Inverse reactions and the statistical evaporation model: Ingoing-wave boundary-condition and optical models

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The calculation of transmission coefficients for emitted particles is fundamental to applications of the statistical evaporation model for the decay of the compound nucleus. In this work we compare the usual type of optical-model calculation of transmission coefficients for neutron, proton, deuteron, triton, and alpha particles with corresponding ingoing-wave boundary-condition calculations. In the latter case the transmission coefficients simply give the probability for transmission through the real potential barrier. This comparison highlights features that are specific to the optical model such as transparency, shape resonances, and peripheral absorption. It also draws attention to the issue of whether simple barrier transmission coefficients are more appropriate for use in the statistical evaporation model.

I. INTRODUCTION

Nuclear reactions induced by heavy ions of >5 MeV per nucleon are copious producers of hot compound nuclei with temperatures of up to ≈ 6 MeV. There is great current interest in determining the macroscopic properties of these hot nuclei,[1] such as their temperature, moment of inertia, size, shape, etc. Information of this type can be found by measuring and interpreting the spectra and angular distributions of emitted photons, light particles, and fragments. The statistical model of nuclear reactions provides the backbone for these interpretations. One assumes that the reaction occurs in two steps, formation of a compound nucleus followed by its decay. The model addresses only the decay probability after the formation is completed.

The basic ideas of the statistical model were introduced and discussed in classic papers of five decades ago.[2–4] Extensive machinery to handle the inclusion of angular momentum[5–8] was put in place in the 1950s, and a number of statistical-model computer codes have been constructed. The framework has been derived via two different routes: namely, detailed balance and the transition state. Recently, Swiatecki has emphasized certain simplicities in the application of the transition-state method.[9] In both approaches there are two essential ingredients: state densities for hot nuclei and transmission coefficients for the emitted photons, particles, or fragments.

In this paper we discuss the elementary logic of the model and its utilization, focusing on the transmission coefficients for light particle emission. The most commonly used recipe for calculating transmission coefficients is to use an optical-potential model with global parameters obtained by fitting elastic-scattering data. The idea behind this procedure is based on the concept of detailed balance, whereby one can obtain the evaporation rate from the knowledge of the time-reversed capture cross section. The major problem with these parametrizations is that neither elastic scattering nor its counterpart, the total of all reactions, is actually the time-reversed reaction for particle evaporation. In addition, no allowance is made for the difference between the hot nuclei involved in evaporation compared to the cold ground-state nuclei used for elastic-scattering studies. Because of this, features which are specific to elastic scattering, such as volume transparency and surface absorption, are routinely being used to describe the evaporation process.

In this paper we address this problem by making calculations using two procedures: the conventional optical model[10,11] and the ingoing-wave boundary-condition model.[12,13] We discuss their relationships to the logical choice of the time reversed or inverse reaction. Our suggestion is that the latter model does provide a reasonable set of "reference values" for the transmission coefficients. This suggestion arises naturally from the basic hypothesis for the transition-state method and can also be reconciled with the notion of detailed balance. The conventional complex optical-potential model is a useful tool for describing elastic scattering. However, the transition-state evaporation model needs a much more simple item, namely, a penetrability for the escape process.

In the next section we outline the simplest form of these two classic methods for deriving the statistical model. Then, in Sec. III, we present a series of calculations that compare two model calculations; finally in Sec. IV we summarize and discuss our conclusions.

II. BASICS OF THE EQUILIBRIUM STATISTICAL MODEL

Let us first recall Swiatecki's simple presentation of the transition-state method.[9] An ensemble of compound nu-

clei with state density $\rho_A(E)$ is presumed to have been formed. Their decay, by exit channel ν, passes through a transition-state configuration with state density $\rho^*(X)$, where $X=E-B-K$ with B and K the potential barrier and kinetic energies corresponding to the decay mode. The decay rate P_ν can be related to the number of points in phase space that traverse the transition state in the time interval Δt divided by the total number of available states[9]

$$P_\nu \Delta t = h^{-1} \int_0^{p_{\max}} dp \int_{-v\Delta t}^{0} dq\, \rho^*(X) W(K)/\rho_A(E) \ . \quad (1)$$

