LBL-26474 c.2

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

RECEIVED
LAWRENCE
BERKELEY LABORATORY
JUN 7 1989
LIBRARY AND
DOCUMENTS SECTION

Presented at the International Workshop on Gross
Properties of Nuclei and Nuclear Excitations
Hirschegg, Austria, January 16–21, 1989

Development of a Transition-State Treatment of Multifragmentation

J. Randrup and J.A. López

December 1988

TWO-WEEK LOAN COPY
This is a Library Circulating Copy
which may be borrowed for two weeks.

NUCLEAR SCIENCE DIVISION

LBL-26474 c.2

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

Gross Properties of Nuclei and Nuclear Excitations
International Workshop XVII, Hirschegg, Kleinwalsertal, Austria, 16-21 January, 1989

Development of a Transition-State Treatment of Multifragmentation

Jørgen Randrup and *Jorge A. López*
Nuclear Science Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

Highly excited nuclear systems can be produced in the laboratory by use of medium-energy heavy-ion beams (or high-energy protons); these systems typically disassemble into several, or many, (moderately excited) nuclear fragments. The experimental basis for this topic is the fact that such multifragmentation processes are presently of central interest in nuclear physics and in spite of vigorous efforts, both experimental and theoretical, they are not yet well understood.

For the nuclear multifragmentation problem, several statistical models have been developed in recent years, based on excitable fragments within a specified freeze-out volume.[1,2,3] Such a scenario is of direct relevance to the study of dilute nuclear matter (at not too high temperatures) and the formulation of the associated statistical mechanics is relatively straightforward, even when fragment interactions are incorporated.[1b]Application of such statistical models to the disassembly of a nuclear "source" has usually been made by simply assuming that the yield of a given final channel is proportional to the corresponding statistical weight.

Although capable of reproducing a variety of features of the data, such approaches are not entirely satisfactory. A principal problem is that there is no inherent way of determining the freeze-out volume, which therefore must be prescribed by some argument external to the model. A related problem is that the potential barriers are not given appropriate consideration, although experience from binary fission has shown that the potential-energy barriers have a controlling influence on the decay widths. Moreover, the propagation of the fragmenting system from the freeze-out configuration to asymptotia is dependent on how the potential energy is treated. These problems are particularly serious at relatively moderate excitations and they need to be adequately solved before it is possible to clarify such key questions as the transition from the ordinary sequential-binary type of decay characteristic of low excitation to the nearly simultaneous multifragment breakup apparently occurring at high excitation.

This unsatisfactory situation has motivated us to develop[4] a refined treatment of statistical multifragmentation based on a suitable generalization of the transition-state approximation for ordinary binary fission[5]. Thus, we consider the irreversible transition of a very excited compound nucleus into a number of prefragments. These prefragments are still interacting and may in general experience significant change during their dynamical evolution subsequent to the transition. The main objective will be to characterize the "transition state", the family of configurations at which the system irreversibly makes the transition into the specified prefragments.

We describe the disassembling system as a collection of a number of interacting (pre)fragments. In this manner, the degrees of freedom associated with a given final channel are included explicitely already at the transition stage, even though the fragments may not yet have been fully developed as separate entities. The physical scenario is then quite similar to that addressed in current statistical multifragmentation models, and we shall adapt our formalism from [1]. As in the binary case, a central problem associated with such a formulation is the construction of a suitable potential energy function in terms of the spatial configuration of the prefragments. The internal level density must also be carefully modified to take account of the particular "shape" of the transition configuration.

*This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The total density of states $\rho_A(E_0^\star)$ can conveniently be decomposed according to mass partition $A_1, ..., A_N$,

$$\rho_A(E_0^\star) = \frac{dN_A(E)}{d\mathbf{R}\, d\mathbf{P}\, dE} = \frac{1}{N!}\sum_N \prod_{n=1}^{N} \left[\sum_{A_n}\right] \delta(\sum_{n=1}^{N} A_n - A)\, \frac{dN_{A_1\cdots A_N}(E)}{d\mathbf{R}\, d\mathbf{P}\, dE} . \tag{1}$$

