A Microscopic Description of Proton-induced Reactions at Intermediate Energies

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Abstract:

A short introduction of the Quantum molecular dynamics model and its application to proton induced reactions is presented. There exist various models that describe heavy ion reactions microscopically in terms of the dynamics of the interacting nucleons. The most important models of this group are the Vlasow–Uehling–Uhlenbeck (VUU) model and the quantum molecular dynamics (QMD) model. The VUU model provides a useful tool to describe the one particle observables of heavy ion reactions. However, phenomena like fragment formation can hardly be described in such a single particle theory, since they are intimately connected to many–body correlations. The correct propagation of correlations is lost in the VUU model, in contrast to the Molecular Dynamics models, by using the testparticle method to obtain an ensemble average of the one particle distribution function. If one wants to treat correlations exactly, one has to get rid of the testparticle method. For this reason in the QMD model a single Gaussian Wigner density is used to describe the nucleons.

The QMD model has been very successful in describing collective and many-body effects in heavy ion collisions at intermediate and high energies ($E = 50-1000$ MeV/nucl.) There is, however, no limitation to the QMD that restricts it to the description of nucleus-nucleus collisions. Therefore we present in this article some results for p-induced reactions in the energy regime from 80 to 800 MeV.

1 The QMD model

In the QMD model nucleons are described as Wigner densities of a boosted Gaussian wave packet with fixed width

$$f_i(\mathbf{r}_i, \mathbf{p}_i, t) = \frac{1}{(\pi\hbar)^3} \exp\left\{ -\frac{(\mathbf{r}_i - \mathbf{r}_{i0}(t))^2}{2L} - (\mathbf{p}_i - \mathbf{p}_{i0}(t))^2 \frac{2L}{\hbar^2} \right\} \quad , \tag{1}$$

where $\mathbf{r}_{i0}$ and $\mathbf{p}_{i0}$ are the centroids of particle i in coordinate and momentum space. Those nucleons interact in the basic version of the QMD model via a local two and three–body Skyrme interaction and a Coulomb and Yukawa interaction.

The Skyrme interaction is therefore used in it simplest form:

$$\hat{V}_{Sk}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) = t_2 \delta(\mathbf{r}_i - \mathbf{r}_j) + t_3 \delta(\mathbf{r}_i - \mathbf{r}_j)\delta(\mathbf{r}_i - \mathbf{r}_k) \quad . \tag{2}$$

Since the momentum dependence of the Skyrme interaction is (for large momenta) in sharp contrast with experimental data we neglect the momentum dependent effects of the Skyrme interaction and we also assume spin-isospin saturated matter (lateron we will reintroduce the momentum dependent interactions in a phenomenological way).

With the Gaussian nucleons (eq.(1)) one calculates the following Hamiltonfunction.

$$\begin{aligned}
H &= \sum_{i=1}^{N} \left(\sqrt{\mathbf{p}_{i0}^2 + m^2} - m \right) \\
&+ \frac{1}{2} \sum_{\substack{i,j=1 \\ j\neq i}}^{N} \int f_i(\mathbf{r}_i, \mathbf{p}_i) V_{Yuk}(\mathbf{r}_i, \mathbf{r}_j) f_j(\mathbf{r}_j, \mathbf{p}_j) d^3r_i\, d^3r_j\, d^3p_i\, d^3p_j \\
&+ \frac{1}{2} \sum_{\substack{i,j=1 \\ j\neq i}}^{N} \int f_i(\mathbf{r}_i, \mathbf{p}_i) V_{Coul}(\mathbf{r}_i, \mathbf{r}_j) f_j(\mathbf{r}_j, \mathbf{p}_j) d^3r_i\, d^3r_j\, d^3p_i\, d^3p_j \\
&+ \frac{1}{2} \sum_{\substack{i,j=1 \\ j\neq i}}^{N} \int f_i(\mathbf{r}_i, \mathbf{p}_i) V_{asym}(\mathbf{r}_i, \mathbf{r}_j) f_j(\mathbf{r}_j, \mathbf{p}_j) d^3r_i\, d^3r_j\, d^3p_i\, d^3p_j \\
&+ \frac{1}{2} \sum_{\substack{i,j=1 \\ j\neq i}}^{N} \int f_i(\mathbf{r}_i, \mathbf{p}_i) V_{Sk}^{(2)}(\mathbf{r}_i, \mathbf{r}_j) f_j(\mathbf{r}_j, \mathbf{p}_j) d^3r_i\, d^3r_j\, d^3p_i\, d^3p_j \\
&+ \frac{1}{2} \sum_{i=1}^{N} \frac{1}{3} \sum_{\substack{j=1 \\ j\neq i}}^{N} \sum_{\substack{k=1 \\ k\neq j, k\neq i}}^{N} \int f_i(\mathbf{r}_i, \mathbf{p}_i) f_j(\mathbf{r}_j, \mathbf{p}_j) f_k(\mathbf{r}_k, \mathbf{p}_k) V_{Sk}^{(3)}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) \\
&\qquad \times d^3r_i\, d^3r_j\, d^3r_k\, d^3p_i\, d^3p_j\, d^3p_k \quad .
\end{aligned} \tag{3}$$