Here a single degree of freedom for the disintegration direction has been assumed and is denoted by q, its conjugate momentum is p, its velocity v, and $W(K)$ is the barrier penetrability factor. Simplifying, one obtains

$$P_\nu = [h\rho_A(E)]^{-1} \int_0^E dX\, \rho^*(X) W(K) \ . \quad (2)$$

The detailed balance approach[3,4,14] also begins with the presumed existence of an ensemble of compound nuclei; their decay by exit channel ν proceeds by the reaction $A \rightarrow B + \nu$. The condition of detailed balancing can be written as follows:[14]

$$\rho_A w_{ab} = \rho_B w_{ba}^* \ . \quad (3)$$

The density of states for the final (initial) system is denoted by ρ_B (ρ_A) and the transition probability from A to B (B to A) is denoted by w_{ab} (w_{ba}^*). The rate P_ν from A to B is then given by the integral of w_{ab} over all states in B,

$$P_\nu = \int w_{ab} = \int \rho_B w_{ba}^* / \rho_A \ . \quad (4)$$

To make contact with Swiatecki's simplified description[9] we consider the decay process in a single dimension, and enclose the emitters in a one-dimensional box of length L. Then the probability for capture of the particle ν by the nucleus B is given by $w_{ba}^* = v_\nu T_\nu(\epsilon_\nu)/L$, where v_ν and ϵ_ν are the particle velocity and energy and $T_\nu(\epsilon_\nu)$ is the capture probability. The state density ρ_B for the combined system of residual nucleus B and particle ν is

$$\rho_B = h^{-1} \int_0^L dq \int_0^{p_{\max}} dp\, \tilde{\rho}_B(E-\tilde{B}-S_\nu-\epsilon_\nu) \ , \quad (5)$$

where S_ν = the separation energy for channel ν, the potential energy of the residual nucleus is $\tilde{B}$, and its state density is $\tilde{\rho}_B$. After substitution into Eq. (4) we obtain

$$P_\nu = [h\rho_A(E)]^{-1} \int_0^{\epsilon_{\max}} \tilde{\rho}_B(E-\tilde{B}-S_\nu-\epsilon_\nu) T_\nu(\epsilon_\nu) d\epsilon \ . \quad (6)$$

(In this discussion angular momentum has been omitted; it could be included as discussed in Refs. 5–8.)

Now let us try to reconcile Eq. (2) from the transition-state approach to Eq. (6) from detailed balancing. Both equations have the same structure and lead to a product of factors for state density and reaction probability. In the transition-state method, it is clear that the factor $W(K)$ in Eq. (2) is simply the barrier penetration factor for ν as it attempts to exit the initial compound nucleus. Similarly we can identify T_ν in Eq. (6) as the barrier penetration factor for reentry of ν by the inverse or time-reversed reaction $\nu + B \rightarrow A$.

The state density factors seem, at first glance, to be different since $\rho^*(E-B-K)$ refers to a transition state nucleus, while $\tilde{\rho}_B(E-\tilde{B}-S_\nu-\epsilon_\nu)$ refers to a residual nucleus after the exit of particle ν. However, the basic assumption of Eq. (3) for detailed balancing is that the initial and final systems must be imagined as capable of complete communication as if in chemical equilibrium. Hence the state B must be imagined to correspond to the final configuration available to the system for such communication. In fission, for example, it would not make sense to use a final state of infinitely separated fragments. A state of two fragments in contact or a deformed saddle-point configuration would be more reasonable. Thus the states B must be thought of as final decision-point configurations for statistical counting, and this idea carries the meaning of statistical equilibrium. Moreover, it is in this sense that one can identify the state densities ρ^* and $\tilde{\rho}_B$ with the same final decision point configuration, and thus conclude that Eqs. (2) and (6) are actually identical. (Some additional discussion of this point is given in Appendix C.)

III. CALCULATIONS AND COMPARISONS OF THE OPTICAL MODEL AND THE INGOING-WAVE BOUNDARY-CONDITION MODEL

Our objective here is to compare two models for the transmission factors. We make calculations with standard complex optical-potential parametrizations[11] (OM), and compare them to results obtained using purely real potentials with ingoing-wave boundary conditions[13] (IWBC). Even though we use the same real potentials, there are three qualitative differences in the results from these two approaches: (a) The usual OM includes reactive scattering outside the real potential well (due to the tail of the imaginary potential) in addition to absorption inside the well. (b) The optical model produces both penetration into the well as well as some subsequent repenetration to escape reaction, i.e., transparency. (c) The optical model supports size resonances due to standing waves inside the well.

