The Quantum Molecular Dynamics Calculation of Nucleon-Nucleus Reactions

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Abstract

The Quantum Molecular Dynamics (QMD) theory is being applied systematically to the nucleon(N)-induced nuclear reactions. It was found that the QMD can give a remarkable agreement with the data of the (N,xN') type reactions over the energy region from several tens MeV to several GeV without adjusting any parameter. The QMD gives a unified picture on the major three reaction mechanisms (i.e., compound, pre-equilibrium and spallation) of nucleon-nucleus reactions.

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I. Introduction

Nuclear reactions reveal various aspects as a function of projectile/target mass, projectile energy and impact parameter. In nucleon induced reactions, the compound nuclear process is dominant in MeV region, while the pre-equilibrium and spallation processes become more likely as projectile energy increases. In heavy-ion (HI) nuclear physics, the reactions are also interpreted with different concepts which are applicable to each specific process.

Recently, the method of microscopic simulation has been developed quite rapidly in heavy ion physics[1]. The Quantum Molecular Dynamics (QMD)[2] is one of those simulation methods. The basic ingredients of this model are the self-consistent nuclear mean field (calculated from the effective N-N interaction) and the stochastic N-N collision term taking account of the Pauli blocking. The mean field plays an important role in low energy domain (e.g., success of TDHF theory) since Pauli blocking prohibits the N-N collision. On the other hand, nuclear reactions are described well by the collision term alone in a very high energy region as the cascade model indicates. Because of these two ingredients, QMD has been able to give a unified description for the various reaction mechanisms of the HI-HI reactions over the projectile energy of several MeV to GeV/nucleon. This capability of QMD made it possible to investigate the compressibility of nuclear matter (nuclear equation of state), mechanisms of formation of intermediate-mass fragments, subthreshold particle production, etc., in a consistent framework.

The same prosperity is expected for nucleon-nucleus (N-A) reactions, because the mean field of QMD corresponds to the real part of the optical model potential (OMP), while the N-N collision is responsible for the imaginary part of the OMP. The QMD gives a (self-consistent) microscopic description of these quantities that are most important in understanding the N-A reactions.

In spite of its success in the heavy ion physics, the validity of QMD in nucleon-induced reactions is still uncertain, because QMD has not been applied intensively to the latter field except for an analysis of (p,xn) reaction carried out by Peilert et al[3]. In their analysis, however, contribution of the statistical decay from the residues produced in the QMD calculation was not considered. The purpose of this work is to validate the usefulness of **QMD with subsequent statistical decay model** in nucleon-induced nuclear reactions and to have a better understanding of the reaction mechanisms.

II. The Quantum Molecular Dynamics[2,4]

In QMD, j-th nucleon (mass m_j) is represented by a Gaussian wave function of variance L;

$$\phi_j(\boldsymbol{r}_j) = \frac{1}{(2\pi L)^{3/4}} \exp\left[-\frac{(\boldsymbol{r}_j-\boldsymbol{R}_j)^2}{4L} + \frac{i}{\hbar}\boldsymbol{P}_j\cdot\boldsymbol{r}_j\right] \tag{1}$$

where $\boldsymbol{R}_j$ and $\boldsymbol{P}_j$ denote the centers of position and momentum. The total wave function is assumed to be a direct product of these wave functions. The time evolution of $\boldsymbol{R}_j$ and $\boldsymbol{P}_j$ is determined, on the basis of the time-dependent variational principle, by Newtonian equations;

$$\dot{\boldsymbol{R}}_I = \frac{\partial\langle\phi|H|\phi\rangle}{\partial \boldsymbol{P}_I}, \quad \dot{\boldsymbol{P}}_I = -\frac{\partial\langle\phi|H|\phi\rangle}{\partial \boldsymbol{R}_I} \tag{2}$$

The Hamiltonian H consists of the classical "kinetic + mass" energy operator, the Skyrme-type effective N-N interaction, and conventional Coulomb and symmetry forces;

$$H = \sum_i \sqrt{m_i^2c^4 + P_i^2c^2} + \sum_{i>j} \{t_0\delta(r_i-r_j) + t_3\delta(r_i-r_j)\cdot\rho[(r_i+r_j)/2]^\gamma + c_i\cdot c_j\cdot e^2/|r_i-r_j| + \text{Symmetry Energy}\} \tag{3}$$

where c_i = 1 for proton and =0 for neutron. The constants t_0, t_3, and γ were determined to reproduce the properties of the saturated nuclear matter and stiff equation of state. The relative position of two particles, which is required in obtaining the expectation value of the Hamiltonian H, is calculated in an invariant form under the Lorentz transformation between the laboratory and center-of-mass of particles i and j.