Evaluating the integrals yields

$$H = \sum_{i=1}^{N} \left(\sqrt{\mathbf{p}_{i0}^2 + m^2} - m \right)$$

$$
\begin{aligned}
&+\frac{1}{2}\sum_{\substack{i,j=1\\ j\neq i}}^{N}\frac{V^0_{Yuk}}{2|\mathbf{r}_{i0}-\mathbf{r}_{j0}|}e^{L/\gamma^2_{Yuk}}\\
&\quad\times\left\{e^{-|\mathbf{r}_{i0}-\mathbf{r}_{j0}|/\gamma_{Yuk}}\left[1-\operatorname{erf}\left(\frac{(2L/\gamma_{Yuk})-|\mathbf{r}_{i0}-\mathbf{r}_{j0}|}{\sqrt{4L}}\right)\right]\right.\\
&\quad\left.-e^{+|\mathbf{r}_{i0}-\mathbf{r}_{j0}|/\gamma_{Yuk}}\left[1-\operatorname{erf}\left(\frac{(2L/\gamma_{Yuk})+|\mathbf{r}_{i0}-\mathbf{r}_{j0}|}{\sqrt{4L}}\right)\right]\right\}\\
&+\frac{1}{2}\sum_{\substack{i,j=1\\ j\neq i}}^{N}\frac{e^2\cdot\sigma_i\cdot\sigma_j}{|\mathbf{r}_{i0}-\mathbf{r}_{j0}|}\operatorname{erf}\left(\frac{|\mathbf{r}_i-\mathbf{r}_j|}{\sqrt{4L}}\right)\\
&+\sum_{i=1}^{N}\left[\frac{\alpha}{2}\frac{1}{(4\pi L)^{3/2}\varrho_0}\sum_{\substack{j=1\\ j\neq i}}^{N}e^{-\frac{(\mathbf{r}_{i0}-\mathbf{r}_{j0})^2}{4L}}+\frac{\beta}{\gamma+1}\left(\frac{1}{(4\pi L)^{3/2}\varrho_0}\sum_{\substack{j=1\\ j\neq i}}^{N}e^{-\frac{(\mathbf{r}_{i0}-\mathbf{r}_{j0})^2}{4L}}\right)^{\gamma}\right]\\
&+\sum_{i=1}^{N}\Omega\frac{1}{(4\pi L)^{3/2}\varrho_0}\sum_{\substack{j=1\\ j\neq i}}^{N}e^{-\frac{(\mathbf{r}_{i0}-\mathbf{r}_{j0})^2}{4L}}\cdot 2(\sigma_i-\frac{1}{2})\cdot 2(\sigma_j-\frac{1}{2})\quad .
\end{aligned}
\tag{4}
$$

where σ_i is equal to 1 for protons and 0 for neutrons.

The first term denotes the kinetic energy of the centroids of the nucleons; the second and third term are the Yukawa and Coulomb interactions, respectively, for Gaussian shaped wave packets (1) of the nucleons. The last term represents the Skyrme part of the interaction which can for infinite nuclear matter, be considered as a density dependent interaction.