These three features of the OM are all related to important aspects of elastic scattering from ground-state nuclei. A great deal of work has gone into obtaining working descriptions of these scattering reactions by parametrization of real and imaginary potentials. However, the task of the statistical model is different and indeed more straightforward and less demanding; it is simply to calculate the penetrability for exit of a particle from a hot nucleus or the time-reversed path of particle entry into a hot nucleus. Hence, one wants to describe only the transmission coefficient for one traversal of a projectile from outside to inside the well. In fact, this simple step is precisely what is done by the IWBC model.[12]

In Figs. 1–4 we compare calculated results for these two approaches: let us examine the differences in some detail. We have chosen the compound nuclei ^{67}Ga and ^{149}Tb since several recent studies have been reported for these cases.[15–18] First, in Fig. 1 we show T_l vs energy for several l values for n, ^{1,2,3}H and ^{4}He. For the deuterons

and tritons (and alphas to some degree) we note that, at low energies, the OM gives significantly larger T_l values than the IWBC model. Since both calculations use the same real potential, this difference must be due to the treatment of absorption. We conclude that this difference arises from the radial tail of the imaginary potential as parametrized in the OM; this causes reactive scattering in peripheral and distant collisions that do not penetrate the real barrier, as shown by comparison to the IWBC model. By its very nature the IWBC model only allows reaction by penetration.

The pattern for the protons and neutrons is much more complex. We have displayed their behavior in more detail for $l=(0-4)\hbar$ in Fig. 2. Here the differences in T_l values are much stronger and vary with both l and ϵ. The major qualitative difference is that for the IWBC model the T_l values always asymptotically approach unity for increasing ϵ, while those from the OM often do not. In addition, even at lower energies, the OM values are usually significantly smaller than those from the IWBC model. This is not because the particles reflect on incidence; it is because they penetrate both into and again out of the well. This distinction can be drawn by comparison to the T_l values calculated by the IWBC model for penetration of the same real potential; the latter set of T_l values approach unity. The same transparency effect appears to a small degree for ^{2}H, but it is essentially absent for the more strongly absorbed ^{3}H and ^{4}He particles. Consider the possible emission of a 10-MeV neutron of $l=0$ from ^{67}Ga. The IWBC model gives $T_l \approx 1$, whereas the OM gives $T_l=0.76$ [see Fig. 1(a)]. The low T_l value from the optical model arises from the rather large chance that an incident neutron will both penetrate to enter and subsequently penetrate again to reemerge from the target. Therefore, if we use the T_l value of 0.76 from the OM, we are reducing the single penetrability value from $T_l=1$ due to the dual barrier penetrations in the optical model (i.e., transparency).

In Figs. 1 and 2 we have illustrated only the rapid rise of T_l values with energy and their leveling off at above-barrier energies. In fact, on a very fine scale, one sees that the OM gives rise to oscillatory structure, while the IWBC model is quite monotonic. This is related to size resonances due to standing waves inside the well. In Fig. 3 we have chosen to show this effect by plotting fractional differences between values from the two models. We show results for protons (a) and neutrons (b) as their oscillations have the largest amplitudes. The tips of the ar-