The collision term is considered in QMD essentially the same as in the cascade model: when two nucleons approach each other within a distance determined from the N-N cross section, a scattering takes place. The probability that a collision is prohibited by the Pauli principle is calculated based on the density overlap of identical-nucleons in the phase-space. The N-N cross section is taken from refs. 5-7. The following inelastic channels, pion production and reabsorption are included;

N + N	→	N + △,	N + △	→	N + N
N + N	→	N + N*,	N + N*	→	N + N
△	→	N + π,	N*	→	N + π
N + π	→	△,	N + π	→	N*

where N* refers to N*(1440).

The QMD calculations are performed up to a certain time (about 100 ~ 200 fm/c depending on the system under interest). The surviving clusters are identified at that time according to the relative position of nucleons, and excitation energy of each cluster is calculated. The, the statistical decay of residues[4] are considered assuming a sharp cut-off model of the transmission coefficients and the Fermi gas level density formula with a=A/8. Finally, the double-differential cross sections are calculated by averaging the results of various impact parameters. Typically 50,000 events are generated.

The only parameter in QMD calculation, the variance L of the wave function, was adjusted to obtain a stable ground state of target nucleus with an adequate binding energy and density profile. Consequently, no parameter was adjusted to fit the calculated cross section to the experimental data.

III. Results and Discussion

The "QMD + statistical decay model" calculations have been carried out for (N,xN') reactions on C, Al and Fe in the energy region of 25 MeV to 3 GeV. In Figs 1 to 4 shown are the typical results of (p,xn) reactions for Fe and C with experimental data[8,9] and predictions of cascade+evaporation code

(Nucleus[10]). At 113 MeV, the cascade model gives lower values compared with the experimental data at the most backward angle, which fact has been interpreted as an evidence of the pre-equilibrium contribution to be added to the cascade model calculations. The present results, on the contrary, reproduce the measured data satisfactorily over the whole angular region. Moreover, the agreement of the present calculation with the low energy neutron data confirms that the QMD gives a proper excitation spectra of residues from which the statistical neutron emission takes place. Therefore, it is clear that the present calculation based on QMD + statistical decay includes the major three reaction mechanisms of nucleon induced reaction, i.e., the cascade (spallation), pre-equilibrium and statistical decay of compound system, in a unified framework. This fact was also verified form the mass and multiplicity distributions produced from p + C reactions. At 800 MeV and 1.5 GeV, the agreement of the present calculation with the measured data is also remarkable.

At 3 GeV, the cascade model overprotects the C(p,n) data at forward angles. These discrepancy has been discussed in terms of the multi-fragmentation or phase transition which are not included in the cascade calculations. The present calculation, on the other hand, reproduce the data in general, which shows that QMD includes complicated reaction processes automatically. However, the prediction of (p,xn) cross section at this energy depends also on the inelastic N-N collision channels quite strongly. The difference in this process in the present approach and Nucleus code might be attributable to this disagreement. This possibility is now under investigation.

Figures 5 and 6 show how the QMD describes the transition of reaction mechanisms as a function of incident energy. In Fig. 5, the particle multiplicity distribution from p + ^{12}C reaction at several incident energies are exhibited. This was calculated at the time of 4.5 to 6.0x10^{-22} [sec] after the contact of p and C; the time up to which the QMD calculation has been carried out. This time corresponds to the typical time scale of the pre-equilibrium process, but much shorter than that of the equilibrium process. Consequently, this figure shows the number of fragments before the statistical decay takes place. The mass distribution of the fragment at the same time is shown in Fig. 6. Figure 5 shows that, at the incident proton energy is as low as 5 MeV, the number of fragment is mostly just unity, showing that the compound nucleus has been created, corresponding to the mass 13 fragment in Fig. 6. As the incident proton energy increases, the number of fragment increases more and more. At 20 and 50 MeV, multiplicity of 2 and 3 become dominant, indicating that one or two particles (mostly nucleons) are emitted from the pre-equilibrium process. The QMD thus includes automatically the multi-particle pre-equilibrium emission. Figure 6 shows that multiplicity of nucleons increases rapidly at this energy region. Above 100 MeV, on the contrary, the multiplicity and mass distribution become flatter. In this energy region, high multiplicity events increaes drastically, and the reaction exhibits a feature what is known as the "spallation" process. In Fig. 6 also shown are that the QMD predicts emission of mass 2 particle from the pre-equilibrium time scale, although the probability is not high. Therefore, the QMD also includes the emission of composite particles form the pre-equilibrium process. In summary, the QMD describes quite naturally the transition of the major three reaction mechanisms of the nucleon-