The parameters α, β, and γ are adjusted to reproduce the properties of infinite nuclear matter, i.e.,

$$
\begin{aligned}
\left.\frac{E}{A}\right|_{\varrho=\varrho_0} &= -16\ \text{MeV}\\
P=\varrho^2\left.\frac{\partial E/A}{\partial\varrho}\right|_{\varrho=\varrho_0} &= 0\ \text{MeV fm}^3\\
K=9\varrho^2\left.\frac{\partial^2 E/A}{\partial\varrho^2}\right|_{\varrho=\varrho_0} &= \begin{cases}200\ \text{MeV}\quad(\text{Soft eos})\\ 380\ \text{MeV}\quad(\text{Hard eos})\end{cases}
\end{aligned}
\tag{5}
$$

In order to obtain a reasonable simulation of finite nuclei, we adjust the two Yukawa parameters V_{Yuk} and γ_{Yuk} (the Yukawa potential also gives a density dependent contribution to the equation of state, which must be taken into account when adjusting the parameters).

It has been emphasized [1, 2, 3, 4] that non–equilibrium effects will play an important role in a realistic treatment of heavy ion collisions. The most pronounced effect can be expected from the momentum dependence of the nuclear interaction which leads to

an additional repulsion between the nucleons. For the computation of such momentum dependent interactions (mdi) we parametrized the momentum dependence of the real part of the optical p–nucleus potential, in order to substitute the term proportional to k_F^2 in the Skyrme interaction, which is in striking contrast to the data above $E_{Lab} \approx 150$A MeV.

We get

$$U_{mdi} = \delta \ln^2[\epsilon'(\mathbf{p}_i - \mathbf{p}_j)^2 + 1]\delta(\mathbf{r}_i - \mathbf{r}_j) \tag{6}$$

with $\delta = 1.57$ MeV and $\epsilon' = 5 \times 10^{-4}$ MeV^{-2}.

When using the mdi, one has to readjust the force parameters in order to yield the same nuclear matter properties as without mdi.

One deficiency of the model is that the nuclear ground state cannot be simulated in a reasonable fashion, because of the absence of the Fermi motion, generated by the Pauli exclusion principle.

Wilets et al. [5, 6, 7] suggested that the Pauli exclusion principle might be simulated by a momentum dependent repulsive potential. Later on several forms of this potential were introduced, yielding a reasonable reproduction of gross thermostatic properties [8, 9, 10, 11].

We employ the Gaussian Pauli potential introduced by Dorso et al. [8, 11]. With such a potential the total energy of the "free" Fermigas is given by:

$$\begin{aligned} E_{tot}^{FG} = E_{kin} + E_{Pau} &= \sum_i \left(\sqrt{\mathbf{p}_{i0}^2 + m^2} - m\right) \\ &+ \frac{1}{2}\sum_{i \neq j} V_{Pau}^0 \left(\frac{\hbar}{q_0 p_0}\right)^2 \exp\left[-\frac{r_{ij}^2}{2q_0^2} - \frac{p_{ij}^2}{2p_0^2}\right] \times \delta_{\tau_i\tau_j}\delta_{\sigma_i\sigma_j} \end{aligned} \tag{7}$$

where σ_i and τ_i denote the spin–isospin index of nucleon i.

The parameters of the several manifestations of the QMD model can be found in the [13]:

Now the numerical simulation of the collision takes place in three steps. First the projectile and target are initialized in their rest frames. Therefore a Metropolis algorith is used to initialize the nuclei in their groundstate. This procedure yields nuclei that are absolutely stable and do not evaporate any nucleons.

Successfully initialized nuclei are then boosted towards each other with the proper center of mass velocities using relativistic kinematics. The centroids of each Gaussian are then propagated corresponding to the Hamilton equations with the Hamiltonian of eq. (4) in Runge-Kutta integration routine with time steps ranging from 0.2 to 0.4 fm/c.

After each integration step the hard N–N collisions are treated in the same way as in the VUU and INC models via a stochastic scattering term. Two nucleons can scatter if the spatial distance of the centroids of their Gaussians is smaller than $\sqrt{\sigma_{tot}/\pi}$. The energy and angular distributions of the experimental differential scattering cross section $d^2\sigma/d\sqrt{s}d\Omega$ are reproduced on the average. Inelastic collisions lead to the formation of Delta particles, which can be reabsorbed in the inverse reaction. We do not incorporate free (s–wave) pions here, unlike the VUU model. Whenever a collision occurs, we check the phase–space distribution around the final states of the scattering partners. We determine

the ratios P_1, P_2 of the final phase spaces which are already occupied by other nucleons. The collision is then blocked with the probability

$$P_{Block} = \min[1, P_1 \cdot P_2] \quad . \tag{8}$$

Whenever a collision is blocked, the momenta of the scattering partners are replaced by the values they had prior to the scattering.