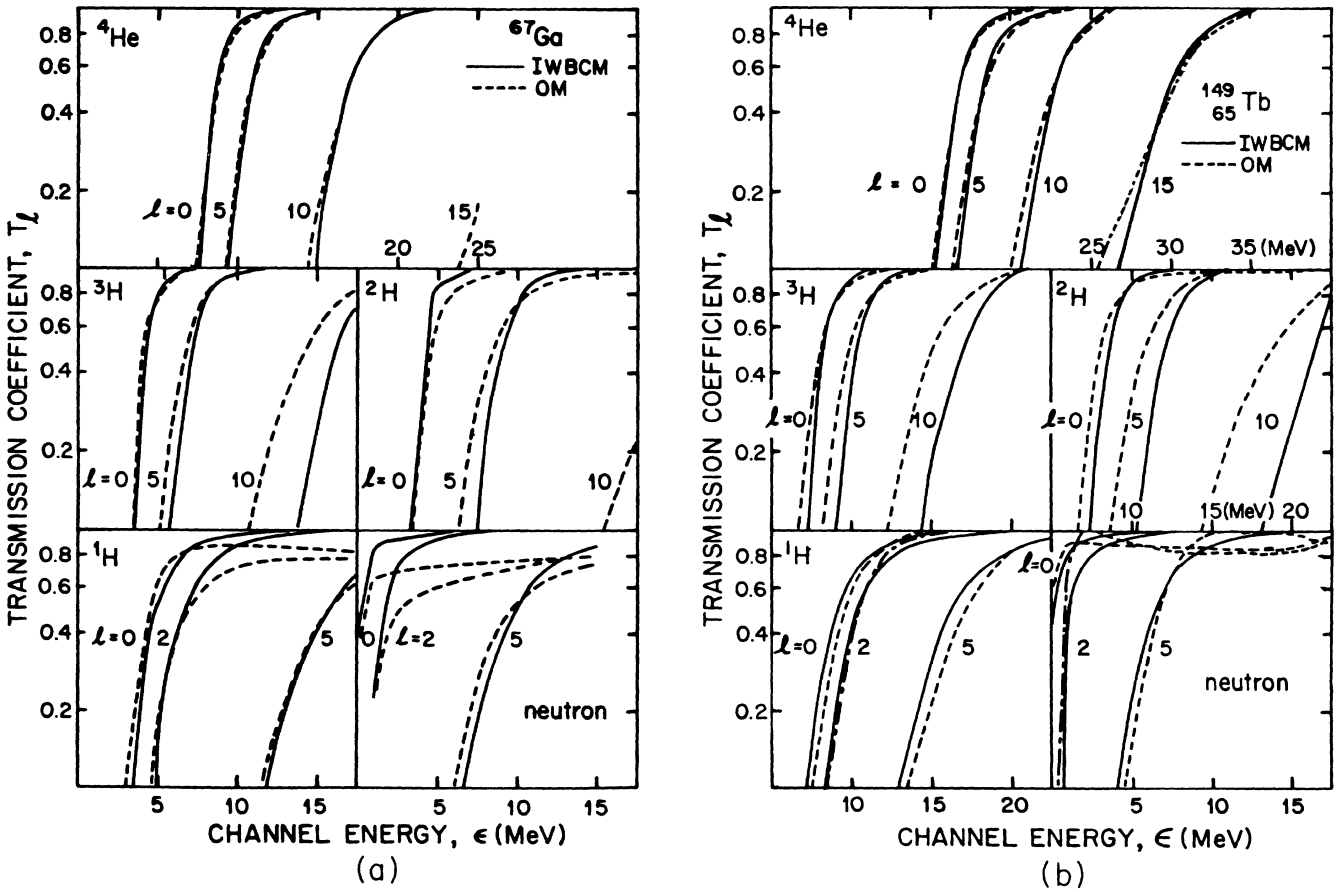
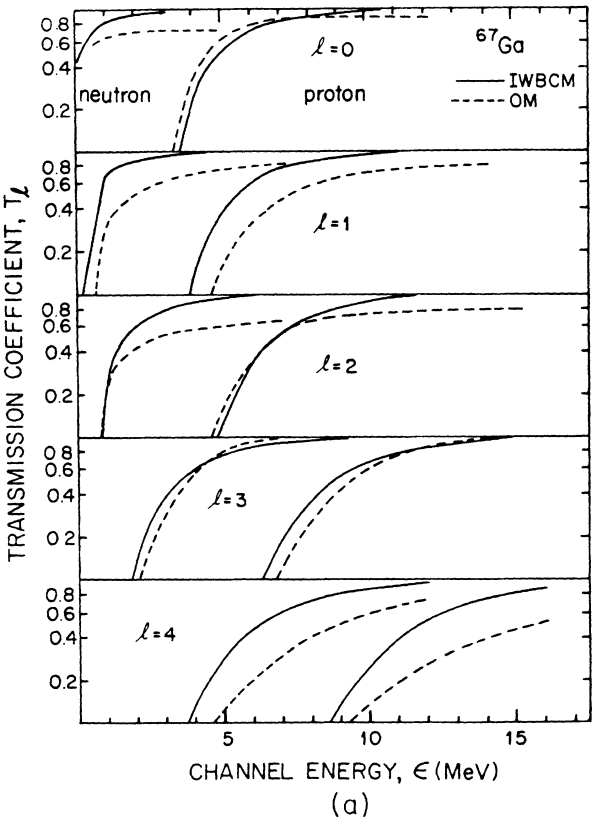


