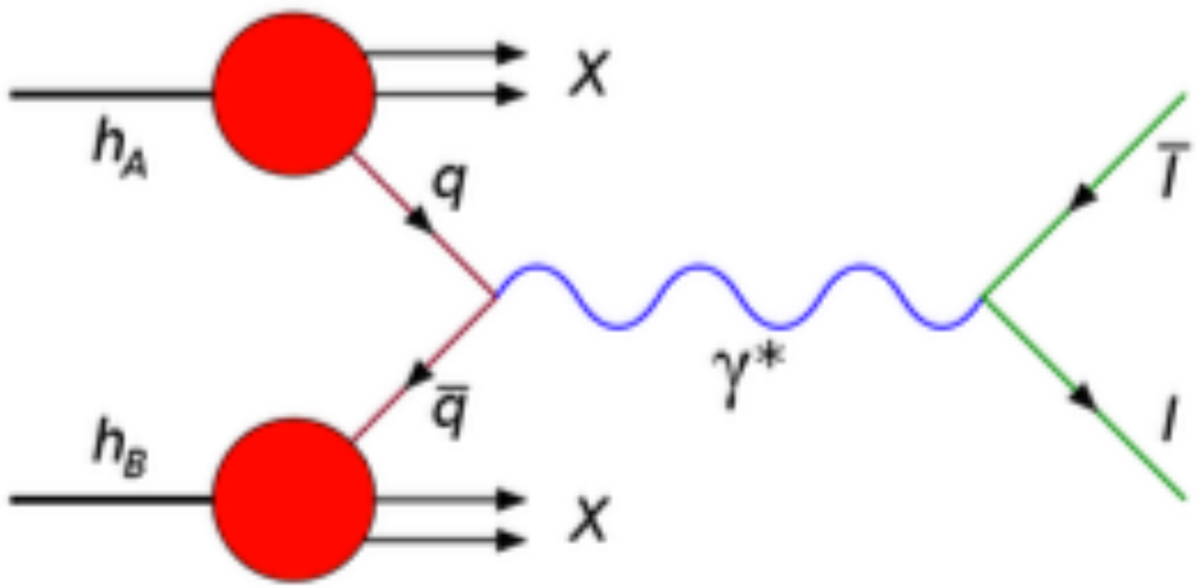
x = fraction of particle’s momentum to proton’s momentum

Quantum Field Theory

- Can FACTORIZE the computation into a hard process and the parton distribution function integration:

$$E_Q \frac{\mathrm{d}\sigma}{\mathrm{d}^3 Q} = \sum_{a_1,a_2} \int_0^1 \mathrm{d}x_2 \mathrm{d}x_1 f_{a_1}^{h_1}(x_1, M^2) f_{a_2}^{h_2}(x_2, M^2)\ E_Q \frac{\mathrm{d}\sigma^{a_1 a_2}}{\mathrm{d}^3 Q}(x_1 P_1, x_2 P_2, M^2)$$

- So for production of leptons:



Quantum Field Theory

- Drell-Yan cross section from CMS:
- J. High Energy Phys. 10, 007 (2011)
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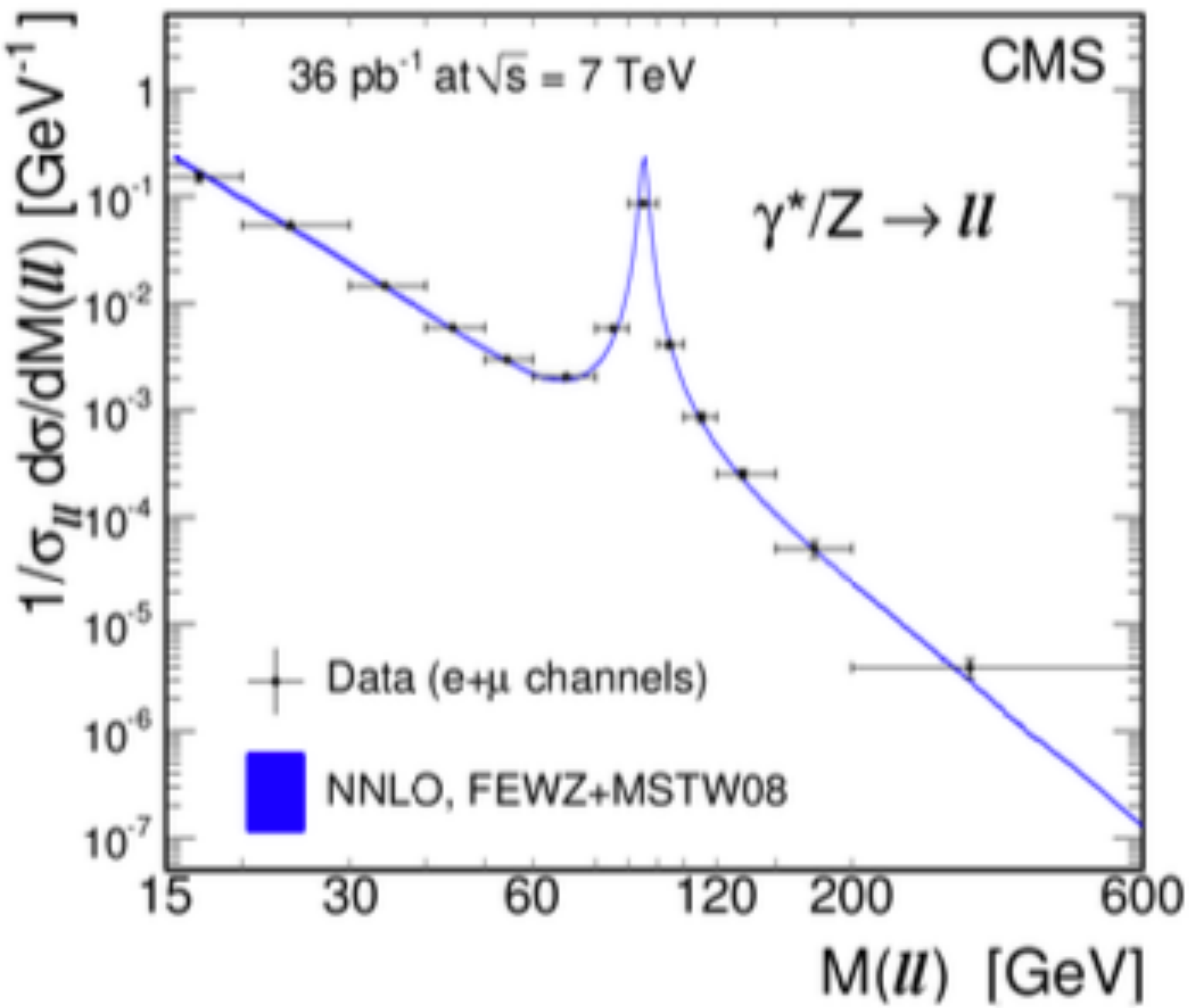
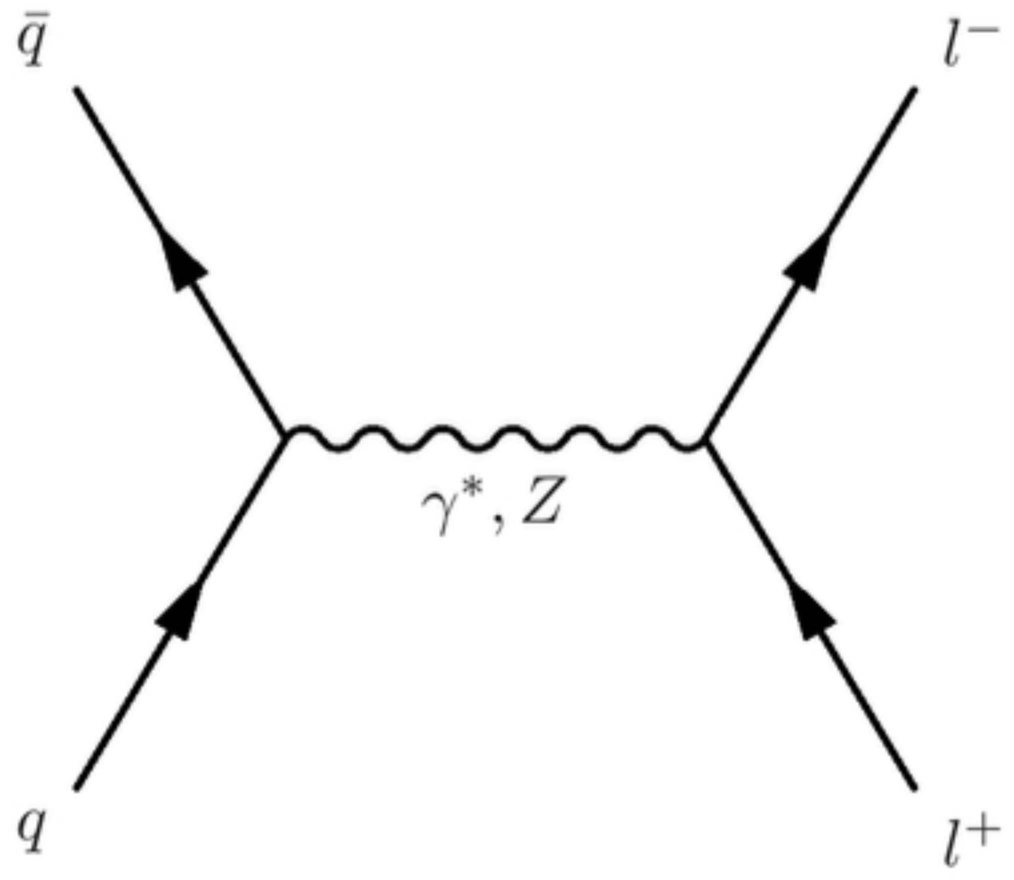


