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РОСАТОМ

Creation of the theoretical data base for the rare nuclear reactions, calculated by the quark-level model of nuclear reactions CHIPS

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Perspectives of the new theoretical data base for cross-sections of the nA reactions



Prediction of the cross-sections of many rare nA reactions, which are not measured and can't be assessed by any empirical model with free parameters:

- the neutron-nuclear exclusive reaction cross-sections for rare isotope targets;
- the exclusive cross-sections of reactions with production of heavy nuclear fragments, which can significantly reduce radiation strength of nuclear materials;
- the anisotropy of differential multiplicities of the generated nuclear fragments.

More accurate fit for the stopping power of the nuclear isotopes at low energy:

- generation of the speed distribution of the γ -radioactive nuclear fragments for more accurate simulation of the Doppler broadening of γ -lines in the measured γ -spectra;
- the bend gap factor in the stopping power of the low energy ions in insulators;
- the electron screening factor in the elastic ion-ion scattering cross-section.

The theoretical data base for the unmeasured lifetimes of nuclear γ -transitions.

- the empirical fit for the measured E1, M1, E2, and M2 γ -transitions in nuclei;
- CHIPS modelling of the γ -radiation during the quark exchange between the excited nuclear cluster (Quasmon) and the cold nuclear clusters in nuclear reactions;
- quark-level calculation of the nuclear excited states and γ -transitions between them.

The quark-level CHIPS algorithm for nuclear reactions in flight and at rest



Nonperturbative physical vacuum

$$T_c = 220.5 \text{ MeV}$$

The Chiral Invariant Phase Space (CHIPS) model considers a nucleon as an ensemble of 3 massless quarks, surrounded by the physical vacuum with the boiling temperature T_c .

The physical vacuum separates clusters, which exchange quarks of the same color through it.

The quark exchange through the vacuum barrier shifts exchanging N nucleons from their mass shells and bound them in *clusters*.

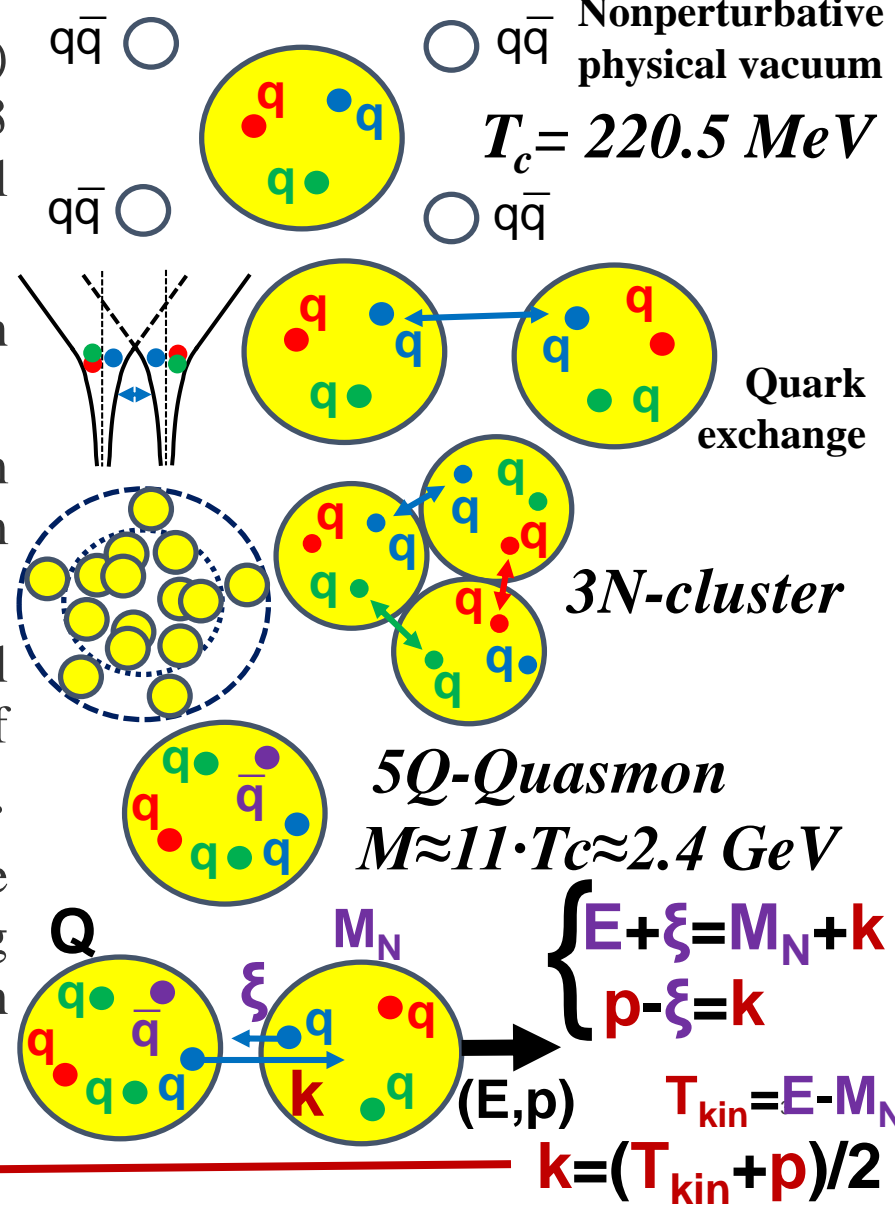
The N -clusters can accumulate the external energy (*Quasmon*) by increasing a number of quarks $n(T_c): M_Q \approx (2n-1)T_c, n \approx (M_Q/T_c + 1)/2$.

The n *Quasmon* (nQ) exchanges a quark of the energy k with the N -cluster quark ξ , knocking out the corresponding nuclear fragment with mass M_N , energy T_{kin} , and momentum p , then