FIG. 1. Transmission coefficients versus channel energy (for n, ^{1,2,3}H and ^{4}He) calculated by the ingoing-wave boundary-condition model (IWBC model) and by the optical model (OM). In (a) the compound nucleus is ^{67}Ga and in (b) it is ^{149}Tb. See Appendix A for the parameters used.



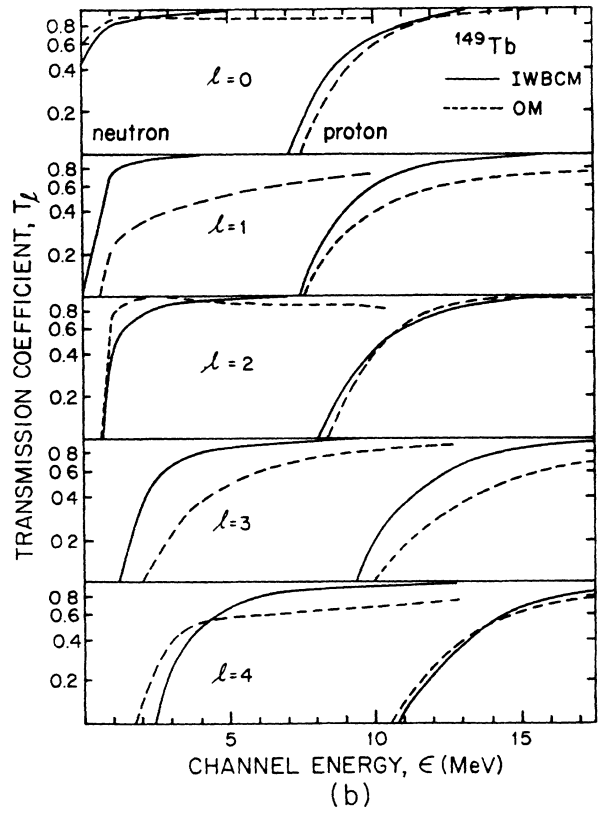


FIG. 2. Same as Fig. 1 but for $l=(0-4)\hbar$ for neutrons and protons.

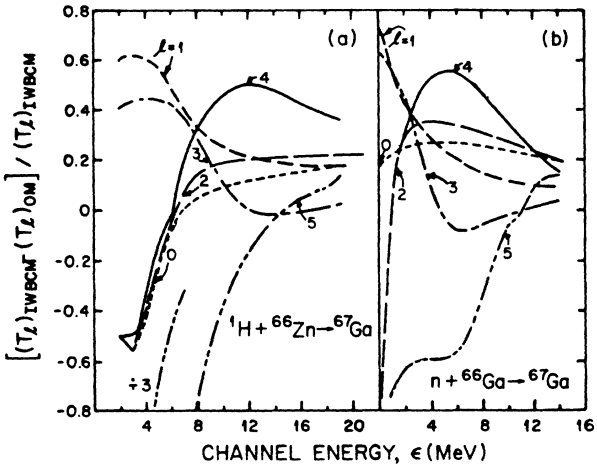


FIG. 3. Fractional differences between the IWBC model and the OM transmission coefficients for neutrons and protons from ^{67}Ga. The IWBC model values are smooth; the oscillations arise from the OM.

rows touch each curve at the energy corresponding to that of the effective barrier (defined by the energy for a T_l value of $\frac{1}{2}$ for IWBC model). The oscillatory pattern is not obviously connected to these effective barriers except that all the differences become positive at higher energies. This again is simply the transparency effect discussed above.

For statistical-model calculations the most important gauges of penetrability are these effective barriers. In Fig. 4 we have plotted effective barriers for each particle: n, ^{1,2,3}H and ^{4}He. First, consider only the solid curves for the IWBC model and the points for the OM. For protons and neutrons the OM values jump around due to the oscillatory behavior discussed above. Values for the IWBC model increase smoothly with l as driven by the centrifugal potential. For ^{2}H and ^{3}H the OM values increase more slowly with l due to reactions outside the well as discussed above. (The dashed line from fusion barriers[19] is discussed in Appendix B.)