2 Results

Preequilibrium neutron emission has been measured recently for the inclusive reactions p + Al, Zr, Pb at $E_p = 80, 120$ and 160 MeV [16] as well as for 256 and 800 MeV [17]. It has been reported [18, 19, 20, 21] that in this energy regime semi classical preequilibrium models, which are based on an intranuclear nucleon–nucleon collision process, fail to reproduce the angular distributions. In order to describe the data more appropriately a multistep model based on the Feshbach–Kerman–Koonin (FKK) [22] formalism with at least two or more incoherent direct nucleon–nucleon interactions has been used [16]. Since the QMD model follows the trajectories of all nucleons microscopically and treats both the hard nucleon–nucleon scattering and the soft nucleon–nucleon interaction, it should be equally successful in describing these reactions.

The experimental and calculated c.m. energy spectra of neutrons emitted at different laboratory angles are shown in figs. 1 for the Pb target at 80,160,256 and 800 MeV incident proton energy. Both the data and the calculations show a characteristic transition from a weak neutron energy dependence at forward angles to an almost exponential shape at backward angles. This clearly indicates that the system is not equilibrated. So we conclude that the failure of the previous preequilibrium models to describe the angular dependence of the data is due to the neglection of second and higher order collisions. The treatment of the collisions within the quantum mechanical model of Feshbach et al. gives a similar agreement with the data, which implies that the quantal treatment of the statistical multistep direct emissions is well reproduced with the stochastic collision term in the QMD model. The detailed form of the nucleon–nucleon potential, which is the essential input for e.g., the Feshbach–Kerman–Koonin theory, seems to be unimportant at these high energies.

A more detailed inspection of 1 shows that the QMD model describes the backward spectra quite good, but fails to give a reasonable reproduction of the neutron spectra at the very forward angles. In this case the QMD fails to reproduce the high energy neutrons.

In addition to figure 1 we show in fig. 2 the angular distributions of the same double differential cross sections for the Al, Zr and Pb target for neutrons with c.m. energies of 35,55,75 and 105 MeV, respectively. Again it can be seen that the QMD model describes the data quite well.

All the results presented here have been obtained with the dynamical QMD model alone. A second step, that describes the statistical evaporation of neutrons from the excited residue, has, up to now, not been included. In the case of the heavy ion reactions it has, however, been shown that such a secondary evaporation (of intermediate mass fragments) is necessary for the description of multifragmentation data (for details see

Ref. [14]). In this case we have used a statistical multifragmentation model for the description of the equilibrium decay of all excited prefragments.

It was for this reason that we have implemented the Paulipotential into the QMD, in order to get a well defined, fermionic ground state for the residue. Having the ground state energy and the total energy of the residue we then can easily calculate the excitation energy and use this value as input for the evaporation step.

Without such a Paulipotential the excitation energy the residue is, in principle, not defined. As a very crude approximation one can use a) the energy this residue would have when it is initialized in the model, or b) the experimental ground state energy. Both cases, however, incorporate a large uncertainty in the excitation energy, especially if the case b) is used.

The effect of the evaporation step on the neutron spectra has not yet been studied, we can however show that the inclusion of the Paulipotential by itself does not change any observables. For this reason we show in fig 3 the neutron spectra for the p (800 MeV) + Al reaction obtained with Paulipotential (open symbols) and without (full symbols). The full line shows the experimental data of [17].

In conclusion we have shown that the semiclassical QMD model gives a reasonable reproduction of both the qualitative and quantitative behavior of neutron spectra in proton induced reactions in the bombarding energy interval between 80 and 800 MeV. The agreement between the calculations and the data is, however, by far not perfect, and may be improved by the inclusion of a secondary evaporation step.

The calculations also suffer from a very poor statistics. All the results presented here have been sampled from about 2000 Monte Carlo events for each system. For detailed comparison to the data at least 20000 events are needed.