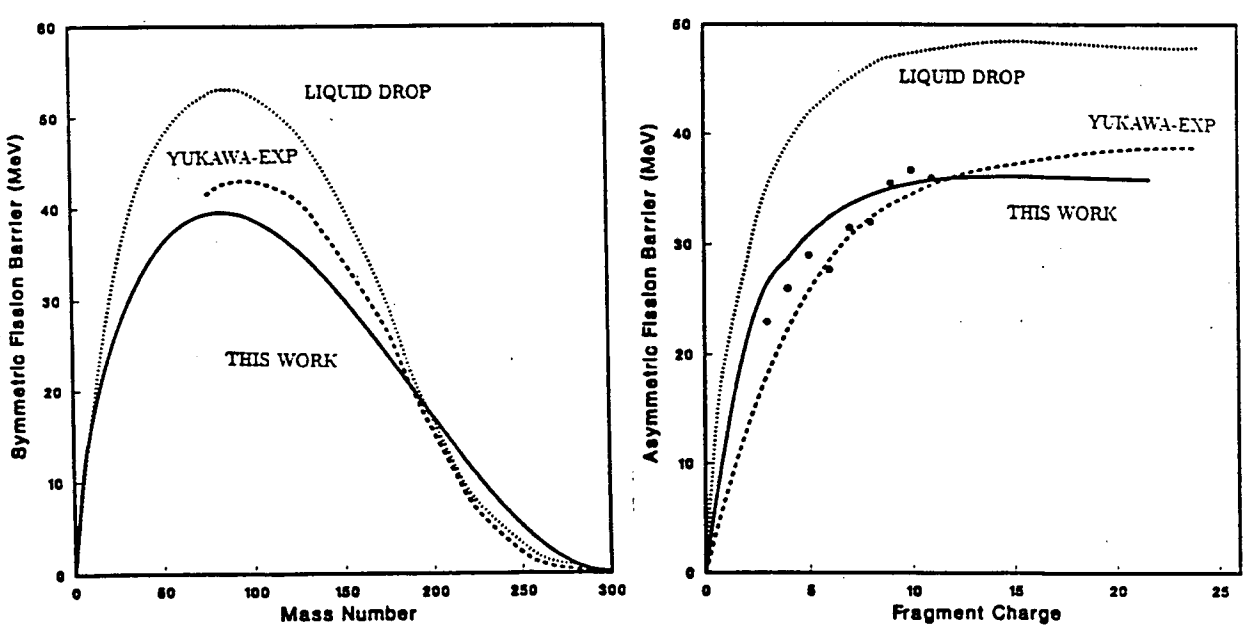
The division by $N!$ compensates for the fact that the summation over fragment mass numbers produces $N!$ terms for which the fragment masses only differ by the order of their labelling. In the above decomposition, the contribution to the density of states from a particular mass partition is given by

$$\frac{dN_{A_1\cdots A_N}(E)}{d\mathbf{R}\, d\mathbf{P}\, dE} = \prod_{n=1}^{N} \left[\int \frac{d\mathbf{r}_n d\mathbf{p}_n}{h^3} \int d\epsilon_n\, \rho_n(\epsilon_n)\right] \delta(E_F - E)\, \delta(\mathbf{P}_F)\, \delta(\mathbf{R}_F) , \tag{2}$$

where $\mathbf{R}_F = \frac{1}{m_0}\sum_n m_n \mathbf{r}_n$ is the overall center-of-mass position and $\mathbf{P}_F = \sum_n \mathbf{p}_n$ is the total momentum. For convenience, we shall henceforth work in the CM reference frame, where both $\mathbf{R}$ and $\mathbf{P}$ vanish. Furthermore, $A_F = \sum_n A_n$ is the total mass number of the particular fragmentation, and E_F is its total energy. This latter quantity is assumed to be of the form

$$E_F = \sum_{n=1}^{N_F} (E_n^0 + \epsilon_n + \frac{p_n^2}{2m_n}) + V(\mathbf{r}_1, ..., \mathbf{r}_N) = E_{1\cdots N}^0 + \epsilon + E_{\text{kin}} + V . \tag{3}$$

Here $E_{1\cdots N}^0 = \sum_n E_n^0$ is the sum of the ground-state energies of the N fragments, and $\epsilon = \sum_n \epsilon_n$ is their total internal excitation energy. The total kinetic energy of the fragments is $E_{\text{kin}} = \sum_n p_n^2/2m_n$, where the inertial mass m_n is approximately equal to A_n times the nucleon mass. Since the transition configurations of interest consist of fairly developed prefragments, we shall assume that the potential energy V can be expressed as a sum of pairwise interaction energies, $V = \sum_{nn'} V_{nn'}$. The specific form of the interaction potential $V_{nn'}(r_{nn'})$ is based on a simple parametrization[6] for the shapes and barrier heights for asymmetric binary fission. This prescription mimics the effect of the finite range of the nuclear interaction and leads to a reasonable global reproduction of fission barriers:



Left: *Symmetric fission barrier heights for nuclei along the line of β stability calculated with the liquid-drop model[7], the Yukawa-plus-exponential model[7], and our modified Swiatecki parametrization[6].* Right: *Asymmetric fission barrier heights for ^{123}Xy as calculated with the same models.*

In order for the density of states (2) to yield a finite result, the fragment positions must be (somehow) confined. This is ordinarily accomplished by requiring the fragment positions to be within a specified volume Ω. While such a scenario is appropriate for studies of infinite matter, which can be approximated by periodic boundary conditions, the nature of the confining agency is less obvious for an isolated finite system, such as may be formed in a nuclear collision. In our present treatment, we shall replace the somewhat artificial volume Ω by a suitable generalized fission coordinate whose function is to constrain the overall spatial extension of the multifragment system so that the position integrals remain convergent. The corresponding density of states is well-defined and can be considered as a function of the disassembly variable. In this manner the breakup problem can be reduced to a one-dimensional form and is then amenable to a transition-state treatment in analogy with ordinary binary fission.

Towards this end we define, for a given fragmentation F, the disassembly coordinate q and its conjugate momentum p as follows,

$$q_F^2 \;=\; \frac{1}{m_0}\sum_{n=1}^{N} m_n r_n^2 \;, \qquad p_F \;=\; \frac{1}{q_F}\sum_{n=1}^{N} \mathbf{p}_n \cdot \mathbf{r}_n \;. \tag{4}$$

The associated inertial mass is given by $m_0 = \sum_n m_n$, since the kinetic energy of the outwards flow is $K = \frac{1}{2}p\dot{q} = p^2/2m_0$. The disassembly variables q and p can be employed as a set of auxiliary degrees of freedom for the multifragment system by applying the identity operation $\int dqdp\; \delta(q_F - q)\delta(p_F - p)$ to the expression (2) for the density of states for the particular mass partition considered. The density of states can then be considered as a function of q and p, which characterize the global extension and outwards motion of the system, resepctively. After performing the constrained integrations over the fragment momenta $\{\mathbf{p}_n\}$, we obtain the following relation,

$$\frac{dN_{A_1\cdots A_N}(E)}{d\mathbf{R}\; d\mathbf{P}\; dE} = \frac{(2\pi m_0)^{-2}}{\Gamma(\frac{3}{2}N-2)}\prod_{n=1}^{N}\left[(\frac{m_n}{2\pi\hbar^2})^{\frac{3}{2}}\int d\mathbf{r}_n\right]\int dqdp\int d\epsilon\; \rho_{1\cdots N}(\epsilon)\kappa^{\frac{3}{2}N-3}\;\delta(\mathbf{R}_{\mathcal{P}})\;\delta(q_{\mathcal{P}}-q)\;. \tag{5}$$

We have also replaced the integrations over the N individual excitations ϵ_n by a single integral over the total internal excitation energy $\epsilon = \sum_n \epsilon_n$. The corresponding total internal level density is denoted $\rho_{1\cdots N}(\epsilon)$ and depends on the particular *positioning* $\mathcal{P}$: $\{\mathbf{r}_n\}$ of the N (pre)fragments. We shall use the convoluted form $\rho_{1\cdots N} = \rho_1 * \cdots * \rho_N$, which would be exact for separated fragments.

For given positions $\{\mathbf{r}_n\}$, the amount of energy available for statistical sharing between the degrees of freedom of the system is given by

$$E^\star \;=\; E - E^0_{1\cdots N} - V(\mathbf{r}_1,...,\mathbf{r}_N) - K \;=\; \kappa + \epsilon\;. \tag{6}$$

This energy is divided between the random kinetic energy κ of the $3N-4$ remaining translational degrees of freedom of the N fragments and their total internal excitation energy ϵ. [Note that κ is the energy of the *statistical* motion of the fragments, *i.e.* their motion in addition to the minimal collective motion required for satisfying the specified constraints on the overall momentum $\mathbf{P}$ and the outwards flow p.] For a specified value of the collective outwards kinetic energy K, the maximum attainable internal excitation is $\epsilon_K = E^\star$, corresponding to $\kappa = 0$. This (unlikely) situation is achieved when all the fragments move in the radial direction, each with a momentum proportional to the distance from the origin. Moreover, we have $\epsilon_K = \epsilon_0 - K$, where $\epsilon_0 = E - E^0_{1\cdots N} - V$ is the largest possible internal excitation energy, as obtained when the collective kinetic energy K vanishes. This quantity is also the largest value K can have (occurring for $\epsilon_K = 0$), for the particular positioning $\mathcal{P}$ considered.

