The GiBUU Model for nonequilibrium nuclear reactions
Theoretical basis and some results

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GiBUU

The Giessen Boltzmann-Uehling-Uhlenbeck Project

GiBUU

- GiBUU
= The Giessen Boltzmann-Uehling-Uhlenbeck Project
- Theory and Code for simulation of nuclear reactions
- degrees of freedom: Hadrons (Baryons, Mesons)
- propagation and collisions of particles in mean fields
- approx. Kadanoff-Baym and Boltzmann-Uehling-Uhlenbeck equations solved
- A+A (~ 1990) 10 – 20 AGeV
- hadron+A (p+A, π+A) (~ 1995) up to 20 GeV
- γ+A (~ 1998) up to GeV
- e+A (~ 2000) up to 300 GeV
- ν+A (~ 2005 -) up to 1 TeV

Institut für Theoretische Physik, JLU Giessen

GiBUU

The Giessen Boltzmann-Uehling-Uhlenbeck Project

- **GiBUU** : **Quantum-Kinetic Theory and Event Generator** based on a BM solution of Kadanoff-Baym equations

- GiBUU propagates phase-space distributions, not particles

- Physics content and details of implementation in:
  Buss et al, Phys. Rept. 512 (2012) 1- 124

  Further details in **Gallmeister et al, Phys.Rev. C94 (2016) no.3, 035502**

- Code from gibuu.hepforge.org, latest version GiBUU 2021

GiBUU: Basics

Essential Properties:

1. Theory is semiclassical, it forgets about quantum coherence and replaces wavefunctions by local plan waves with quantum features: off-shell, Pauli-blocking
2. Consequence:
   1. Heavy-ion reactions are non-equilibrium, no coherence, can be described
   2. Semi-inclusive reactions such as (e,e‘pX) A can be described, but not exclusive (e,e‘p) A
   3. There are no shell-effects anywhere, only ‚average‘ nuclear properties→ energy transfers ~> 50 MeV
   4. FSI do not remember the ‚interactions before‘, except for kinematics

Quantum-kinetic Transport Theory from non-equilibrium Green‘s function method

- Kadanoff-Baym (1962) start from *eq. of motion for 1-particle* Green‘s function which depends on a chain of n-particle Green‘s functions

  - Approximations:
    - Truncate hierarchy of coupled Green‘s functions, i.e. neglect all explicit many-body Green‘s functions, absorb their effect into modeled self-energies.
    - Gradient approximation: assume that densities vary slowly in r- and p-space (good for heavier nuclei, in practice A >~ 12).

Nonequilibrium processes

- ‚Usual' Green's functions describe time-developments from in-state at $t = -\infty$ to out-state at $t = +\infty$ -> cross section

- In statistical (non-equilibrium) physics one is interested in expectation values of operators at finite (real) time t

Green's Functions for nonequilibrium processes

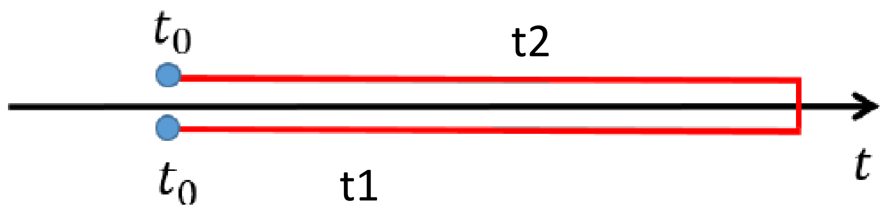
- In *non-equilibrium theory* the one-body density matrix ρ(x,x') is related to Green's function

$$G(x_1, x_2) = \qquad \equiv \frac{1}{\mathrm{Tr}\rho(t_0)} \mathrm{Tr}[\rho(t_0) T\phi(x_1)\phi(x_2)],$$

with $\rho(t_0)$ = density operator at initial time (Heisenberg picture)

$$\begin{aligned}
G(x_1, x_2) &= \frac{1}{\mathrm{Tr}\rho(t_0)} \mathrm{Tr}[\rho(t_0) T U^\dagger(x_1^0, t_0)\phi_I(x_1)U(x_1^0, t_0) \times U^\dagger(x_2^0, t_0)\phi_I(x_2)U(x_2^0, t_0)] \\
&= \frac{1}{\mathrm{Tr}\rho(t_0)} \mathrm{Tr}[\rho(t_0) T U^\dagger(x_1^0, t_0)\phi_I(x_1)U(x_1^0, x_2^0)\phi_I(x_2)U(x_2^0, t_0)] \\
&= \frac{1}{\mathrm{Tr}\rho(t_0)} \mathrm{Tr}[\rho(t_0) T_P \phi_I(x_1)\phi_I(x_2)U_{CTP}(t_0)] \\
&\equiv \langle T_P \phi(x_1)\phi(x_2)\rangle \\
&= \theta_P(x_1 - x_2)\langle\phi(x_1)\phi(x_2)\rangle + \theta_P(x_2 - x_1)\langle\phi(x_2)\phi(x_1)\rangle,
\end{aligned}$$

Green's Functions on Contour



Schwinger-Keldysh Contour

- Green's Functions live on the closed-time path:

$$G(x_1,x_2) = \begin{pmatrix} G^{++}(x_1,x_2) & G^{+-}(x_1,x_2) \\ G^{-+}(x_1,x_2) & G^{--}(x_1,x_2) \end{pmatrix} = \begin{pmatrix} G^{F}(x_1,x_2) & \pm G^{<}(x_1,x_2) \\ G^{>}(x_1,x_2) & G^{\overline{F}}(x_1,x_2) \end{pmatrix},$$

- G^F : ‚normal' Feynman propagator
- $G^>$: t_1 on negative branch, t_2 on positive branch, $t_1 > t_2$

$$\begin{aligned} G^{F}_{\alpha\beta}(x_1,x_2) &= \langle T\psi_\alpha(x_1)\overline{\psi}_\beta(x_2)\rangle\,, \\ G^{\overline{F}}_{\alpha\beta}(x_1,x_2) &= \langle T_A\psi_\alpha(x_1)\overline{\psi}_\beta(x_2)\rangle\,, \\ G^{<}_{\alpha\beta}(x_1,x_2) &= \langle\overline{\psi}_\beta(x_2)\psi_\alpha(x_1)\rangle\,, \\ G^{>}_{\alpha\beta}(x_1,x_2) &= \langle\psi_\alpha(x_1)\overline{\psi}_\beta(x_2)\rangle\,, \end{aligned}$$

Green‘s Functions and Selfenergies

Dyson equation couples Green‘s functions to selfenergy Σ

$$\hat{S}(x_1, x_2) = \hat{S}_0(x_1, x_2) + \hat{S}_0(x_1, x_1') \odot \hat{\Sigma}(x_1', x_2') \odot \hat{S}(x_2', x_2),$$

$$S_{0x}^{-1} = \mathrm{i}\not{\partial}_x - m,$$

$$S_{0x_1}^{-1} S^{<}(x_1, x_2) = \Sigma^{\mathrm{ret}}(x_1, y) \odot S^{<}(y, x_2) + \Sigma^{<}(x_1, y) \odot S^{\mathrm{adv}}(y, x_2),$$