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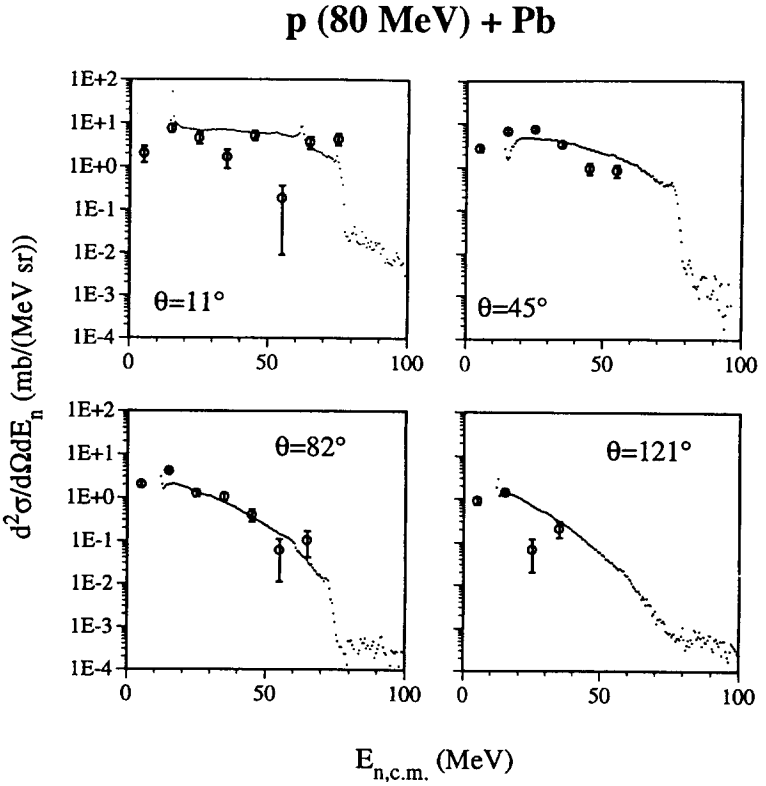

Fig. 1a

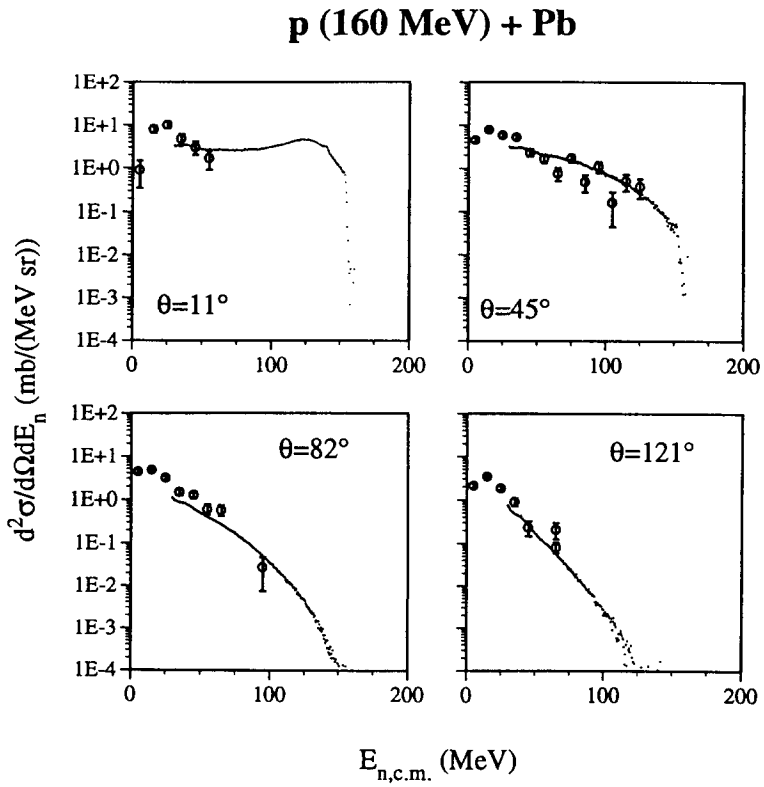

Fig. 1b

Figure 1:
Neutron energy spectra in the c.m. frame for the reactions p(80, 160, 256, 800MeV) + Pb at different laboratory angles as indicated. The symbols show the QMD calculation while the full line represents the data of [16, 17].