hard

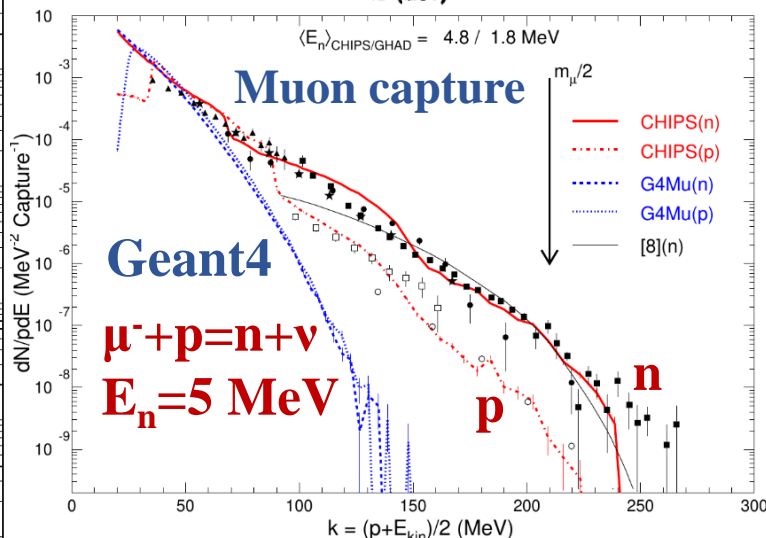
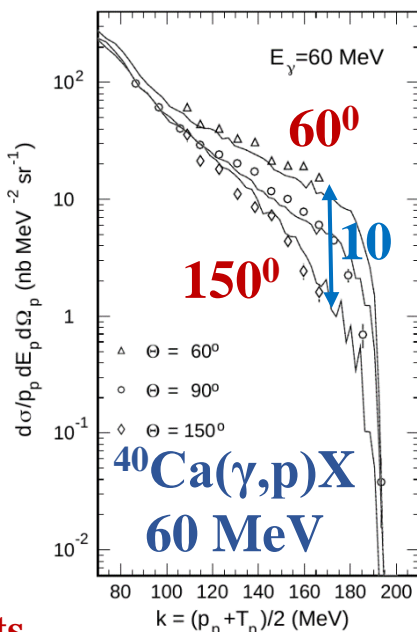
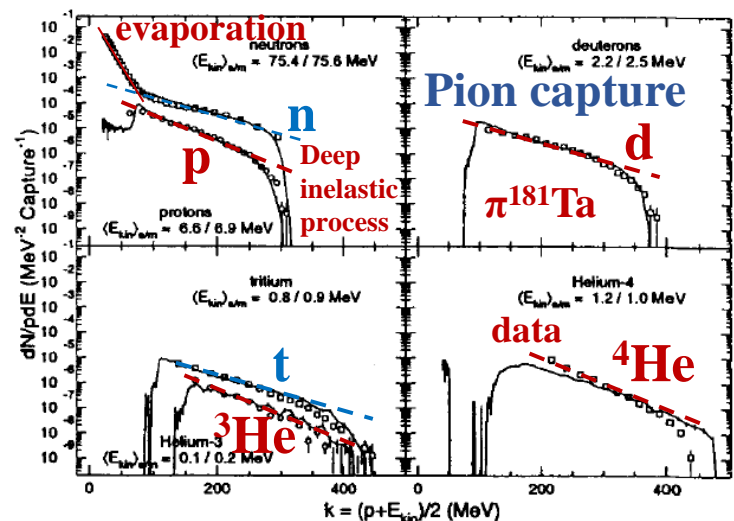
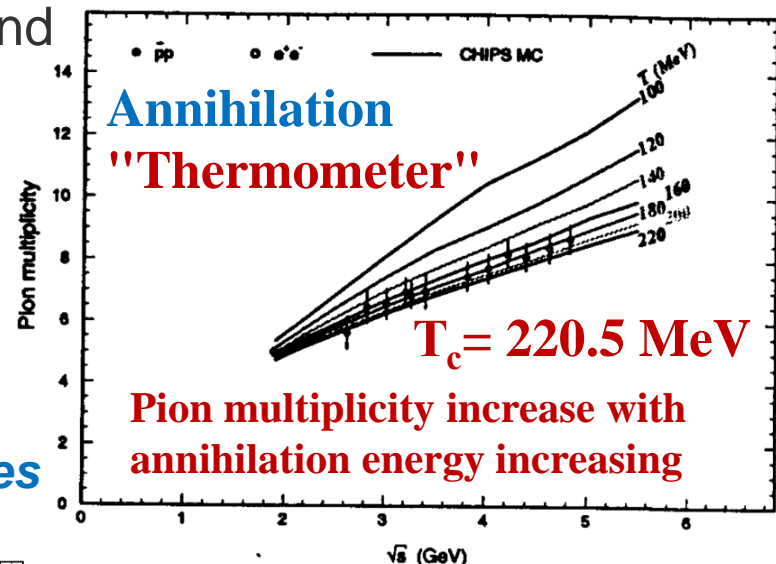
hadronization:

$$k = (T_{kin} + p)/2$$



The most emphatic quark-level effects in nuclear reactions

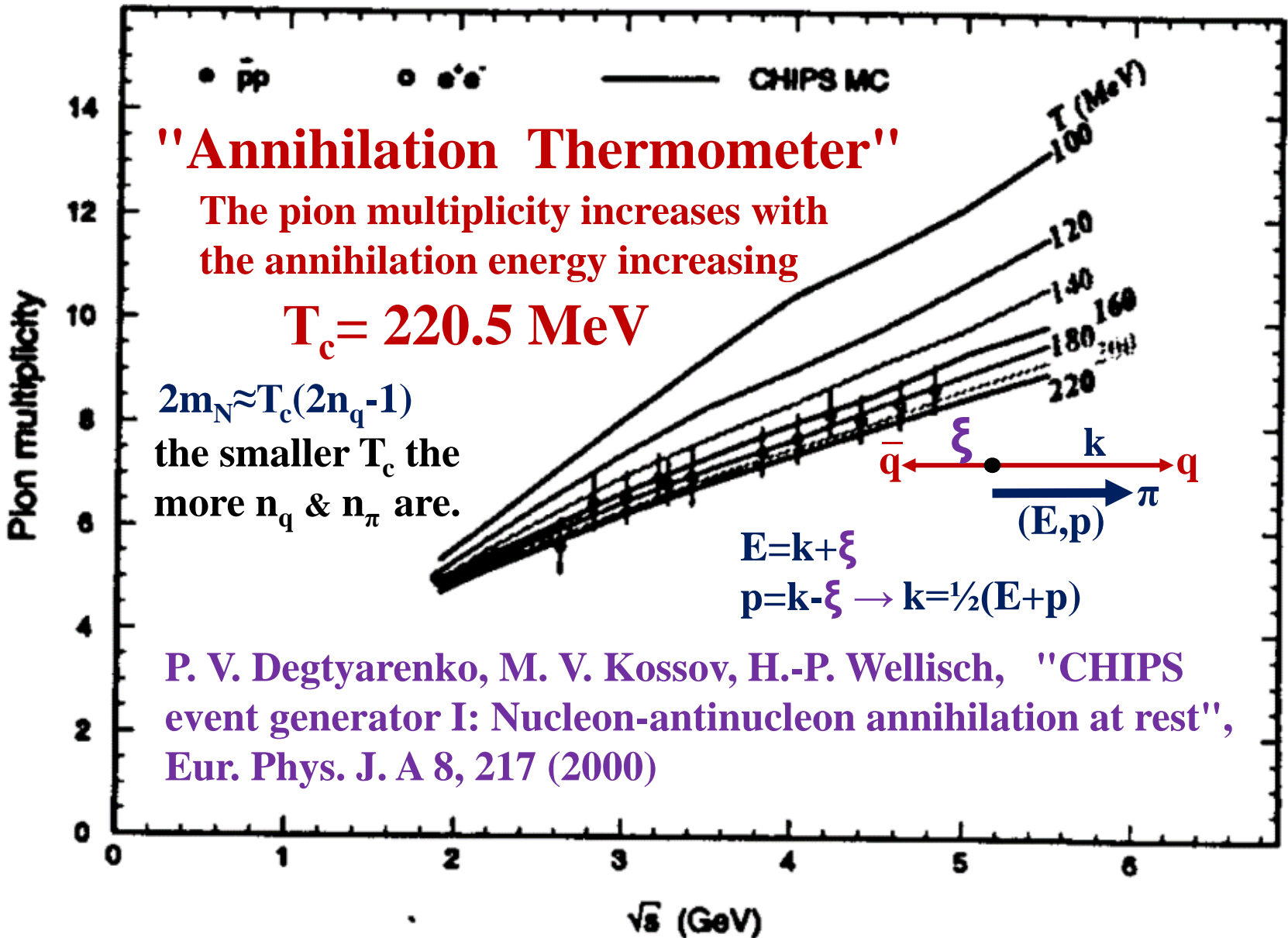
- Pion multiplicity in the proton-antiproton and electron-positron **annihilation**
- Neutron spectra in **pion capture** at rest
- **Anisotropy** of the proton spectra in low energy photonuclear reactions at **60 MeV**
- Neutron spectra in **muon capture** at rest
- **Vacuum temperature T_c and $1s$ hadron masses**