Kadanoff-Baym Equations: System of coupled integro-differential equations

One equation for each particle

Kadanoff-Baym Equations

$$
\begin{aligned}
\mathrm{i}\left(\partial\!\!\!/_{x_1} S^{<}(x_1,x_2) + S^{<}(x_1,x_2)\overleftarrow{\partial\!\!\!/}_{x_2}\right) &- [\mathrm{Re}\,\Sigma^{\mathrm{ret}} \odot S^{<}](x_1,x_2) + [S^{<} \odot \mathrm{Re}\,\Sigma^{\mathrm{ret}}](x_1,x_2) \\
&- [\Sigma^{<} \odot \mathrm{Re}\,S^{\mathrm{ret}}](x_1,x_2) + [\mathrm{Re}\,S^{\mathrm{ret}} \odot \Sigma^{<}](x_1,x_2) \qquad (25) \\
= \frac{1}{2}\Big\{[\Sigma^{>} \odot S^{<}](x_1,x_2) + [S^{<} \odot \Sigma^{>}]\,(x_1,x_2) &- [\Sigma^{<} \odot S^{>}](x_1,x_2) - [S^{>} \odot \Sigma^{<}](x_1,x_2)\Big\}\,.
\end{aligned}
$$

Kadanoff-Baym Equations: 1 equation for each particle

L.P. Kadanoff & G. Baym
Quantum Statistical Mechanics, 1962:

[*These equations*] represent a horribly complex set of integral equations for a. To get detailed numerical answers, it is necessary to solve these equations. The best we can do, ... , is to use some iteration procedure.

Kadanoff-Baym Equations

- Approximations:
  - Model self-energies
  - Assume that densities change smoothly with coordinate and momentum
    -> better for heavier nuclei
  - ➔ Introduce Wigner functions

Wigner Transforms

- *Classical* phase space distribution *f(t,x,p)* allows to calculate average of any observable:

$$\langle A\rangle = \int d^3\mathbf{x} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} A(\mathbf{x},\mathbf{p}) f(t,\mathbf{x},\mathbf{p}).$$

- *Quantum Mechanics*: Average of any operator Â(x,p)

$$\left\langle \widehat{A} \right\rangle = \mathrm{Tr}\left(\widehat{A}\widehat{\rho}\right).$$

with the one-body density matrix ρ(x,x‘)

- Define Wigner Transform

$$W(\mathbf{x},\mathbf{p}) = \int d^3\mathbf{y} \exp\left(\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{y}\right) \left\langle \mathbf{x}-\frac{\mathbf{y}}{2}\right| \widehat{\rho} \left|\mathbf{x}+\frac{\mathbf{y}}{2}\right\rangle$$

useful when density matrix depends only weakly on the cm coordinate of x,x‘

$$\left\langle \widehat{A} \right\rangle = \int d^3\mathbf{x} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} A(\mathbf{x},\mathbf{p}) W(\mathbf{x},\mathbf{p}),$$

Green‘s Functions and densities

Vector current density: $F_V^\mu(x,p) = -\mathrm{i}\,\mathrm{tr}[\tilde{S}^<(x,p)\gamma^\mu]$

$$\partial_\mu F_V^\mu(x,p) - \mathrm{tr}\left\{\mathrm{Re}\,\tilde{\Sigma}^{\mathrm{ret}}(x,p), -\mathrm{i}\tilde{S}^<(x,p)\right\}_{\mathrm{pb}} + \mathrm{tr}\left\{\mathrm{Re}\,\tilde{S}^{\mathrm{ret}}(x,p), -\mathrm{i}\tilde{\Sigma}^<(x,p)\right\}_{\mathrm{pb}} = C(x,p).$$

with ‚collision term‘

$$C(x,p) = \mathrm{tr}\left[\tilde{\Sigma}^<(x,p)\tilde{S}^>(x,p) - \tilde{\Sigma}^>(x,p)\tilde{S}^<(x,p)\right].$$

$$-\mathrm{i}\tilde{S}^<(x,p) = -2\,f(x,p)\;\mathrm{Im}\,\tilde{S}^{\mathrm{ret}}(x,p),$$
$$\mathrm{i}\tilde{S}^>(x,p) = -2\,[1-f(x,p)]\;\mathrm{Im}\,\tilde{S}^{\mathrm{ret}}(x,p),$$

Pauli Principle

f = Lorentz scalar function

$S^<$ = (scalar) density of particles, $S^>$ = (scalar) density of holes

From now on: S = G !

Quantum-kinetic Transport Theory from non-equilibrium Green's function method

$$\mathrm{i}G^{<}(x,p) = +2f(x,p)\,\Im G^{\mathrm{ret}}(x,p)$$
$$\mathrm{i}G^{>}(x,p) = -2(1-f(x,p))\,\Im G^{\mathrm{ret}}(x,p)$$

This allows to introduce the Spectral Function

A(x,p) = imaginary part of sp propagator

$$F_V^{\mu} = (p^{*\mu}/E^{*})F,$$

$$F(x,p) = 2\pi g f(x,p) A(x,p)$$

$$\mathcal{D}F(x,p) + \mathrm{tr}\,\left[\Re G^{\mathrm{ret}}(x,p), -\mathrm{i}\Sigma^{<}(x,p)\right]_{\mathrm{PB}} = C(x,p)$$

Botermans-Malfliet approx

$$\mathcal{D}F(x,p) - \mathrm{tr}\left\{\Gamma(x,p)f(x,p), \Re G^{\mathrm{ret}}(x,p)\right\}_{\mathrm{PB}} = C(x,p)$$

Width of spectral function

Quantum-kinetic Transport Theory from non-equilibrium Green's function method

On-shell drift term — Off-shell transport term — Collision term

$$\mathcal{D}F(x,p) - \mathrm{tr}\left\{\Gamma f, \mathrm{Re}S^{\mathrm{ret}}(x,p)\right\}_{\mathrm{PB}} = C(x,p) \ .$$

$$\mathcal{D}F(x,p) = \{p_0 - H, F\}_{\mathrm{PB}} = \frac{\partial(p_0 - H)}{\partial x}\frac{\partial F}{\partial p} - \frac{\partial(p_0 - H)}{\partial p}\frac{\partial F}{\partial x}$$

H contains mean-field potentials

Describes time-evolution of *F(x,p)*

$$F(x,p) = 2\pi g f(x,p)\,\mathcal{P}(x,p)$$

Spectral function: $\mathcal{P}(x,p)$

Phase space distribution: $f(x,p)$

KB equations with BM offshell term

Essential for any in-medium physics

One such equation for each kind of particle: neutrino, nucleon, resonance, meson,
All coupled through mean field potential and collision term *C*

Giessen Model: Theory and Generator

Initial State Interactions

- Nucleons are bound in a momentum-dep mean-field potential
- Treats all ISI processes: QE, RES, 2p2h, DIS (switch to DIS = PYTHIA at W ~ 2 - 3 GeV)
- The low-energy part similar to Valencia model, but binds nuclei
- Contains large number of N* resonances and mesons, up to charm
- Not restricted to the low energies of Valencia model