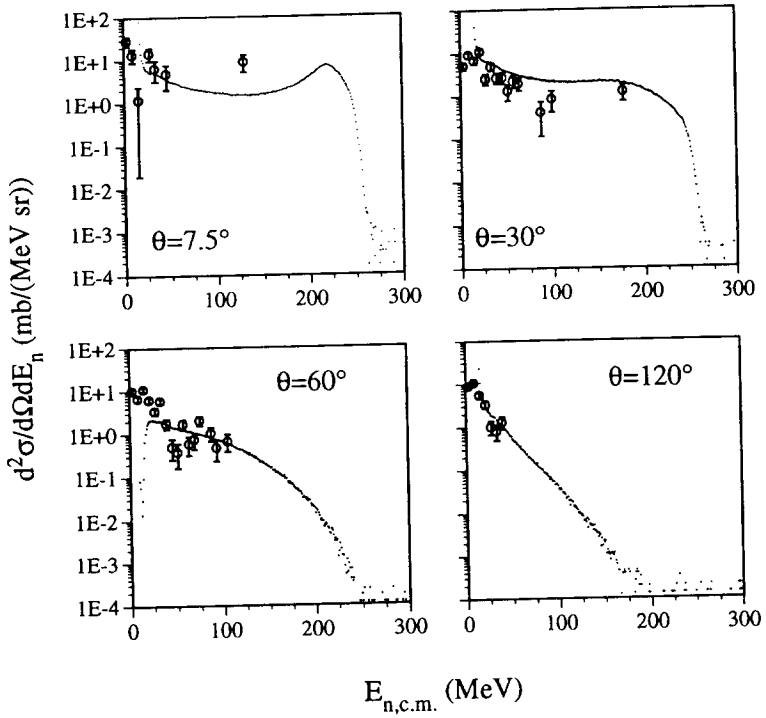
p (256 MeV) + Pb
θ=7.5°
θ=30°
θ=60°
θ=120°
d²σ/dΩdE_n (mb/(MeV sr))
E_n,c.m. (MeV)

Fig. 1c

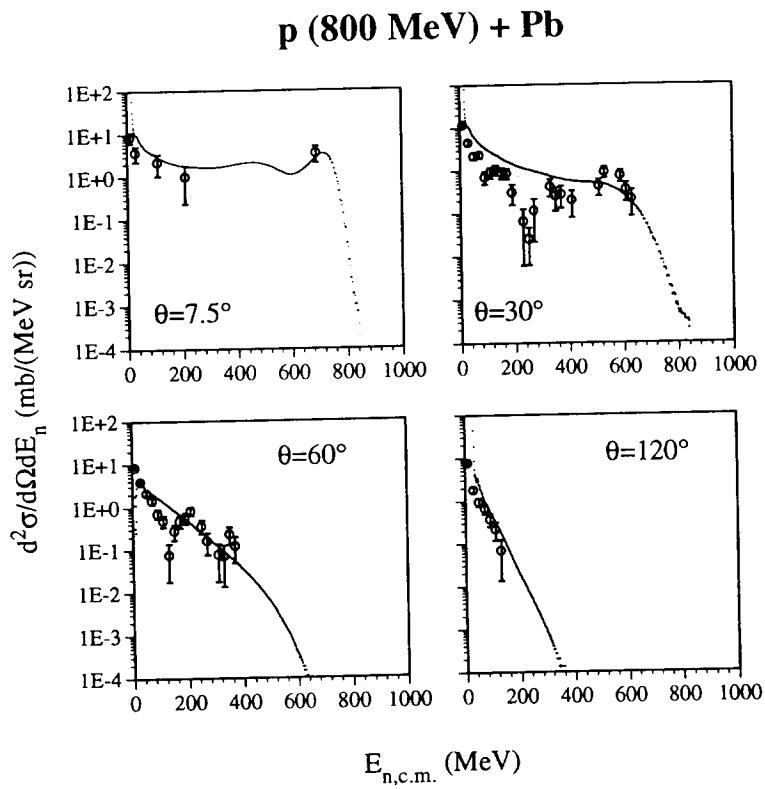
p (800 MeV) + Pb
θ=7.5°
θ=30°
θ=60°
θ=120°
d²σ/dΩdE_n (mb/(MeV sr))
E_n,c.m. (MeV)