IV. DISCUSSION, CONCLUSIONS, AND SUMMARY

A reasonable first task for statistical-model calculations is to provide a reference calculation for hypothetical hot nuclei that have the sizes and shapes of their cold counterparts. In this spirit the T_l^ν values should address simply the inverse of particle emission. The parametrization of the optical model (via data on elastic scattering) has been mainly directed toward a description of distorted-wave functions for elastic-scattering reactions. Therefore, it gives rise to a number of special properties some of which we have illustrated in Figs. 1–4.

The presence of transparency in the OM is a problem. We actually want the escape probability for a particle that is initially inside the hot compound nucleus. Its chance for escape should not be reduced because a view from outside the ground state shows that it is likely to both enter and emerge on one pass. Within the transition-state framework, the time reversed reaction is

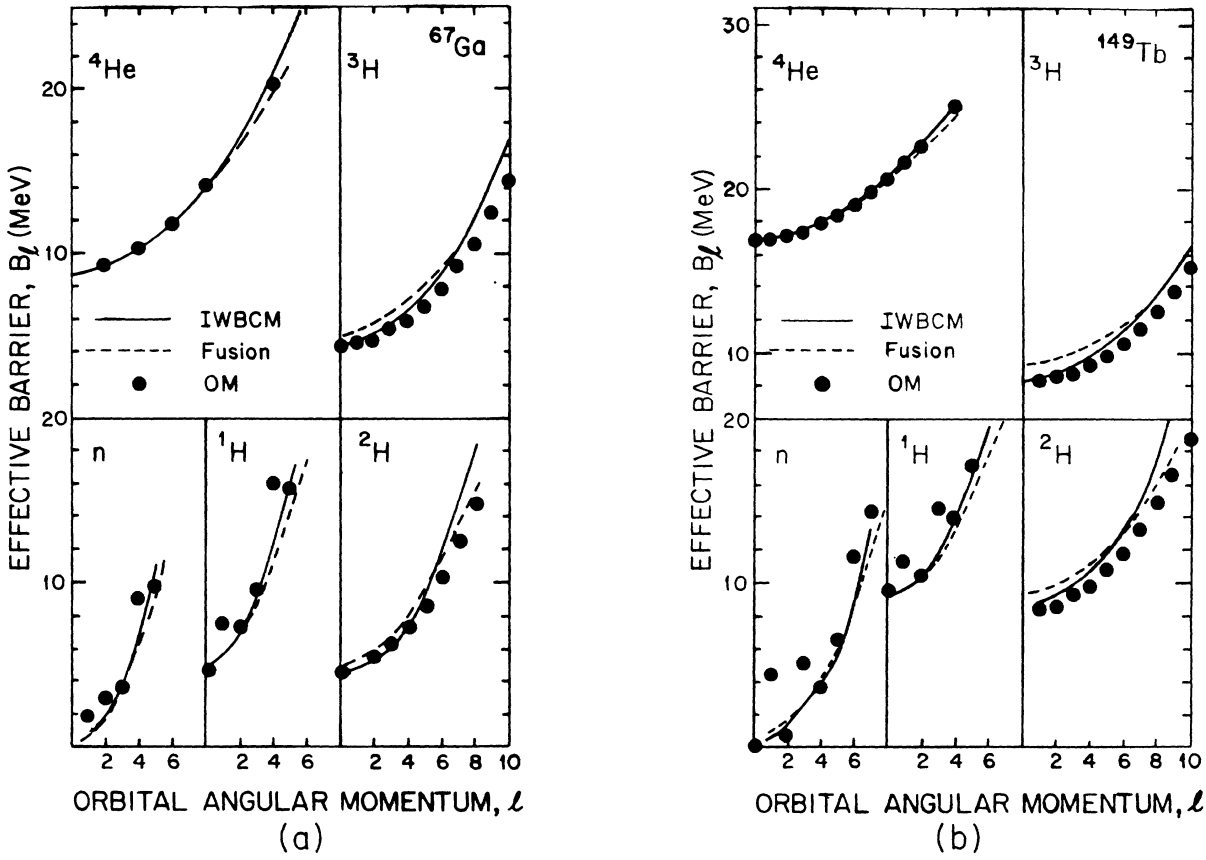


FIG. 4. Effective barriers (defined by the energies for $T_l=\frac{1}{2}$) vs l for n, ^{1,2,3}H and ^{4}He. Values are shown from the IWBC model, the OM, and empirical fusion barriers (s-wave barriers from Ref. 19 as employed in Refs. 15 and 18; see Appendix B).