Final State Interactions: quantum-kinetic transport theory

- Contains elastic and inelastic FSI, tries to respect time-reversal invariance
- Fully relativistic transport in potential, trajectories numerically integrated
- Relativistically correct collision criteria for FSI
- Allows for off-shell transport of broad spectral functions
- Contains modelling of color transparency, formation times

Giessen model ingredients

Baryon Resonances up to *W ~ 2* GeV transported explicitly, with properties from PDG, *lifetime determined by widths*

DIS Processes (*W > 2* GeV) described by string fragmentation (PYTHIA), *lifetime determined by fragmentation time-scale*, no external `formation times`:

K. Gallmeister, U. Mosel
``Time Dependent Hadronization via HERMES and EMC Data Consistency''
Nucl. Phys. A **801**(2008) 68

K. Gallmeister, T. Falter
``Space-time picture of fragmentation in PYTHIA/JETSET for HERMES and RHIC''
Phys. Lett. B **630** (2005) 40

Problem: Cross section development during these `formation times`, often taken to be *0* , e.g. GENIE: no interactions within *0.342* fm/c !

Contradicts experiments!

GiBUU Ground State

- Start with empirical density distribution, use reasonable energy-density functional for nuclear matter→ calculate mean field potential, dependent on *r* and *p*

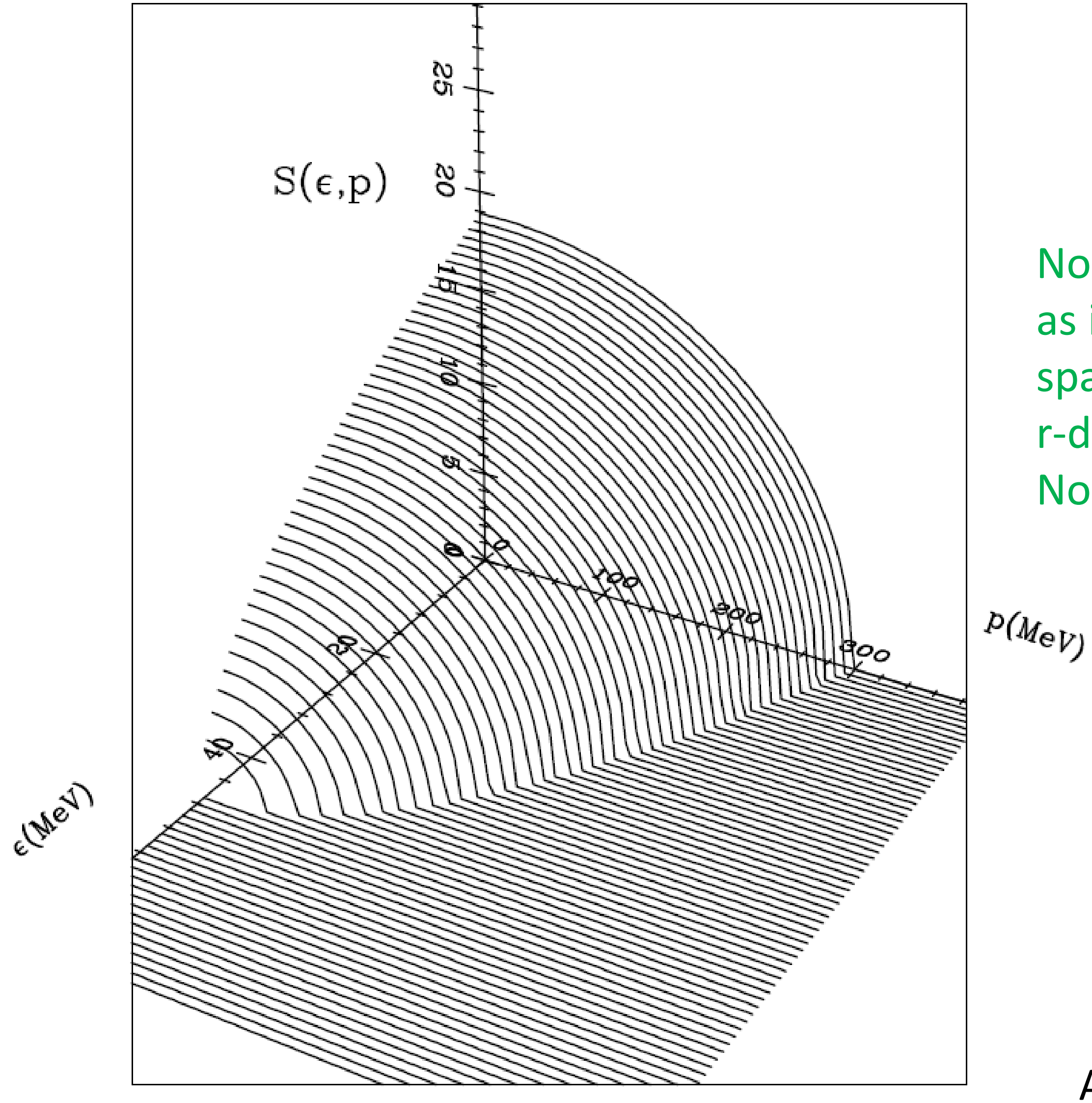
- Use density to obtain momentum distribution by local Thomas-Fermi model: $k_F^3(r) \sim \rho(r)$

- Readjust k_F slightly to maintain constant Fermi energy

- Spectral Function: $$\mathcal{P}_h(\mathbf{p},E) = \int_{\text{nucleus}} \mathrm{d}^3x\, F(\mathbf{x}, t=0, \mathbf{p}, E)$$

$$= g \int_{\text{nucleus}} \mathrm{d}^3x\, \Theta\left[p_{\mathrm{F}}(\mathbf{x}) - |\mathbf{p}|\right] \Theta(E)\, \delta\left(E - m + \sqrt{\mathbf{p}^2 + m^{*2}(\mathbf{x},\mathbf{p})}\right)$$

Semiclassical Spectral Function



No spiky behavior
as in RFG because of
spatial integration over
r-dependent potential,
No shell effects

Alberico et al,
Nucl.Phys. A634(1998) 233

Collision term

$$C(x,p) = \mathrm{tr}\left[\Sigma^{<}(x,p)G^{>}(x,p) - \Sigma^{>}(x,p)G^{<}(s,p)\right]$$

gain term loss term

$G^{<}$ = particle density ~ f*a

$G^{>}$ = hole density ~ (1 –f)*a

$\Sigma^{>}$: collision rate out of phase-space element (x,p),

$\Sigma^{<}$: collision rate for transition into that element

In thermal equilibrium gain = loss
Transport does not need any a priori assumptions about thermal equilibrium, but will tell you if and when it is reached.