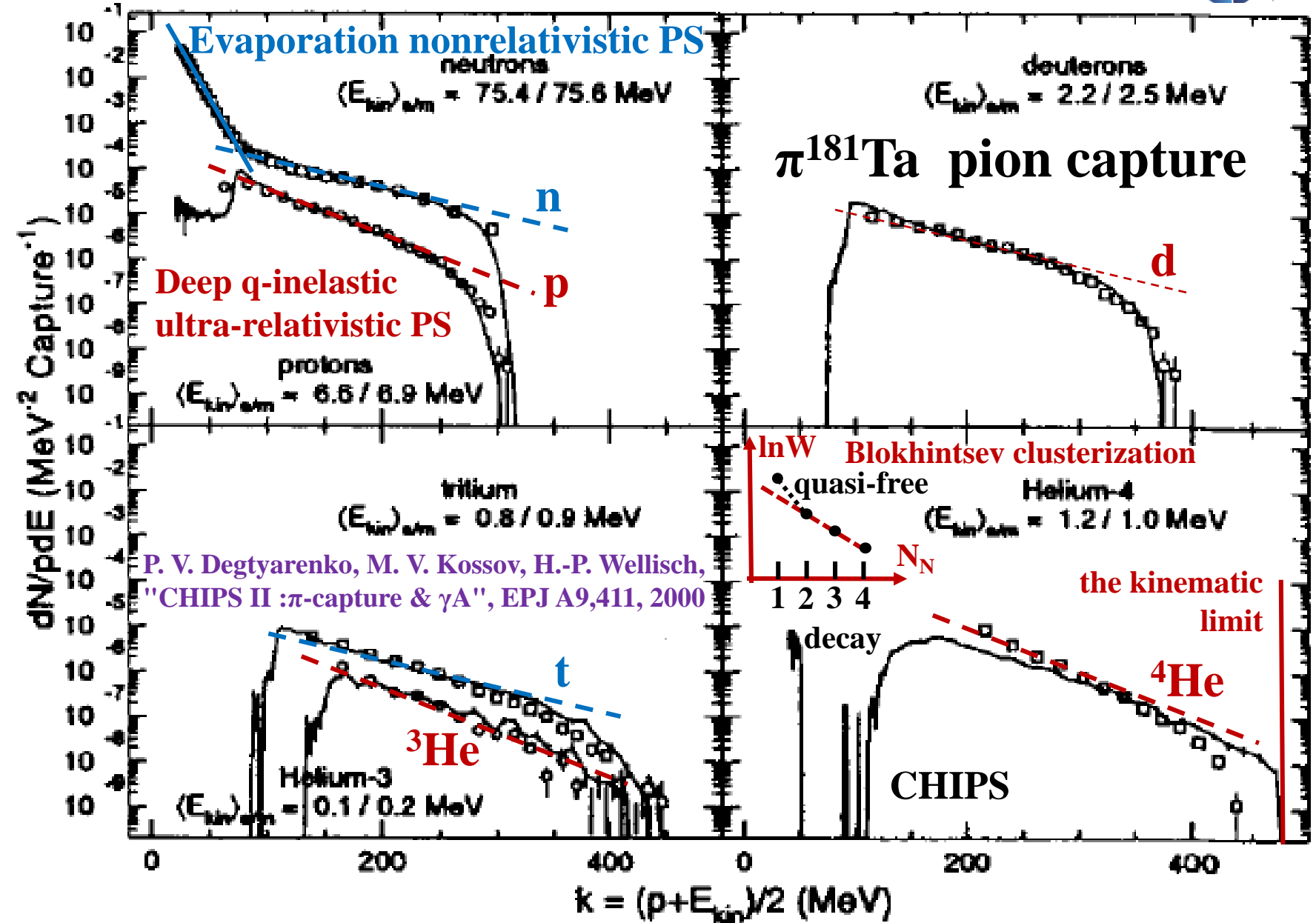
The deep inelastic (quark-level) processes + the neutron evaporation. Production of heavy nuclear fragments.

The additional quark-level CHIPS processes: $\mu^- + u \rightarrow d + \nu$ ($m_\mu/2$) и $\mu^- \rightarrow d + \bar{u} + \nu$ (m_μ)