Fig. 1d

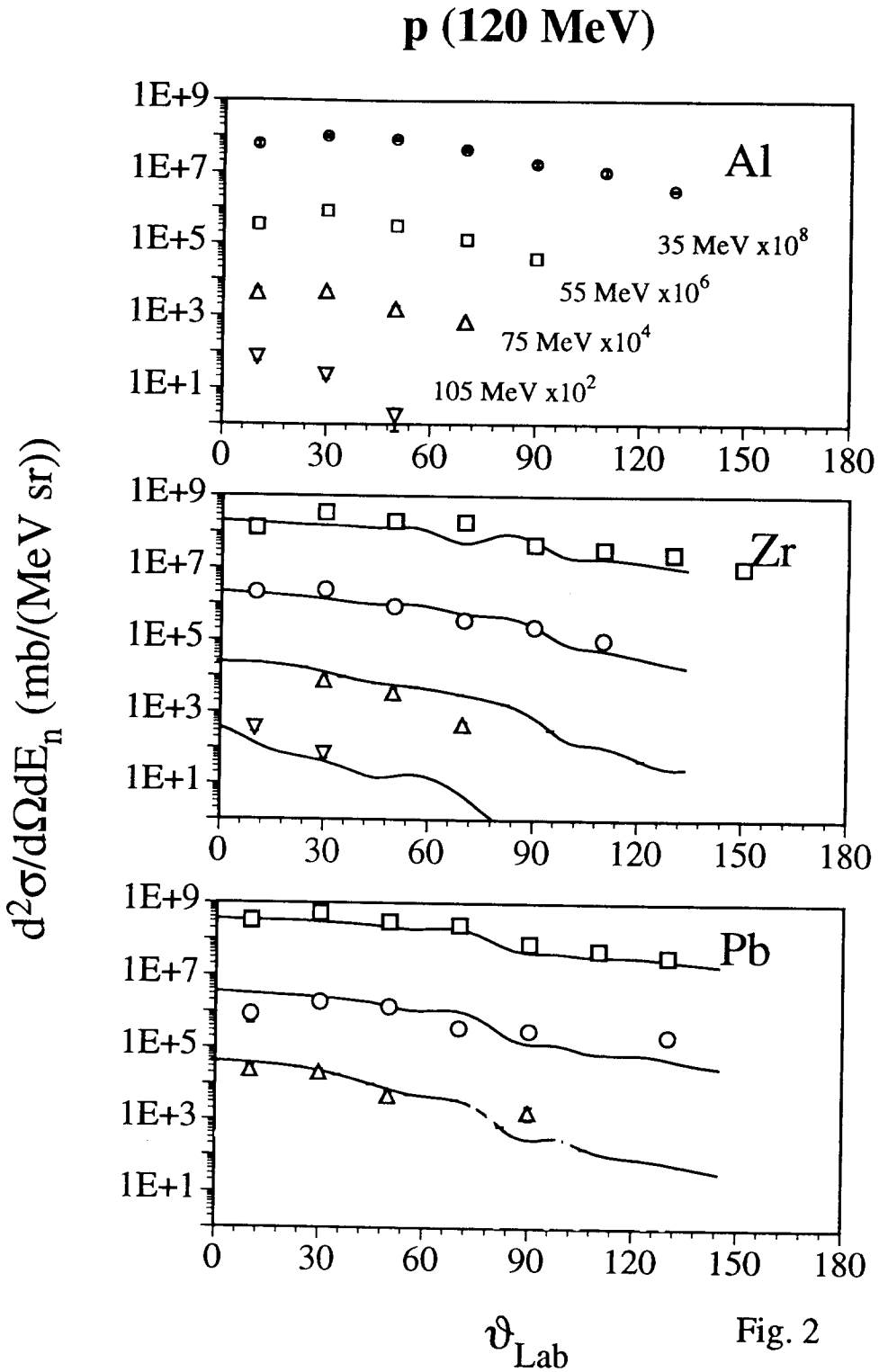

Figure 2:
Angular distributions for neutron with c.m. energies of 35, 55, 75, and 105 MeV in reactions p(120MeV) + Al, Zr, Pb. The symbols show the QMD calculation while the full line represents the data of [16].