Short-Range Correlations in Transport Theory

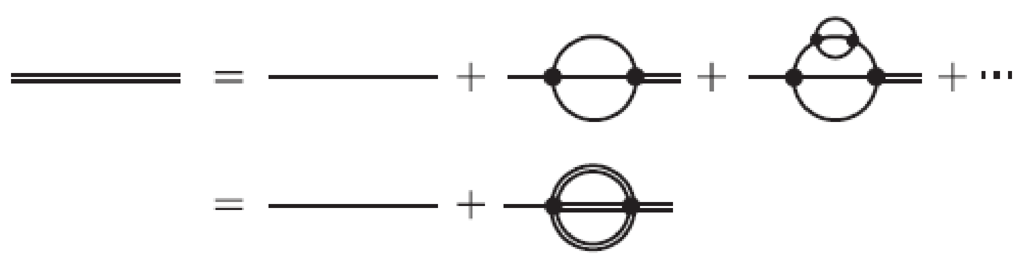
- ~ 1990: SRC found in correlated nuclear many-body calculations (Fantoni et al, Benhar, degli Atti):
  2 correlated nucleons with low cm momentum, but large (>p_F) momenta.

$$a(\omega,p) = \frac{\Gamma(\omega,p)}{(\omega - \frac{p^2}{2m_N} - \mathrm{Re}\Sigma(\omega,p))^2 + \frac{1}{4}\Gamma^2(\omega,p)},$$

$$\Gamma(\omega,p) = 2\mathrm{Im}\Sigma(\omega,p) = i(\Sigma^>(\omega,p) - \Sigma^<(\omega,p)).$$

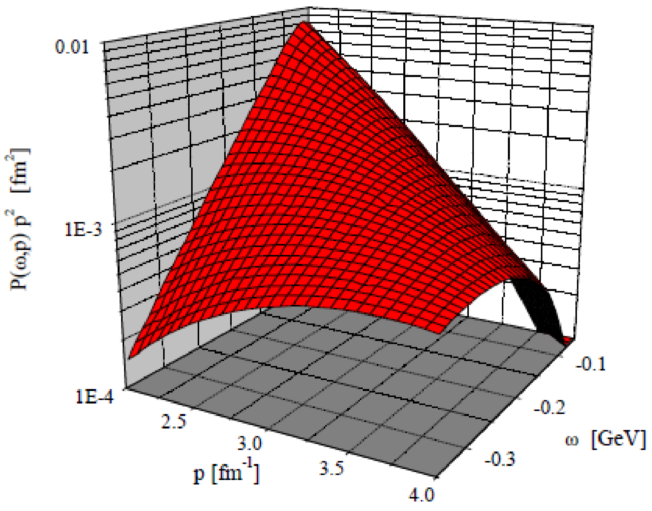
$$\Sigma^>(\omega,p) = g\int \frac{d^3p_2 d\omega_2}{(2\pi)^4}\frac{d^3p_3 d\omega_3}{(2\pi)^4}\frac{d^3p_4 d\omega_4}{(2\pi)^4}(2\pi)^4\delta^4(p+p_2-p_3-p_4)\,\overline{|\mathcal{M}|^2} \times g^<(\omega_2,p_2)g^>(\omega_3,p_3)g^>(\omega_4,p_4) \quad (2)$$

$$\Sigma^<(\omega,p) = g\int \frac{d^3p_2 d\omega_2}{(2\pi)^4}\frac{d^3p_3 d\omega_3}{(2\pi)^4}\frac{d^3p_4 d\omega_4}{(2\pi)^4}(2\pi)^4\delta^4(p+p_2-p_3-p_4)\,\overline{|\mathcal{M}|^2} \times g^>(\omega_2,p_2)g^<(\omega_3,p_3)g^<(\omega_4,p_4), \quad (3)$$