Vacuum temperature in annihilation



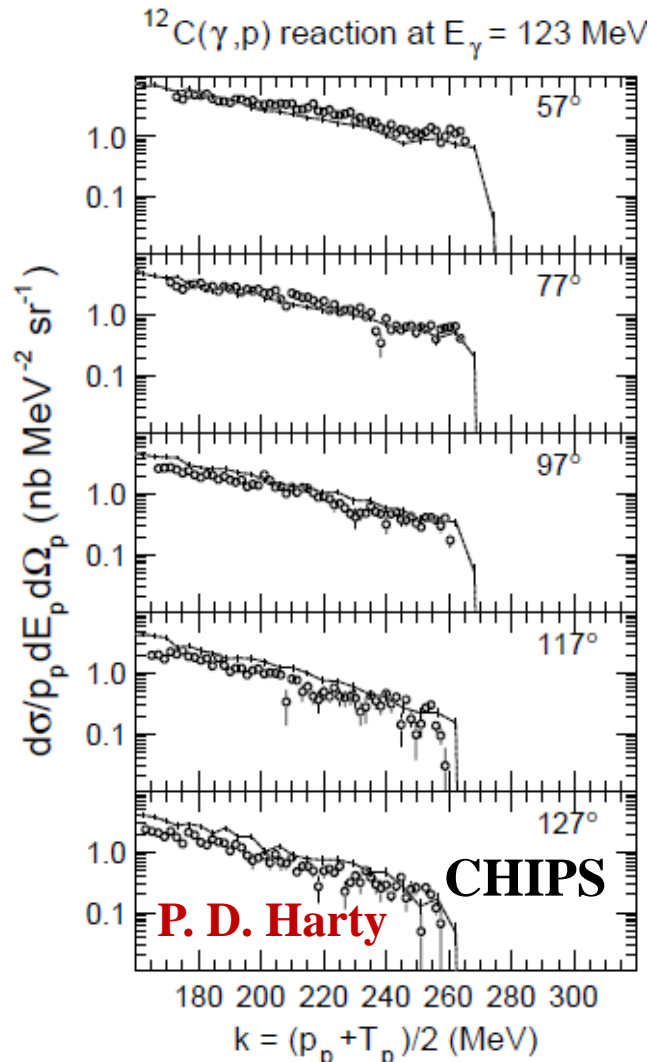
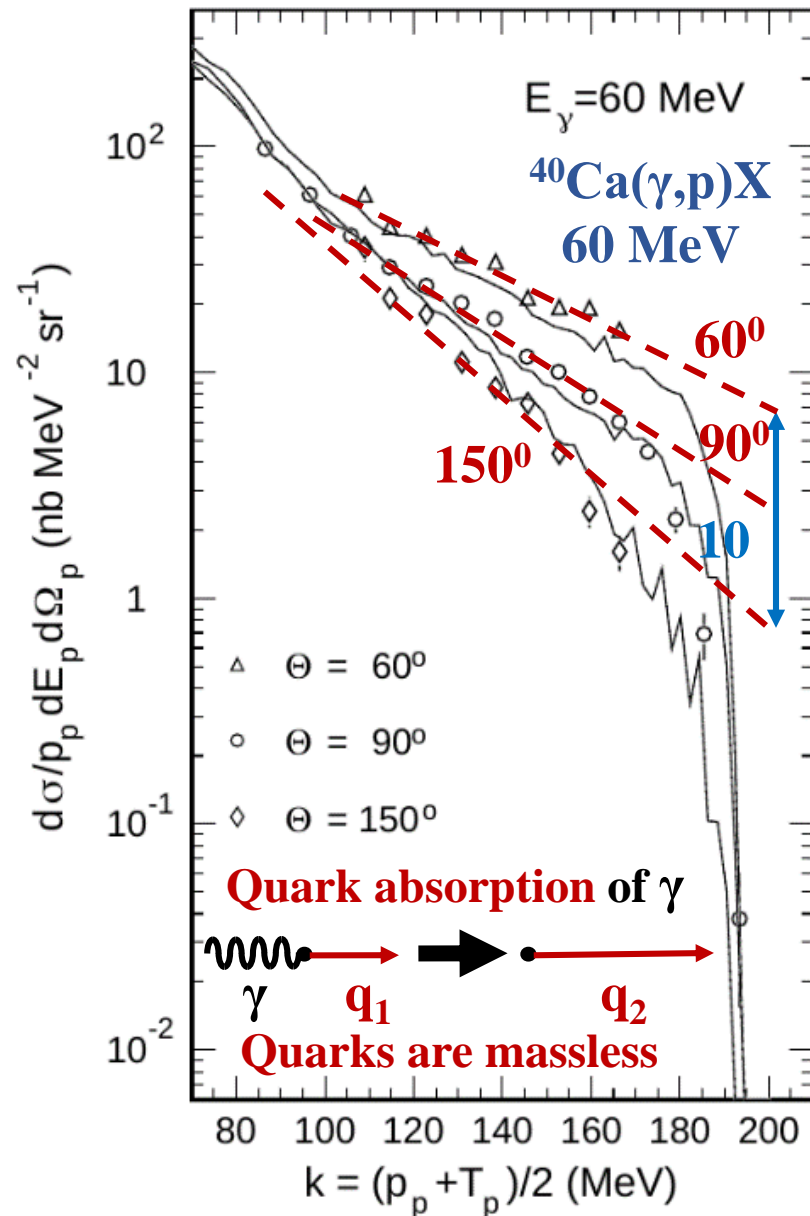
Pion capture fragmentation spectra



Photonuclear reactions below $\Delta(3,3)$



P. V. Degtyarenko, M. V. Kossov, H.-P. Wellisch,
 "CHIPS event generator III: Photo-nuclear
 reactions below Δ ", Eur. Phys. J. A 9, 421 (2000)