Quantum Field Theory

- Look at the Drell-Yan matrix element:



- Differential Cross Section is:

$$\frac{d\sigma}{d\Omega} = \frac{N_c^{\text{final}}}{N_c^{\text{initial}}} \times \frac{1}{256\pi^2 s} \times \frac{s^2}{(s - M_Z^2)^2 + s\Gamma_Z} \times \left[(L^2 + R^2)(L'^2 + R'^2)(1 + \cos\theta) + (L^2 - R^2)(L'^2 - R'^2) 2\cos\theta \right] ,$$

$$s = (p_i + p_j)^2 = (E_i + E_j)^2 - (\mathbf{p}_i + \mathbf{p}_j)^2$$

$$L = \sqrt{\frac{8G_F m_Z^2}{\sqrt{2}}} (T_3 - \sin^2\theta_W Q) , \quad R = -\sqrt{\frac{8G_F m_Z^2}{\sqrt{2}}} \sin^2\theta_W Q ,$$

- So look back at the master formula:

$$\frac{d\sigma}{d\Omega} = \sum_{a_1,a_2} \int_0^1 dx_2 dx_1 f_{a_1}^{h_1}(x_1, M^2) f_{a_2}^{h_2}(x_2, M^2)\ E_Q \frac{d\sigma^{a_1 a_2}}{d^3Q}(x_1 P_1, x_2 P_2, M^2)\ ,$$

- Your homework problem will be to perform a MC simulation of the pp —-> Z ——> e+e- cross section!

- u(total) = u(valence) + u(sea)
- ubar (total) = u(sea)
- d(total) = d(valence) + d(sea)
- dbar (total) = d(sea)
- s(total) = s(sea)
- sbar(total) = s(sea)