The above formula (5) "counts" the total number of states (within the given tolerance dE on the total energy) by going through all possible fragmentation F consistent with the constraints $\mathbf{R}_F = \mathbf{0}$, $q_F = q$, and $p_F = p$, and for each such positioning summing over all values of (q,p). The disassembly coordinate q controls the overall spatial extension of the multifragment system, while the constrained positionings represent orthogonal macroscopic degrees of freedom analogous to the additional deformation parameters employed in refined descriptions of ordinary fission.

Our transition-state approximation to the disassembly problem is most conveniently formulated in terms of the outwards probability current, *i.e.* the number of elementary multifragment states that pass by a given value of q per unit time. This quantity can be obtained from (5) by extending the q integration over values of from 0 to p/m_0, the distance covered by q per unit time, yielding the flux factor p/m_0 in the p integration. Subsequently, it may be used that $(p/m_0)dp = dK$, so that the integrations over K and ϵ may be interchanged and the former one performed analytically. The outwards current is then

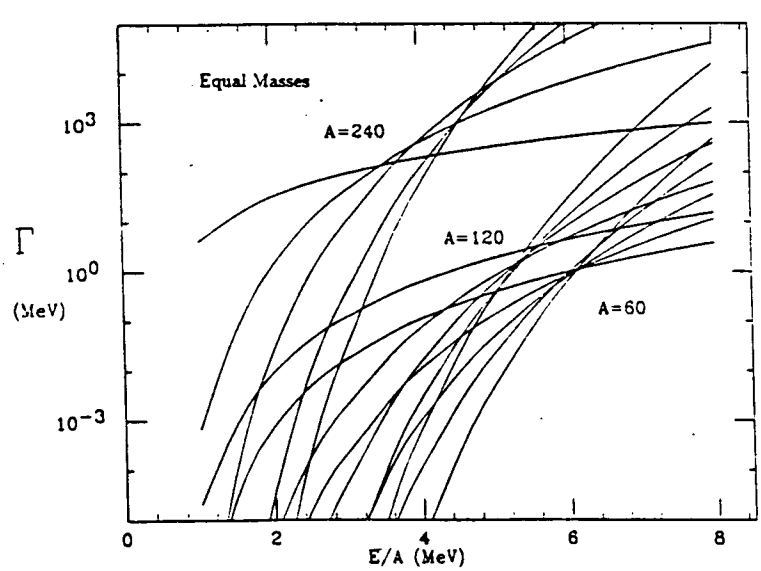
$$\frac{d\nu_{1\cdots N}}{dE} = \frac{\sqrt{4\pi}}{\Gamma(\frac{3}{2}N-\frac{3}{2})}\,\frac{1}{\Gamma(\frac{3}{2}N-1)}\,\langle\,(\frac{m_0 q_0^2}{2\hbar^2})^{\frac{3}{2}N-2}\int_0^{\epsilon_0} d\epsilon\;\rho_{1\cdots N}(\epsilon)\;[\epsilon_0-\epsilon]^{\frac{3}{2}N-2}\,\rangle'\,. \qquad (7)$$

The statistical average $\langle\cdot\rangle'$, is over the fragment positions, constrained by some (arbitrary) value of the disassembly coordinate q. [It is an important feature of the result that is independent of which particular value q' has been chosen to constrain the reduced positions, since the subsequent stretching will bring the system to the same transition configuration.]

For given values of the constrained positions $\{\mathbf{r}'_n\}$, the integrand in the flux (7) has a minimum at some value q_0, because the potential energy exhibits a maximum as the system is stretched from a compact configuration towards separated fragments. [The minimium in the integrand is shifted slightly inwards relative to the barrier top due to the factor q^{3N-4}.] As in the treatment of binary fission, it is natural to identify the value $q = q_0$ with the local bottle neck in the evolution towards breakup. Accordingly, the total rate at which the system makes an irreversible transition towards disassembly is approximated by the above current (7), with the proviso that the local value of q be chosen as that value q_0 for which the integrand has its minimum.