simply reentry, and the probability for subsequent escape is not relevant. Similarly the excess subbarrier reactions [with $(T_l)_{\rm OM} > (T_l)_{\rm IWBC\ model}$] that occur outside the real well are best ascribed to inelastic collisions that do not lead to capture. Such reactions are not appropriate for the inverse reactions we seek even though they are observable as inelastic scattering, transfer, etc. Finally, size resonances are related to the delicate interactions between cold nuclei and are not obviously part of the time-reversed reaction of evaporation from hot nuclei. By contrast, the simple IWBC model addresses only the two possibilities of reflection by or penetration of the potential barrier as required for the transition-state approach to statistical evaporation.

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APPENDIX A: POTENTIAL PARAMETERS USED IN THE CALCULATIONS

For these calculations we have selected parameters from "global" optical-model potentials given in the input options for the statistical-model code CASCADE: neutrons,[20] protons,[21,22] deuterons,[22,23] tritons[22,24] and alphas.[25] Our comparison calculations do not include the spin-orbit part of these potentials. The particular parameter values that we have used are listed below in the notation of Ref. 22 (energies in MeV, lengths in fm). Potentials for n, p, and t have an energy dependence as indicated by E_L, the laboratory energy in MeV.

Neutron potential parameters:

$V=49.72-0.3E_L-17(1-2Z_T/A_T)$, $r_0=1.256$, $a_0=0.626$,

$W_D=5.22+0.4E_L-10(1-2Z_T/A_T)$, $r_D=1.26$, $a_D=0.0045E_L+0.555$.

Proton potential parameters:

$$V=53.3-0.55E_L+0.4(Z_T/A_T^{1/3})+27(1-2Z_T/A_T),\ r_0=1.25,\ a_0=0.65,\ r_c=1.25\ ,$$

$$W_D=3A_T^{1/3},\ r_D=1.25,\ a_D=0.47\ .$$

Deuteron potential parameters:

$$V=91.13+2.2Z_T/A_T^{1/3},\ r_0=1.05,\ a_0=0.86,\ r_c=1.30\ ,$$

$$W_D=218/A_T^{2/3},\ r_D=1.43,\ a_D=0.5+0.073A_T^{2/3}\ .$$

Triton potential parameters:

$$V=165-0.17E_L-6.4(1-2Z_T/A_T),\ r_0=1.20,\ a_0=0.72,\ r_c=1.30\ ,$$

$$W_v=46-0.33E_L-110(1-2Z_T/A_T),\ r_v=1.40,\ a_v=0.84\ .$$

Alpha potential parameters:

$$V=50,\ r_0=1.17+1.77/A_T^{1/3},\ a_0=0.576,\ r_c=1.17\ ,$$

$$W_v=1.65(A_T)^{1/2}-2,\ r_v=r_0,\ a_v=a_0\ .$$

The ingoing-wave boundary-condition calculations make use of only the real parts of these optical potentials. The imaginary parts are replaced by an ingoing-wave boundary condition inside the barrier, as discussed in Ref. 11. The position of the boundary condition has been chosen to be close to the location of the "pocket" inside the barrier in each case. The boundary condition is such that if the pocket is *above* the center-of-mass energy, then total reflection (no transmission) occurs. This always happens for rather large partial waves, and corresponds to the pure elastic-scattering limit where no reactions occur.