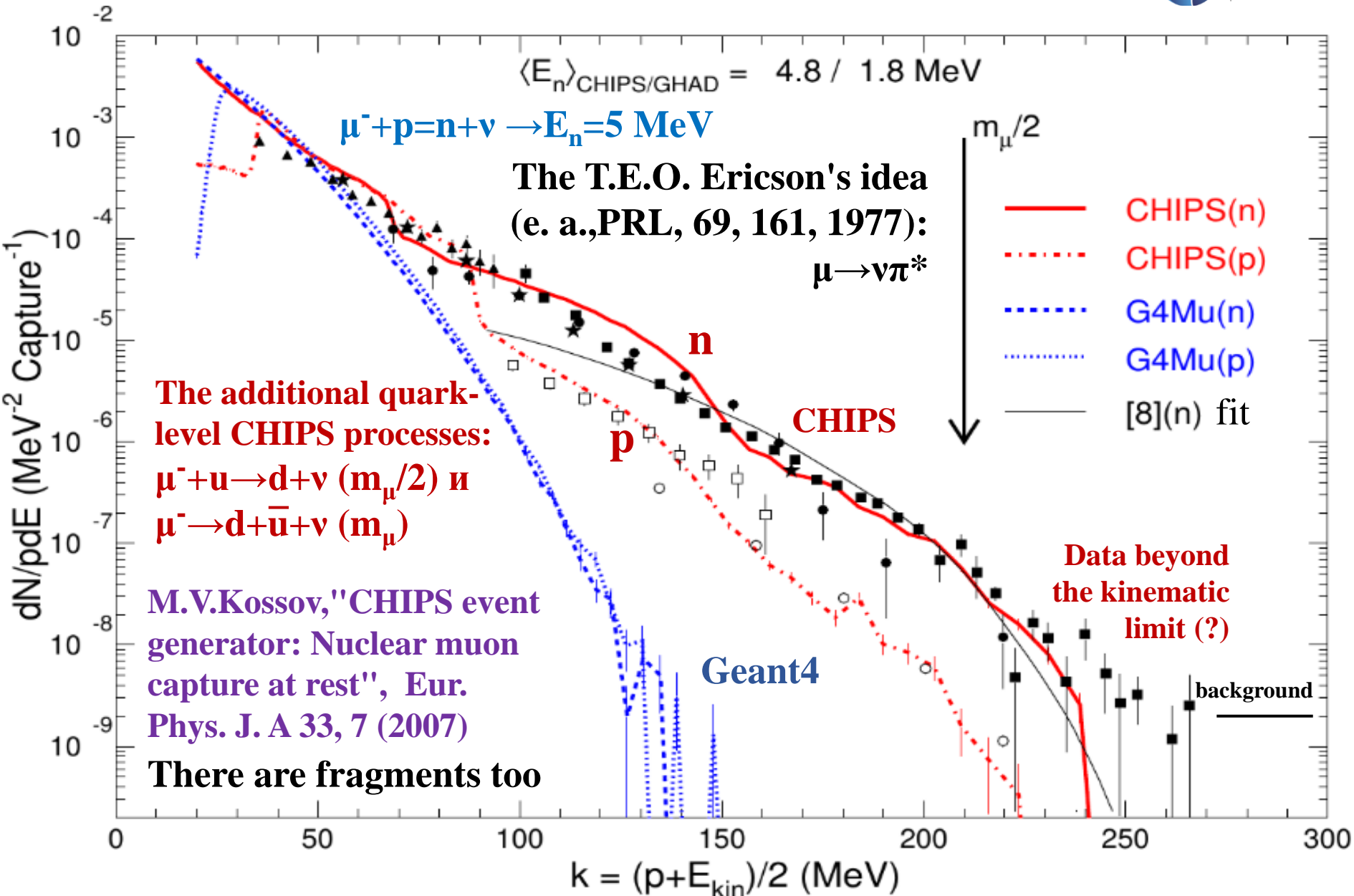


The unpublished paper of P.D.Harty was cited in PRC 49, 2704 (1994). Nobody could believe that 100 MeV gamma can accelerate the carbon nucleus so much (the boost of massless quarks). Even the nucleon-quasimon can't move so fast. The absorption of γ by the nucleon quark solves the problem.

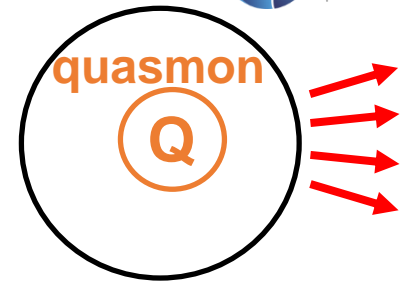
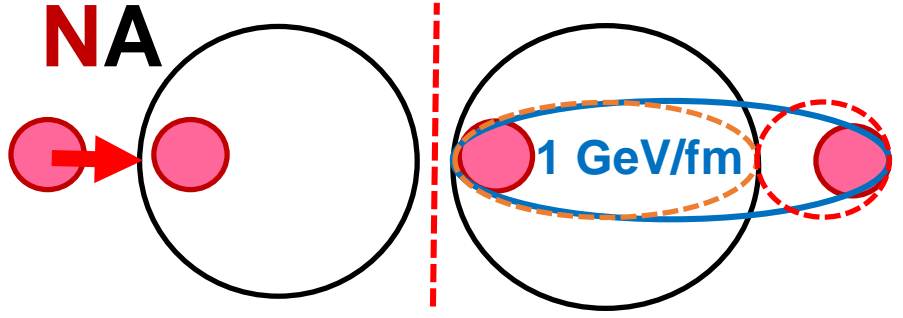
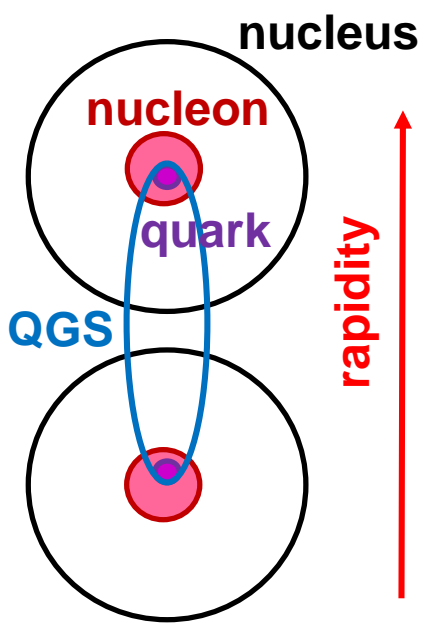
Muon capture fragmentation spectra



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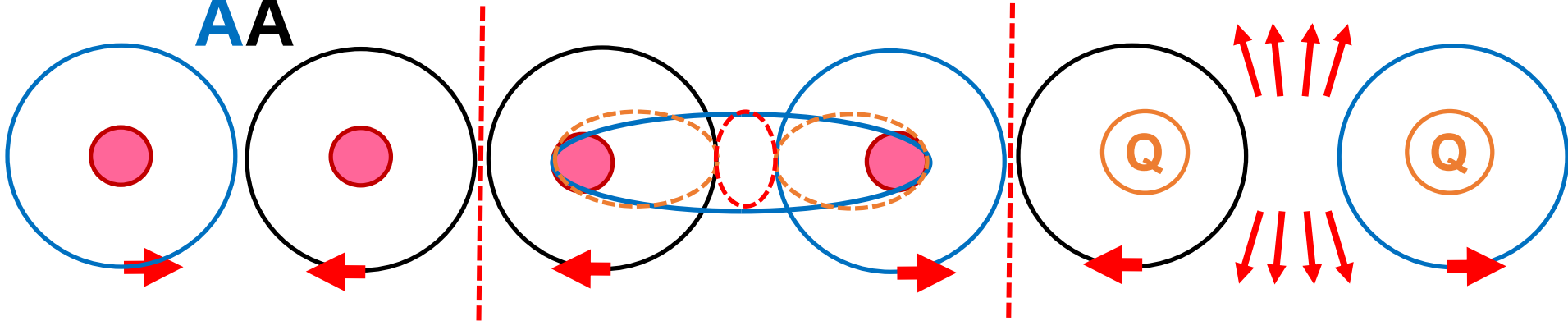
CHIPS simulation of ion-ion interaction



A Niedermaier string is split in nuclear and vacuum parts

In the ion-ion interactions the Niedermaier string is split in the two nuclear parts and the vacuum part in-between. There can be a few quasmon-pairs creation in the collision. The multi-quasmon fragmentation algorithm is verified.

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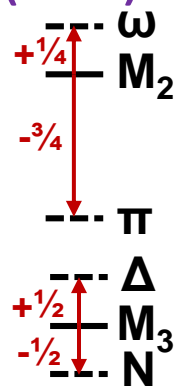


The CHIPS ion-ion algorithm is a decay-algorithm. It is much faster than the cascade-algorithms of the other models (DPMJET, UrQMD, FRITIOF, VENUS).