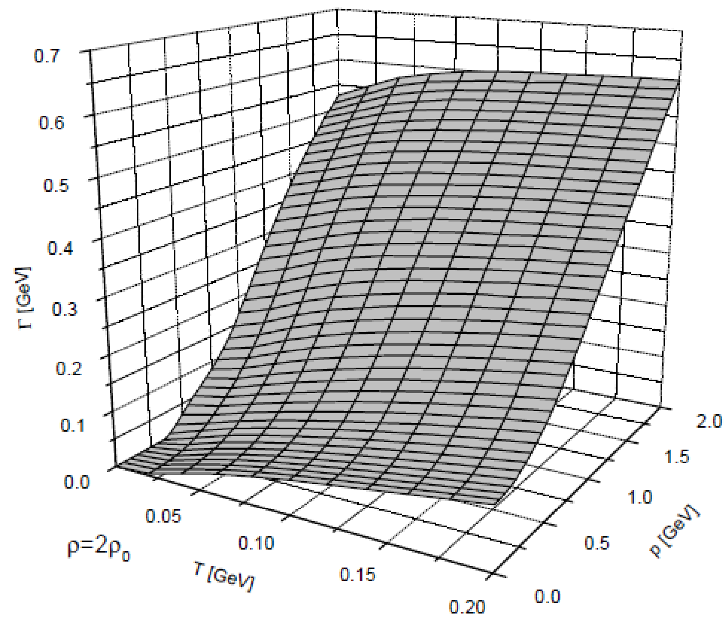


Short-range Correlations

Interaction constant in momentum space -> δ-force in r-space



Groundstate



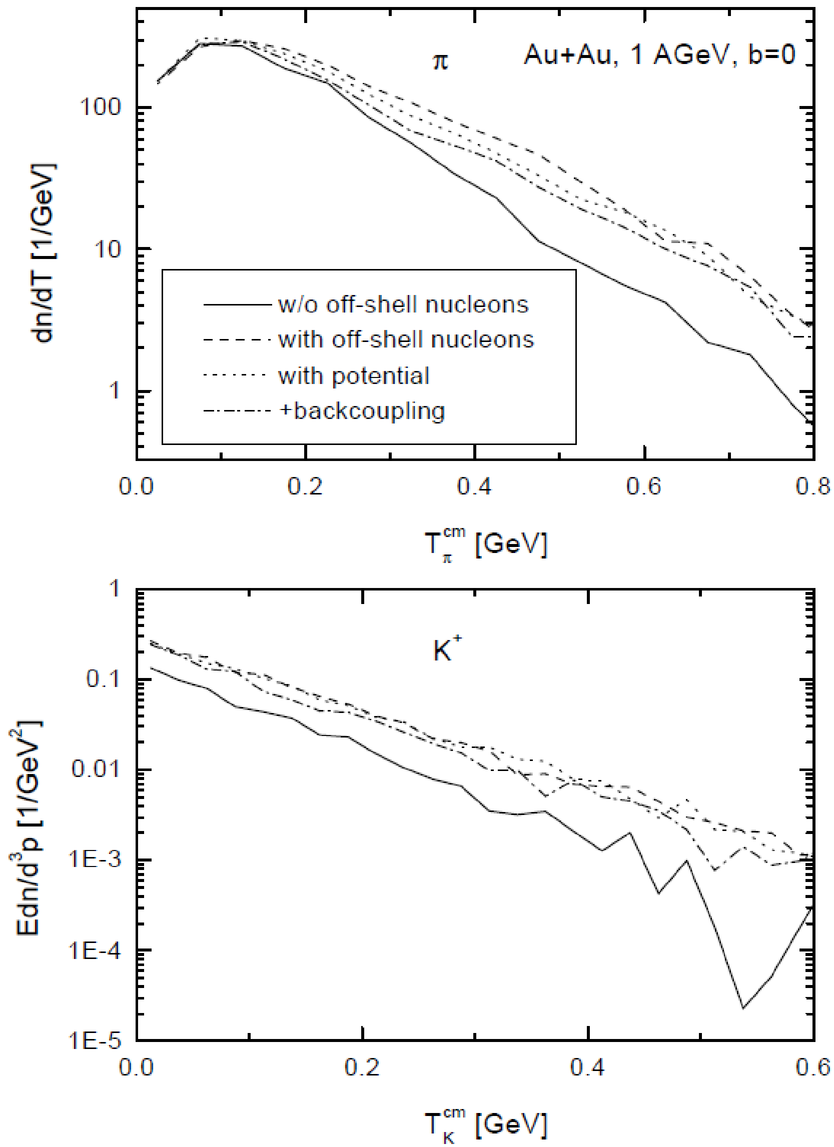
Excited state

A nucleon in the groundstate of a nucleus does not have the free mass, but must be described by a spectral function.

If this nucleon is kicked out of the nucleus in a reaction, one needs off-shell transport to ensure that the free nucleon has the correct, sharp mass

Now some applications´, from 1990 - now

Src in Heavy-Ion Collisions



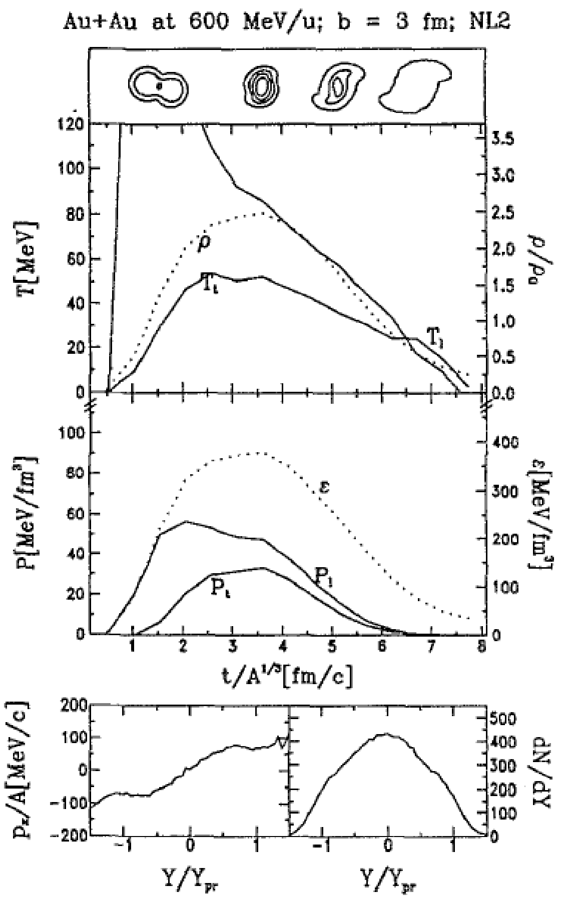
Effenberger et al
Phys.Rev.C 60 (1999) 051901

src affect threshold behavior

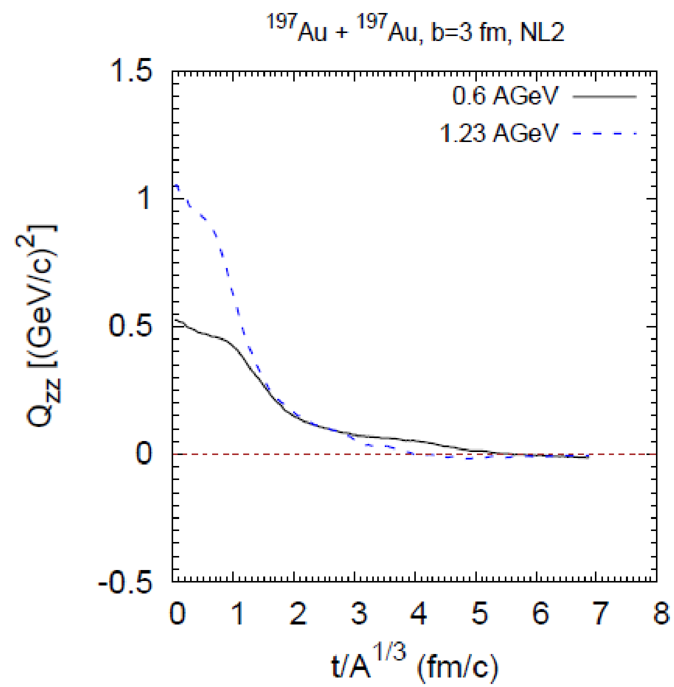
Do heavy-ion reactions really thermalize?

Nowadays often used model for particle production in HI collisions: ‚Coarse Graining', assumes local equilibrium.

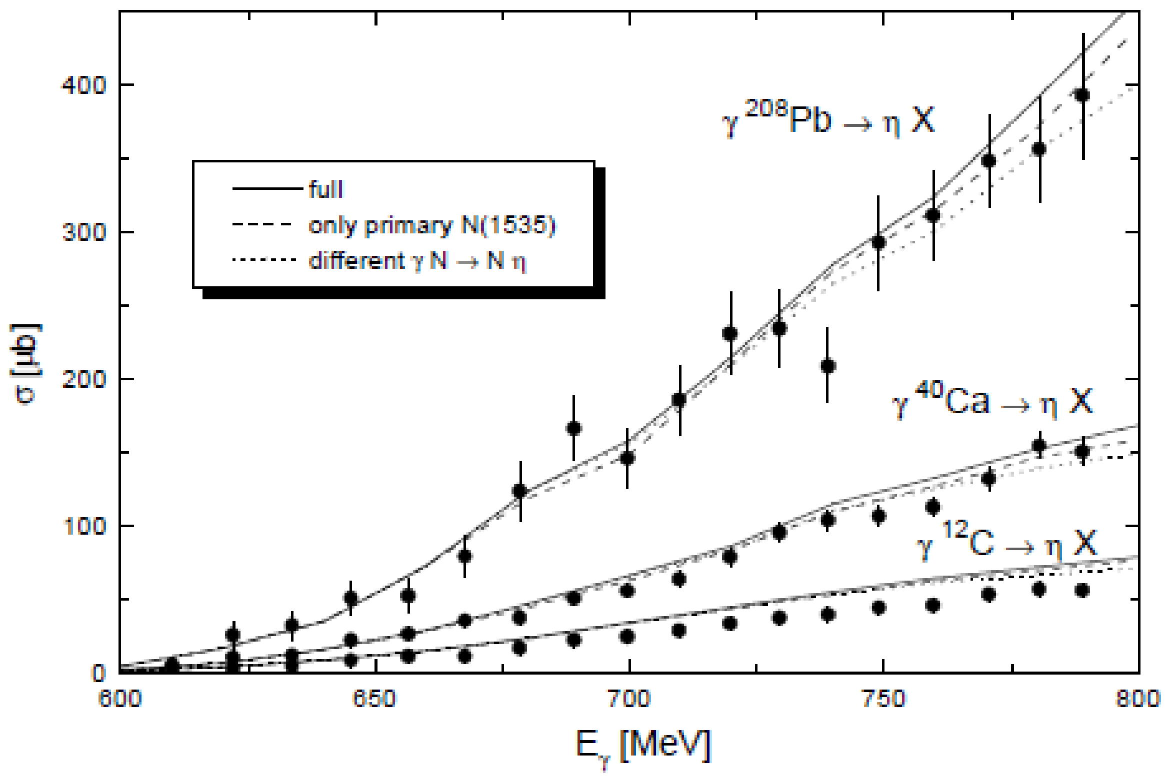
BUT: is this the correct physics at SIS energies? A relativistic transport calculation (Lang et al, 1991) said something else:



Recent check (2021) by Larionov confirms Lang:



Photoproduction of mesons



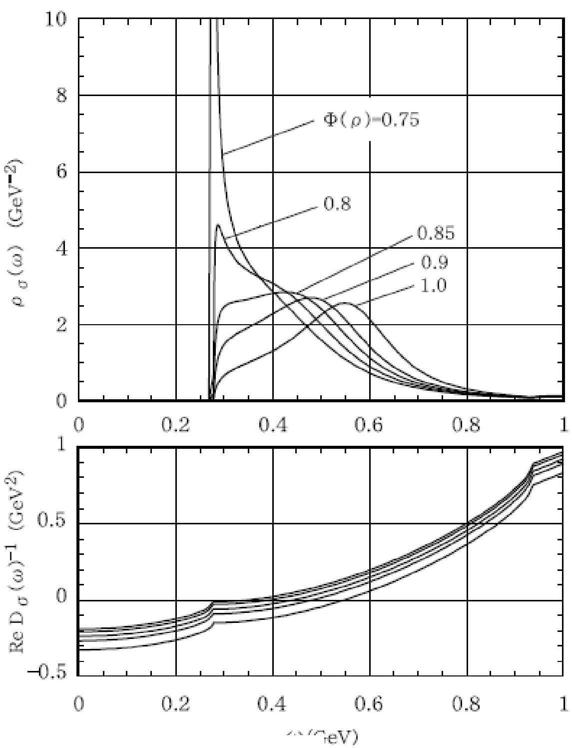
Theory: Effenberger et al, 1997
Data: Metag et al, TAPS

Chiral Condensate in Nuclei

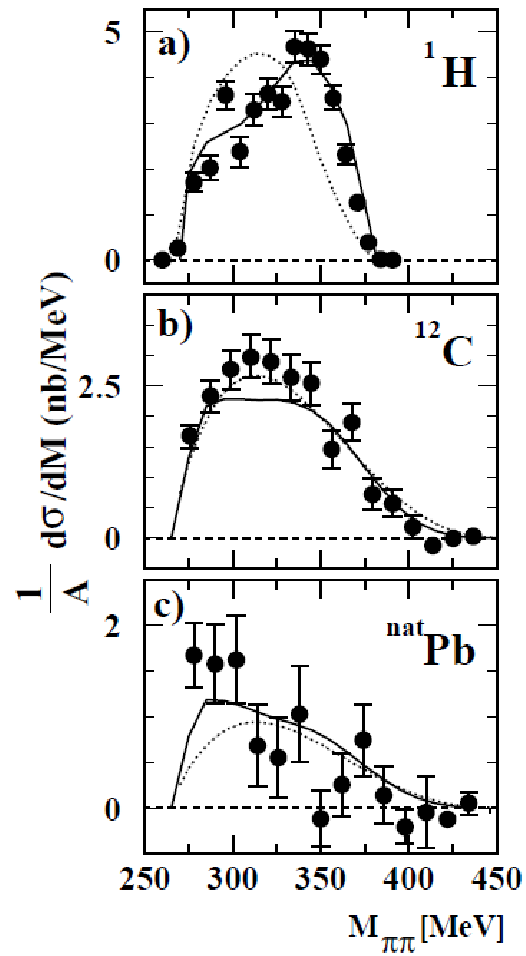
Hatsuda, Kunihiro, Shimizu, PRL 82 (1999):

Chiral symmetry is nearly restored inside nuclei.

Observable: Lowering of σ mass in nuclei:

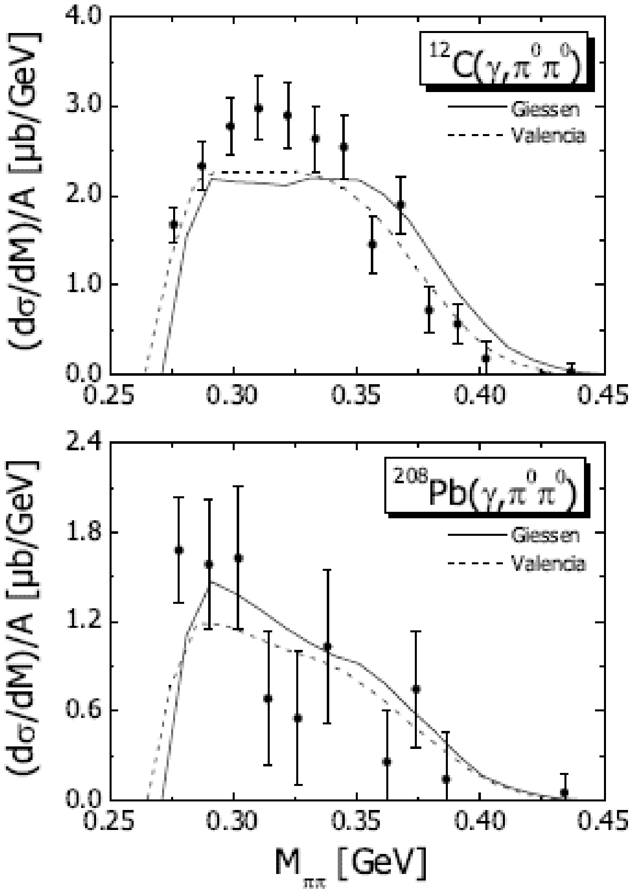


$$\langle\sigma\rangle \equiv \sigma_0\ \Phi(\rho).$$



Exp: TAPS, Messchendorp et al, 2002

Chiral Symmetry in Nuclei restored?