nucleus reaction in a unified framework without adjusting any parameter; the formation of compound nucleus (which is dominant at low energy), pre-equilibrium process (including multi-particle emission and emission of composite particles), and the spallation reaction.

VI. Concluding Remarks

The Quantum Molecular Dynamics + statistical decay model has been applied to analyze the nucleon-induced nucleon emission cross sections from several tens MeV to several GeV. It was proved that the present calculation could reproduce the measured data quite satisfactorily without assuming any additional reaction mechanisms and without adjusting any parameters. The QMD gives a unified framework of the major three reaction mechanisms of nucleon-induced nuclear reactions; the spallation, pre-equilibrium (including multi-particle and composite-particle emissions) reaction and compound nucleus formation.

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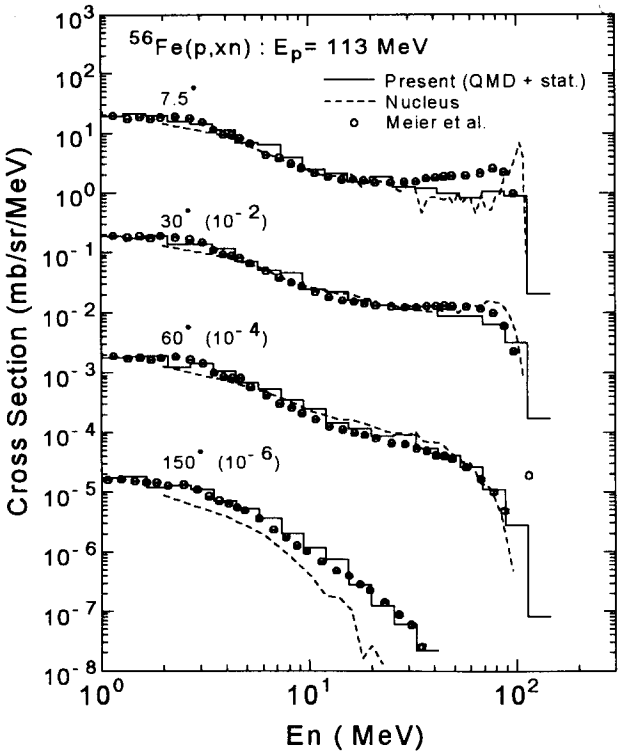