Vacuum temperature $T_c = 220.5$ MeV for calculation of 1s hadron masses



- The T_c dependence of the mass of n partons: $M = 2T_c \sqrt{n(n-1)}$
- Mesons spin products $\langle s_1, s_2 \rangle = \frac{1}{2}S(S+1) - \frac{1}{2}(\frac{1}{2}+1) = +\frac{1}{4} - \frac{3}{4}$
- Mesons: $M_2 = 2T_c \sqrt{2} = 624$ MeV, $(3m_\omega + m_\pi)/4 = 621$ MeV
- Baryons spin products $2\langle s_1, s_2 \rangle = \frac{1}{3}S(S+1) - \frac{1}{2}(\frac{1}{2}+1) = +\frac{1}{2} - \frac{1}{2}$
- Baryons: $M_3 = 2T_c \sqrt{6} = 1080$ MeV, $(m_N + m_\Delta)/2 = 1074$ MeV
- The light quark hadron masses are published [M.V.Kossov, EPJ, A14, 265 \(2002\)](#)
- All **92** 1s-hadron masses (**be published**)
- Masses of glueballs (f-mesons) **without the color-magnetic shifts** are close to M_2 , M_3 , $M_4 = 1528$ MeV, $M_5 = 1972$ MeV
- The T_c could be a third fundamental constant: $\Delta E = T_c \Delta I$ ($I = -S$)



The TPT algorithm for exclusive and inclusive cross-sections of reactions with production of nuclear fragments



To normalize the differential multiplicity the inelastic cross-section σ_{in} is used

- The CHIPS algorithm generates the final states of nuclear reactions, which can be sorted and collected for different exclusive channels of the nuclear reaction in a form of the 3N-histograms, where N is a number of the final state fragments with $[p_x, p_y, p_z]$;
- Below the separation energies of the secondary fragments only the γ -excited residual nucleus can exist, so the "closest" γ -excitation level is selected, and the last decay in the fragment is recalculated with the corresponding fixed residual nucleus A^* mass;
- To calculate the inclusive spectra of the identical fragments "i" all these fragments are collected to the common differential multiplicity histogram $\rho_i(\mathbf{p}) = dn_i/E/d\mathbf{p}$ ($n_i = N_i/M_n$), which can be converted to the invariant inclusive cross-section $f_i(\mathbf{p}) = \sigma_{in} \cdot \rho_i(\mathbf{p})$.

The γ -decays of the excited nuclei are simulated by the γ -cascade tables RIPL

- The "closest" level choice for the CHIPS simulated nuclear excitations can be done, taking into account the width and the strength of the surrounding γ -excitation levels;
- The TPT models for the probabilities of the E1, M1, E2 и M2 γ -transitions are under development in the TPT software package to assess the unknown γ -transitions.

The TPT stopping power solutions for simulation of the Doppler line broadening.

- For simulation of the γ -lines Doppler broadening the lifetime of the excited γ -levels and the stopping power of ions are necessary. The data provide knowledge of them.
- If the stopping power is known at low energies, one can find the lifetime? And if the lifetime is known, one can find the stopping power from the Doppler broadening form.

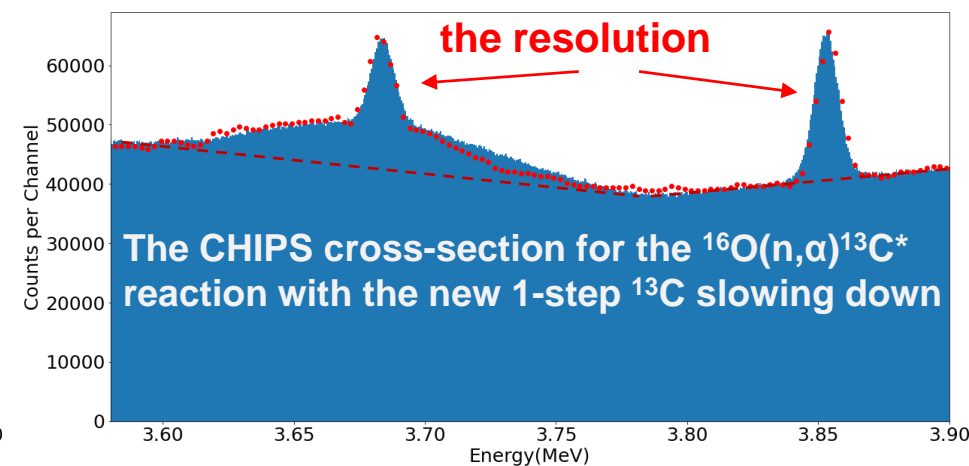
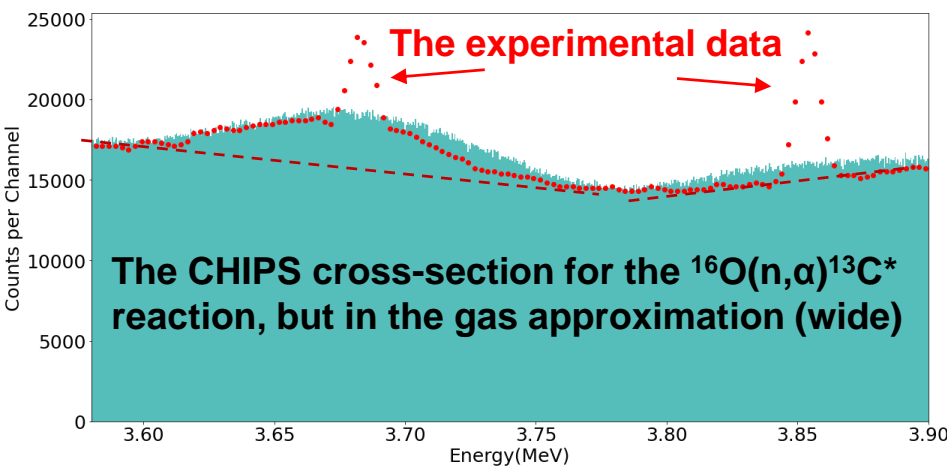
The TPT simulation of the γ -line Doppler broadening in the $^{16}\text{O}(n,\alpha)^{13}\text{C}$ reaction