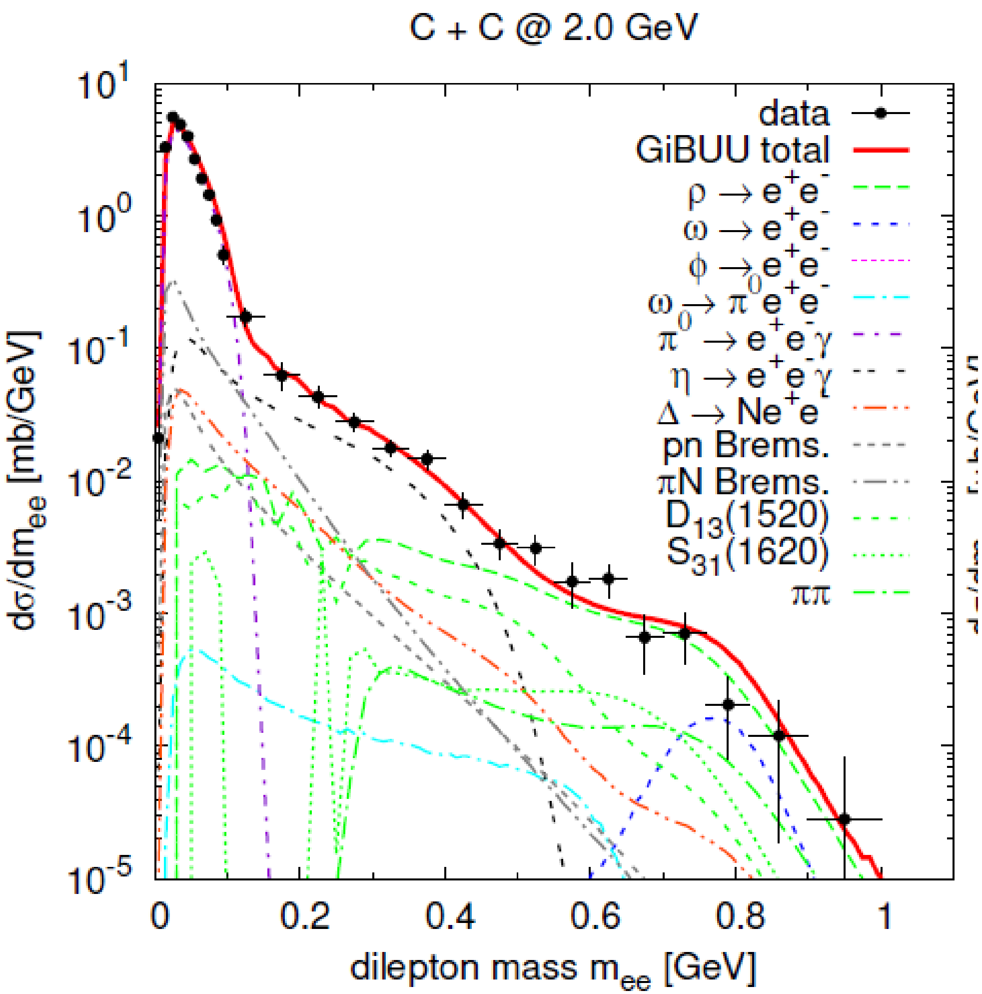


Lowering of σ-spectral function described:

Effect of final state interactions in pions

Muehlich et al, 2004

Timelike photon (= dilepton) production



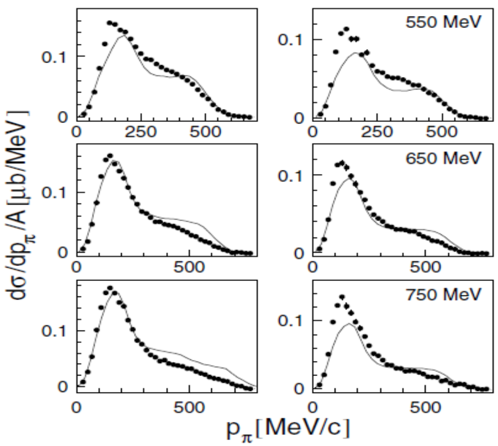
Data: HADES,
Theory:
Larionov et al, 2021

Dilepton spectrum in the HADES experiment

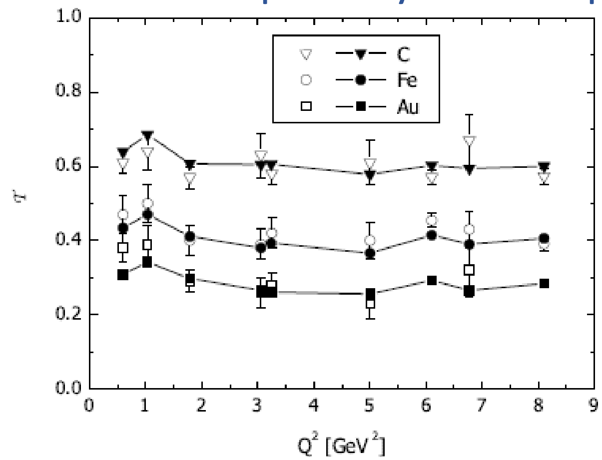
Check: pions, protons

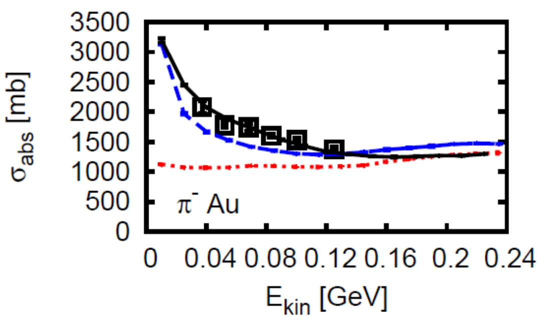
(Leitner et al, https://inspirehep.net/literature/819969 (2009))

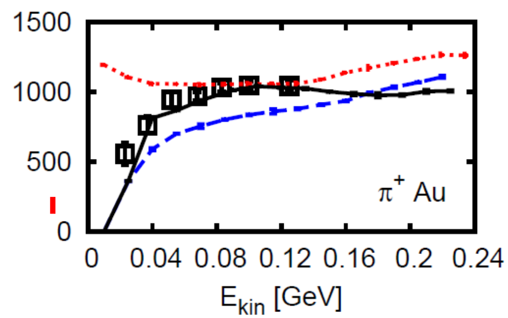
$\gamma \rightarrow \pi^0$ on Ca Pb



Proton transparency in eA -> p + X







Pion reaction Xsect.