Fig. 1 ^{56}Fe(p,xn) cross section at 113 MeV

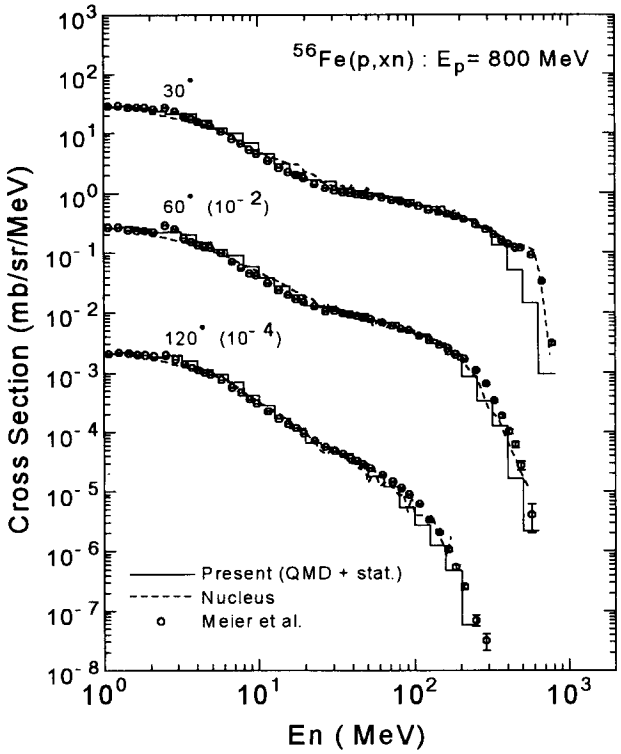

Fig. 2 ^{56}Fe(p,xn) cross section at 800 MeV

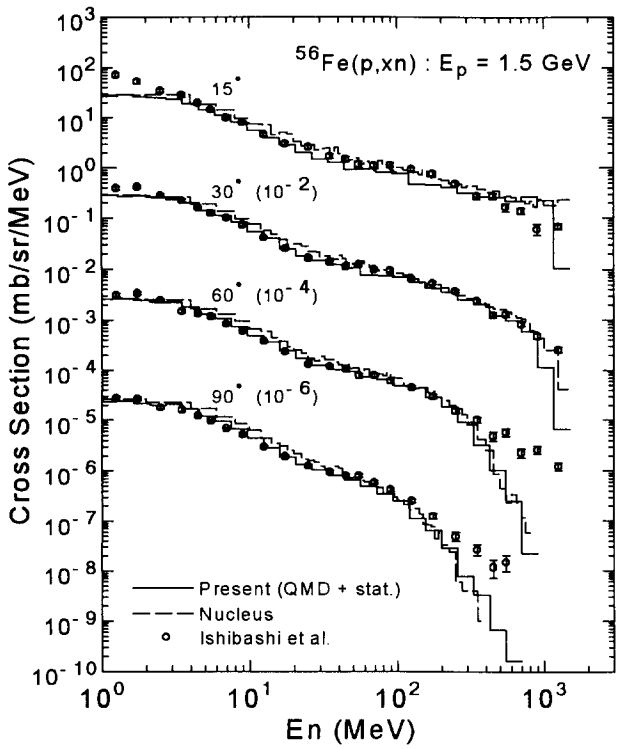

Fig. 3 ^{56}Fe(p,xn) cross section at 1.5 GeV

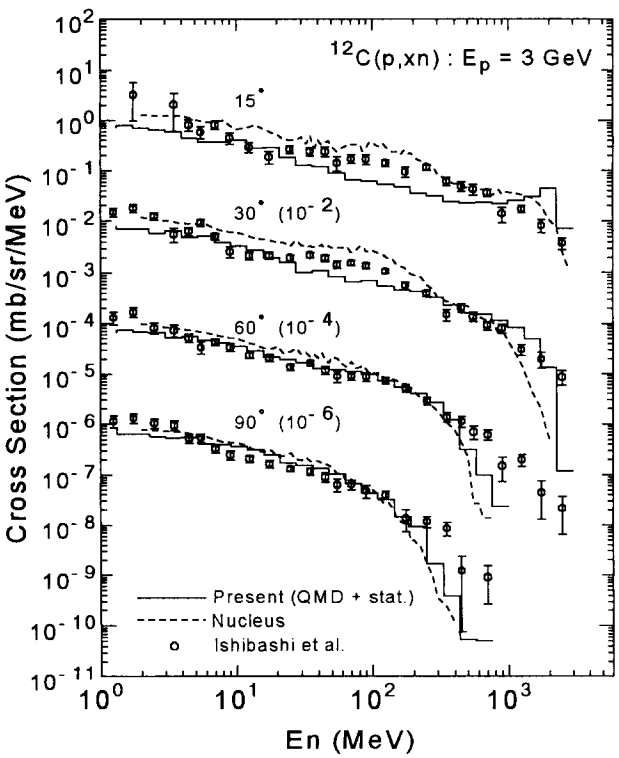

Fig. 4 ^{12}C(p,xn) cross section at 3 GeV