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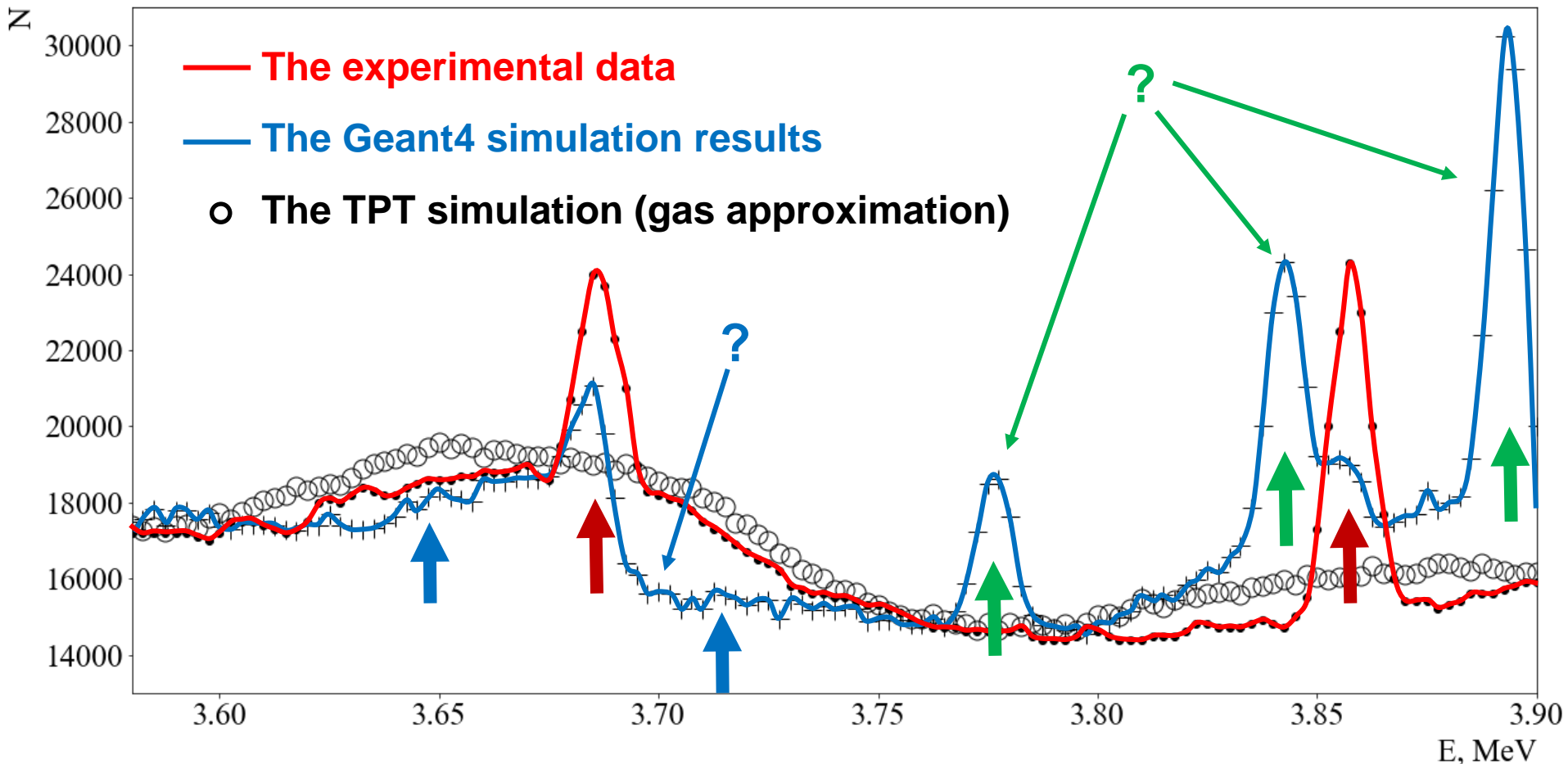
To slow down an ion only small steps can be used in the simulation, as the energy loss drops down significantly with energy decreasing. The first ion transport TPT algorithm was realized in the gas approximation without any slowing down, but now the one step slowing down algorithm is used:

1. The TPT algorithm, taking into account the ion slowing down in the $dt \rightarrow \alpha n$ reaction, was implemented in 2022.
2. The TPT low energy neutron elastic scattering algorithm for the logging simulation was implemented in 2023.
3. The 1-step slowing down algorithm for the γ -cascade was implemented in 2024



The adequate to the experimental data $^{16}\text{O}(n,\alpha)^{13}\text{C}^*$ reaction cross-section is absent in Geant4 NewtronHP and in the open data bases. For the TPT software package it was generated by the CHIPS model. The Doppler broadening of the γ -line depends on the lifetime (RIPL) and the stopping power dE/dx for the excited ^{13}C isotope in the BeO media (Geant4). The demonstrated experimental γ -spectrum (red dots) shows, that the line 3.686 MeV has two widths: the first one for the direct excitation (wide), and the second one is the result of the 167 keV γ -decay of the long lived 3.853 MeV level (narrow). The data are perfectly reproduced by the TPT simulation.

For comparison the Geant4 simulated γ -spectrum is shown



1. All the Geant4 spikes are narrow, so they correspond to the ^{13}C decay **at rest** without any Doppler broadening. **To the left** of the **3.686 MeV** line there is **a dense set of lines**, but this is not a Doppler effect, as **to the right of the line there is no events**.
2. Geant4 generates **a lot of the strong spikes**, which are not seen in the experiment, while they are much stronger than the lines, which are **seen in the experiment**.