--- no potential

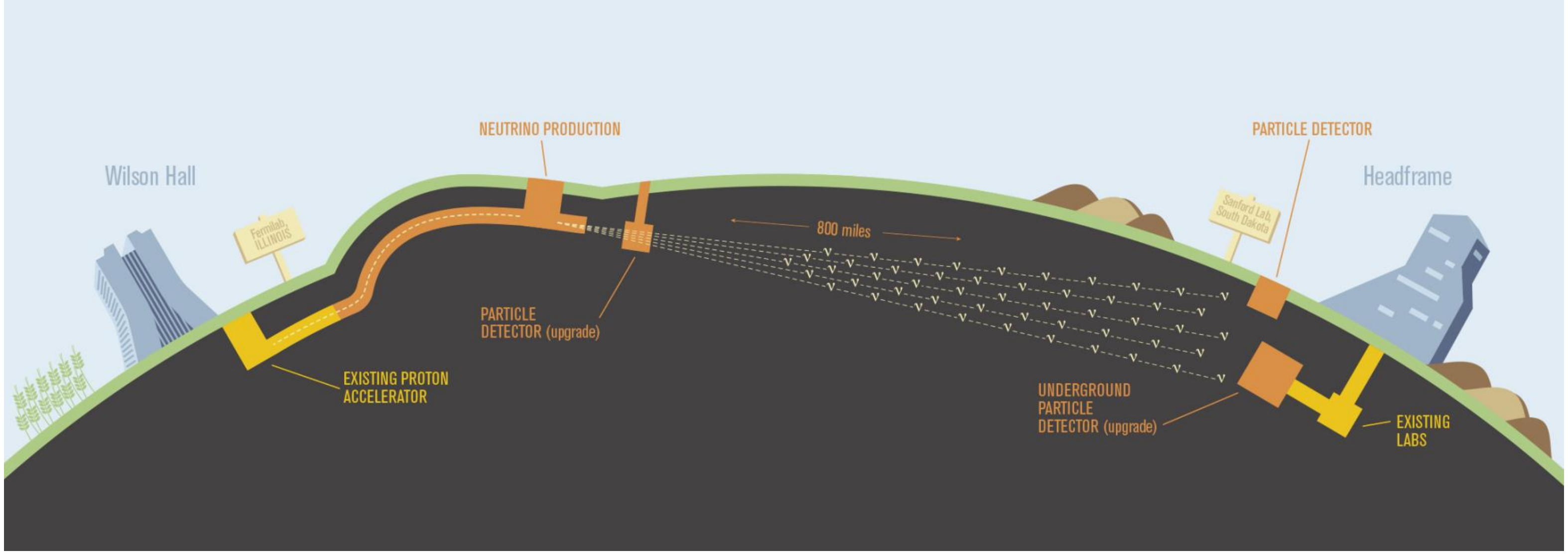
--- Coulomb only

--- Coulomb + nuclear

DUNE

‚Flagship experiment of US high-energy physics‘

p + A -> π, K -> ν +X



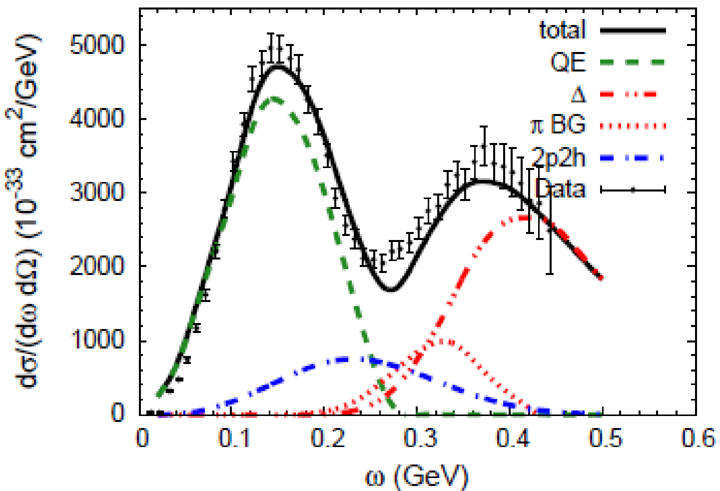
Neutrino beam is very wide (in meters and in energy!)
➔ need to reconstruct the neutrino energy event-by-event,

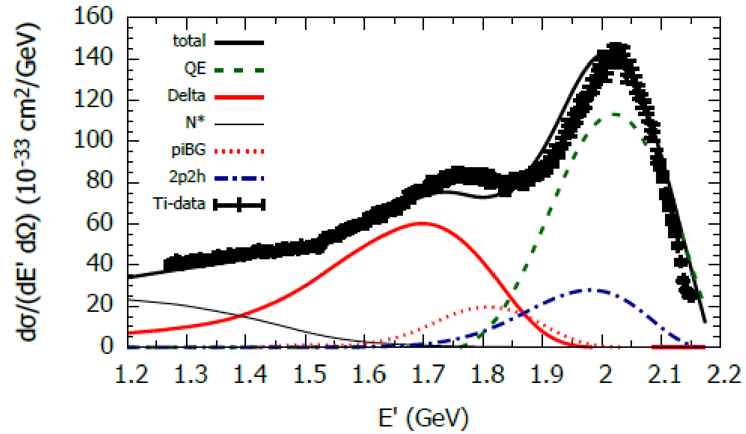
Reconstruction needs quantitative understanding of neutrino-nucleus interactions

Lepton-induced Reactions on Nuclei

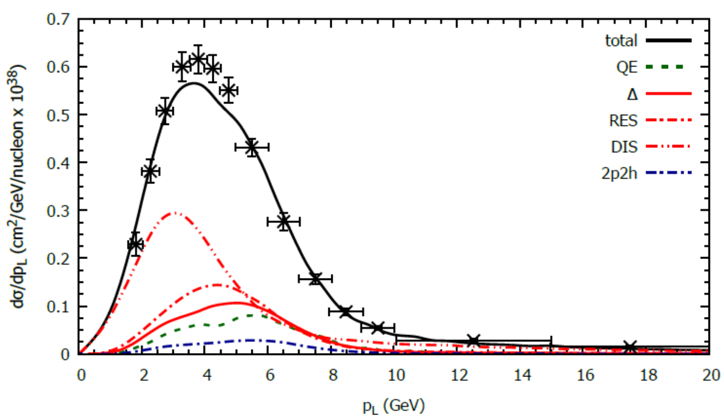
Electrons

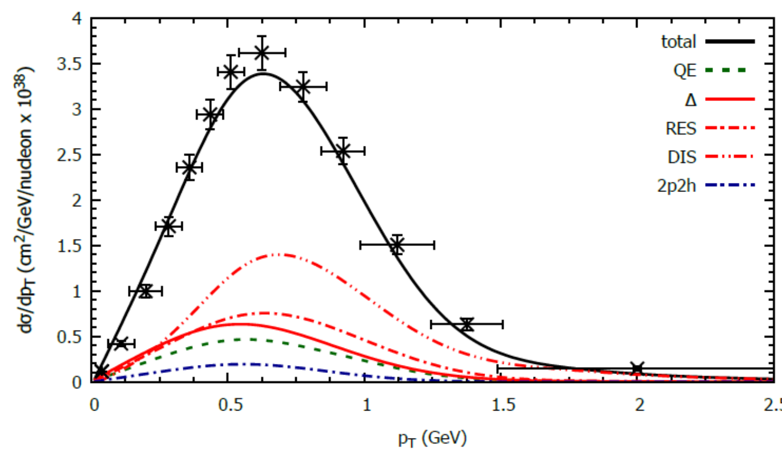
Data: JLAB 2019,
Mosel and Gallmeister,
Phys.Rev.C 99 (2019) 6, 064605





Neutrinos





Data: MINERvA_ME, 2021

Summary

1. Nuclear reactions always involve non-equilibrium phases, must be taken into account when looking for actual observables
2. KB equations are THE tool to describe non-equlibrium phases and their approach to equilibrium (if any)
3. GiBUU is built on an (approximate) solution of the KB equations
4. Produces not only inclusive X-sections (such as Scaling, Spectral Function, GFMC methods), but full event final state files, 4-vectors for all particles
5. GiBUU has been applied to a wide variety of nuclear reactions
6. Experiments like HADES for heavy-ions and DUNE (for neutrinos) use GiBUU