Invoking the usual statistical assumption, the decay width of the system (into the specified mass partition) is given by the magnitude of the transition current, $d\nu_{1\cdots N}/dE$, divided by the total compound level density, $\rho_A(E_0^\star)$, which represents the total number of elementary states in the decaying compound system. Evaluating the ϵ-integral in (7) approximately, we then obtain the following result for the partial width for transition into the specified mass partition,

$$\Gamma_{A_1\cdots A_N}(E) = \frac{1}{\rho_A(E_0^\star)}\frac{d\nu_{1\cdots N}}{dE} \approx \frac{1}{\rho_A(E_0^\star)}\,\frac{\sqrt{4\pi}}{\Gamma(\frac{3}{2}N-\frac{3}{2})}\,\langle\,(\frac{m_0 q_0^2\bar{\tau}_0}{2\hbar^2})^{\frac{3}{2}N-2}\,\rho_{1\cdots N}(\epsilon_0)\;\bar{\tau}_0\,\rangle'\,, \qquad (8)$$



The patital width $\Gamma_{A_1\cdots A_N}(E)$ for transition of a compound nucleus with mass number A into N prefragments with equal masses, as a function of the initial excitation energy per nucleon $E_0^\star/A$.

where $\bar{\tau}_0$ is the internal temperature of the transition configuration. The total width $\Gamma_A^N(E)$ for transition into any N prefragments can be obtained subsequently by summing over all the contributing mass partitions,

$$\Gamma_A^N(E) = \frac{1}{N!}\prod_{n=1}^{N}\left[\sum_{A_n}\right] \delta(\sum_{n=1}^{N} A_n - A)\, \Gamma_{A_1\cdots A_N}(E) \,. \tag{9}$$

The partial width $\Gamma_{A_1\cdots A_N}(E)$ for equal-mass breakup (*i.e.* $A_1 = \cdots = A_N$) is shown at the bottom of the previous page, for a number of instructive cases.

At low excitation, channels with only two prefragments dominate and the formula (8) for the decay width reduces to a form rather similar to the standard Bohr-Wheeler expression[5], but with a modulation factor arising from the orbital motion of the binary complex. The dominant multiplicity increases with excitation and at high excitation the treatment acquires considerable formal similarity with existing statistical multifragmentation models (especially [1b]), although certain notable differences are present. An important advantage of our treatment is that it automatically provides a constraint on the fragment positions so that a finite result obtains; in this regard it is a significant advance relative to current statistical models in which the freeze-out volume must be prescribed separately.

This novel transition-state treatment of multifragmentation provides a well-defined means for calculating the partial widths for transition of the system into a number of interacting prefragments with specified masses and total energy. It is important to be aware that in order to obtain the actual final channel for a particular disassembly process, it is necessary to follow the further propagation of the system from the transition point towards asymptotia, since some prefragment pairs may find themselves inside the barrier of their respective two-body interaction potential and hence may recombine.

A major motivation for undertaking the present work has been the need for a model in which the evolution of the disassembly process from low to high excitation can be addressed. Having attractive limits, the developed model provides such a framework and its utility has been illustrated by our studies of the dependence of the (pre)fragment multiplicity on excitation energy. Though depending on Monte-Carlo sampling, the application of the model is not more computer-demanding than current statistical multifragmentation models, and a variety of instructive applications of the model are foreseen, at this point primarily for the purpose of gaining theoretical insight.

References

[1] S.E. Koonin and J. Randrup, Nucl. Phys. **A356** (1981) 223; **A474** (1987) 173

[2] D.H.E. Gross, Phys. Lett. **161B** (1985) 47;
D.H.E. Gross, Zhang Xiao-ze, and Xu Shu-yan, Phys. Rev. Lett. **56** (1986) 1544

[3] J.P. Bondorf, R. Donangelo, I.N. Mishustin, C.J. Pethick, and H. Schulz, Nucl. Phys. **A443** (1985) 321; J.P. Bondorf, R. Donangelo, I.N. Mishustin, and H. Schulz, Nucl. Phys. **A444** (1985) 460

[4] J.A. López and J. Randrup, LBL-26164, submitted to Nuclear Physics A

[5] N. Bohr and J.A. Wheeler, Phys. Rev. **56** (1939) 426;
W.J. Świątecki, Aust. J. Phys., **36** (1983) 641

[6] W.J. Świątecki, Phys. Scrip. **24** (1981) 113 and private communication (1988)

[7] H.J. Krappe, J.R. Nix and A.J. Sierk, Phys. Rev. **C20** (1979) 992

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
1 CYCLOTRON ROAD
BERKELEY, CALIFORNIA 94720