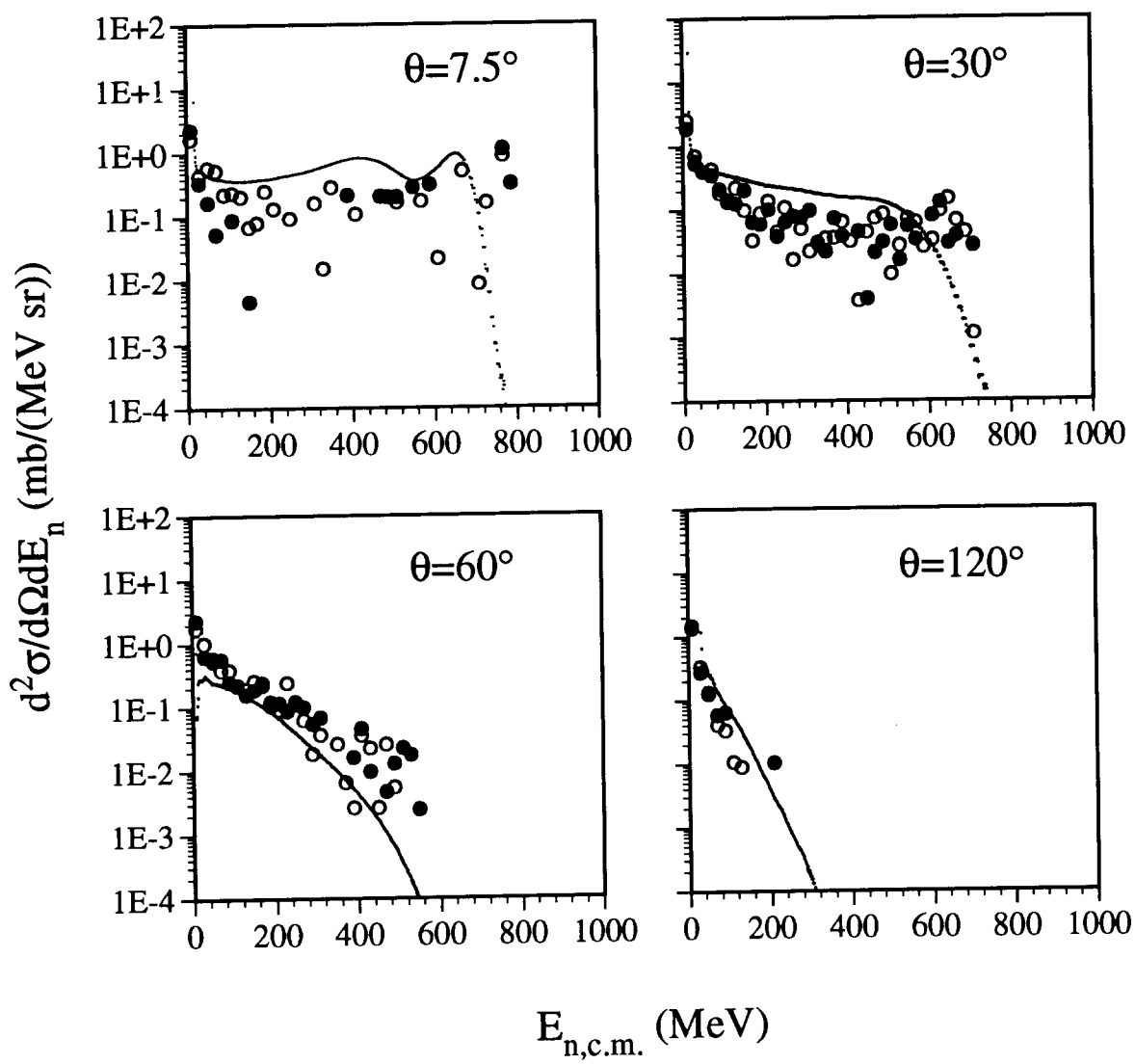

Fig. 3

Figure 3:
Neutron energy spectra in the c.m. frame for the reactions p(800MeV) + Al at different laboratory angles as indicated. The symbols show the QMD calculation with (open symbols) and without (full) symbols) while the full line represents the data of [16].