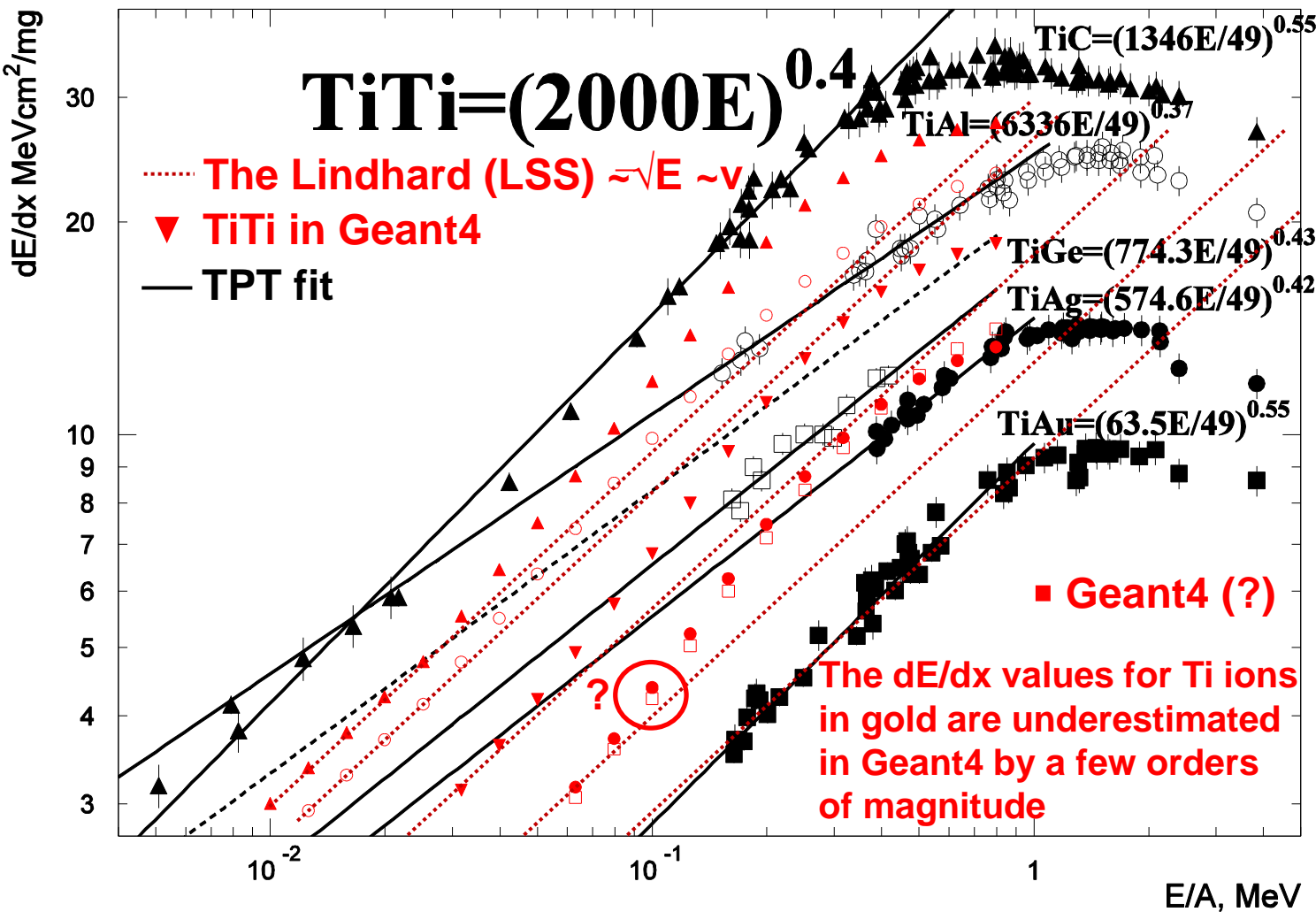
Conclusion

1. The theoretical CHIPS data base can fill a gap in our knowledge of the neutron-nuclear reactions with **production of heavy nuclear fragments**.
2. The heavy fragments production, especially the α -particle production (the helium pores), is very important for simulation of the **radiation hardness of materials of nuclear setups and atomic power plants**.
3. The energetic ions as a result of the material irradiated can be products of **elastic and inelastic neutron-nuclear scattering and the induced ion cascade**.
4. For ions knocked out of the crystal lattice and for ions produced in inelastic neutron-nuclear reactions the dE/dx function should be improved for the robust simulation of the ion cascades, especially for the **low energy ions**.
5. For the simulation improvement it is necessary to fit all IAEA experimental dE/dx data and measure the dE/dx functions **at lowest energies**.
6. The CHIPS model is validated at high energies, where the kinematic limits are not important, but **at relatively low energies the new validation should be done**, which can prove applicability of the quark level model at low energies.
7. We are looking forward to extend the CHIPS model beyond the projectile neutrons to the projectile γ -rays and **other projectile nuclear fragments**.

**Thank you for
your attention**



The perspectives of the improvement of the dE/dx function from **Geant4** to TPT



The black dots are the IAEA data for the dE/dx function of Ti in different media. The data for Ti in Ti are absent. The TPT estimation is shown by the **dashed line**. **The red markers** of the same shape as the **data** correspond to **Geant4**. They are proportional to the ion speed (**the LSS law**). For the low energy ions the Geant4 fit is too far from **the existing experimental data**. One should vary the speed dependence.

In our simulation we used the Geant4 fit of the dE/dx function, because as a result of the α -decay the $^{13}\text{C}^*$ nucleus acquires relatively high speed, for which the **Geant4 fit** is close to the **data**. For the linear dE/dx it's much easier to calculate the step length to the $^{13}\text{C}^*$ decay.

Calculations of the step length to the nuclear decay and the nuclear speed



If $dE/dx=C \cdot v$, then $m \cdot dv=C \cdot dx$. If x is the distance to the stopping point ($x=0$ и $v=0$): $m \cdot v=C \cdot x$. If the decay time t_d is known, one can calculate the distance to the decay x_d , which is passed during t_d . Substituting $v=dx/dt$, we get $m \cdot d \ln x=C \cdot dt$ relation, and it means that the slowing-down time ($x=0$, $v=0$) is infinite. If the radioactive ion was born at $x=m \cdot v/C$ and decay after t_d in the point x_d , then $m \cdot \ln(x/x_d)=C \cdot t_d$ and $x_d=x \cdot \exp(-C \cdot t_d/m)$. The step is $L=x \cdot [1 - \exp(-C \cdot t_d/m)]$. As $x_d=m \cdot v_d/C$, where v_d is the speed at the decay point, $m \cdot \ln(v/v_d)=C \cdot t_d$, and $v_d=v \cdot \exp(-C \cdot t_d/m)$.

If the stopping power is proportional to another power speed, then $dE/dx=C \cdot v^\alpha$, where $\alpha=1$ is the LSS model. Then, substituting $dx=v \cdot dt$, we get $m \cdot dv=C \cdot v^\alpha \cdot dt$ or $m \cdot dv^{1-\alpha}=(1-\alpha)C \cdot dt$, that is $m \cdot v^{1-\alpha}=(1-\alpha)C \cdot (t-t_0)$. For $\alpha < 1$ the slowing-down time ($x=0$, $v=0$, $t_0=0$) is finite $t=m \cdot v^{1-\alpha}/(1-\alpha)C$. If $t_d > t$ the nucleus manages to stop, but if $t_d < t$, it still has $v_d=[(t-t_d)(1-\alpha)C/m]^{1/(1-\alpha)}$, that is (without t) $v_d=[v^{1-\alpha} - t_d(1-\alpha)C/m]^{1/(1-\alpha)}$. For $\alpha > 1$, the same as for $\alpha=1$ (LSS), the slowing-down time is infinite and for any t_d : $v_d=[v^{1-\alpha} + t_d(\alpha-1)C/m]^{1/(1-\alpha)}$. To get the step length $L=x-x_d$, the speed should be integrated $L=\int v(t)dt$ from 0 to t_d : $L=\{[v^{1-\alpha} + t_d(\alpha-1)C/m]^{(2-\alpha)/(1-\alpha)} - v^{2-\alpha}\} \cdot m/C/(\alpha-2)$. This formula is valid for any α , except for the $\alpha=1$, but if $\alpha < 1$ for $t_d > t$ the step is restricted by the stopping point $L=v^{2-\alpha} \cdot m/C/(2-\alpha)$. At this point the radioactive nucleus is at rest, and the γ -decay does not have any Doppler effect. One can see, that if $\alpha \neq 1$ the calculations are a bit more complicated, but the calculations of the step length to the nuclear decay and the nuclear speed at the decay point are still durable.

The TPT fit of the experimental dE/dx values (IAEA) for different ions in gold