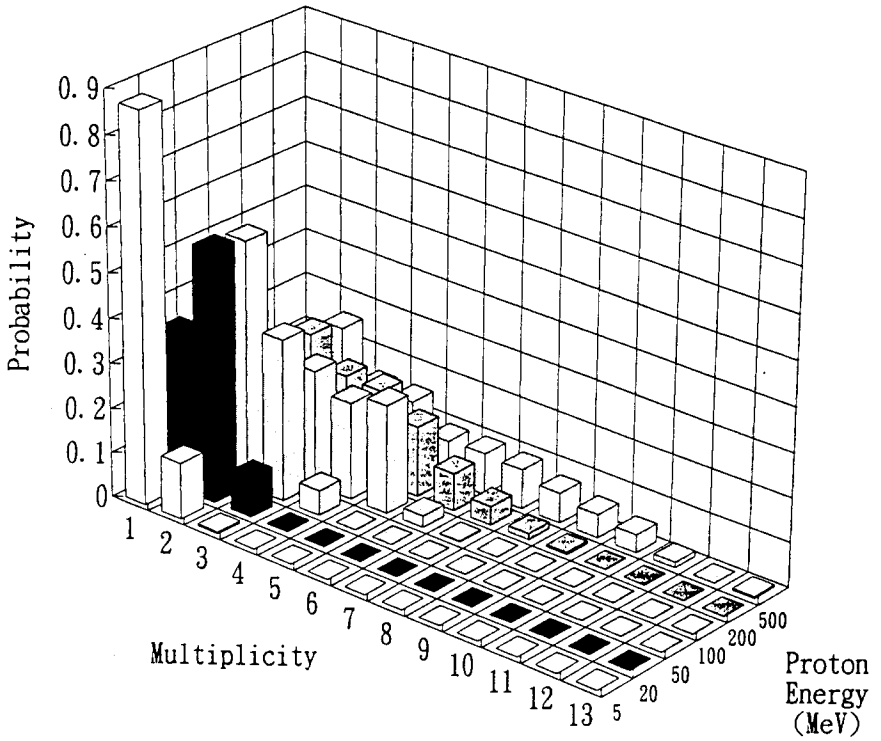

Fig. 5 Particle multiplicity distribution from ^{12}C + p reaction at t = 4.5 ~ 6.0 × 10^{-22} [sec]

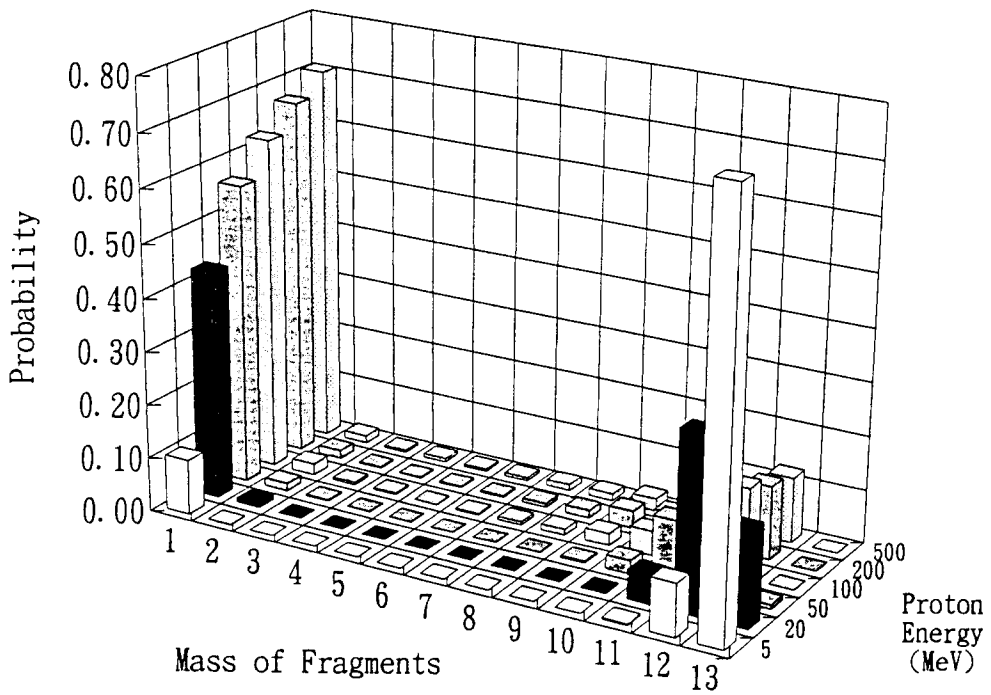

Fig. 6 Fragment mass distribution from ^{12}C + p reaction at t = 4.5 ~ 6.0 × 10^{-22} [sec]