APPENDIX B: EFFECTIVE REAL POTENTIAL BARRIERS

One can easily become confused by the many different theoretical potentials on the market as well as by the many empirical optical potentials from elastic scattering. However, as discussed in Ref. 19, it is the heights of the real-potential maxima that are particularly important for statistical-model calculations of particle evaporation. In that paper, measured fusion cross sections were used to obtain empirical systematics of the effective barriers for capture of ^{1}H and ^{4}He. These empirical fusion barriers were found to have average deviations of only $\approx 3\%$ from similar empirical systematics based largely on real potentials from fits to elastic scattering.[26] Similarly only small deviations were found from barrier heights calculated by the proximity potential.[27] These empirical systematics seem to us to provide a reasonable basis for testing barriers for use in statistical-model calculations. It would be desirable to repeat the fits to fusion data with the IWBC model as opposed to the WKB approximation used in Ref. 19, but the differences are expected to be rather small.

Refs. 15 and 18 have followed this general procedure in statistical-model calculations for the decay of the compound nuclei ^{67}Ga and ^{149}Tb. In Fig. 4 we show the l-dependent barriers used there (dashed line) for comparison to those from the IWBC model and the OM. For n, ^{1}H and ^{4}He their barriers are very similar to those from the IWBC model employed here. They used the same s-wave barriers for ^{2,3}H as for ^{1}H; this gives a small overestimate for the ^{2,3}H barriers. Refs. 15 and 18 also calculated transmission coefficients from a Hill-Wheeler formula with curvature parameter ($\hbar\omega$) of 4 MeV. This gives a reasonably good approximation for ^{4}He but allows too much penetrability for sub-barrier protons.[19] The use of transmission coefficients from the IWBC model, as recommended here, would enhance the deviations between statistical-model calculations and experimental energy spectra as shown in Refs. 15 and 18.

APPENDIX C: A GAS ANALOGY FOR DETAILED BALANCING AND ITS RELATION TO THE TRANSITION-STATE METHOD

Imagine a gas of point particles contained in a permeable cube of volume V_A (edge d_A) inside a larger perfectly reflecting cube of volume V_B (edge d_B). Gas is put into A while B is left empty. Very occasionally, one molecule escapes from A into B. One waits until an equilibrium is set up between the rate of its escape from $A(w_{ab})$ and its recapture into $A(w_{ba}^*)$. The number of states for all the gas molecules inside A is ρ_A and for one molecule in B with the rest inside A is ρ_B. From detailed balancing[3,4] (for an ensemble) we have

$$\rho_A w_{ab}=\rho_B w_{ba}^*\ . \tag{C1}$$

We can write for the recapture rate $w_{ba}^*=(v/d_B)(T_f\sigma/d_B^2)=vT_f\sigma/V_B$, where v is the velocity of the molecule in B, σ is the area of the holes in A, and T_f is the transmission factor for a molecule successfully passing a hole. The number of available states for all the gas molecules but one inside A is $\tilde{\rho}_B$. The number of available states for one molecule of momentum p after escape

into B is $4\pi p^2 V_b dp/h^3$. On substitution into Eq. (C1)

$$w_{ab} = (4\pi p^2/h^3)(vT_f\sigma)(\tilde{\rho}_B/\rho_A)dp \ , \tag{C2}$$

$$w_{ab} = (m\epsilon/\pi^2\hbar^3)(T_f\sigma)(\tilde{\rho}_B/\rho_A)d\epsilon \ . \tag{C3}$$

The result of this equilibrium situation is that no internal dynamical information enters the expression for w_{ab}. We need only determine the probability $(T_f\sigma)$ for capture, i.e., the "external dynamics." These equations, as derived in Ref. 4, are the three dimensional analogue to Eq. (6) in Sec. II.

The use of detailed balancing avoids the internal-decay dynamics by use of an external volume B and waiting for the establishment of equilibrium. This appears to be a big advantage in simplifying the result, but one must look carefully because the actual decay processes are intrinsically irreversible, and the mental exercise of imagining an equilibrium balance might be deceiving. For example, much has been written about the difference between the potential-energy surface for the path toward fission compared to that toward fusion. If the detailed balancing argument is used to obtain the initial escape rate [as in Eqs. (6) and (C3)] then one must assume that the capture processes are the exact inverse of those for emission. The decay products must not change in essential characteristics between the emission and subsequent reentry processes. To achieve this one can imagine shrinking the size of V_B down close to V_A to cause reflection and time reversal just at the decision point for emission. But in this act, elastic scattering from ground-state nuclei becomes irrelevant; the "external dynamics" become merged with the "internal dynamics," and the routes of detailed balancing and the transition state have become indistinguishable.

In sum it seems that both approaches give the same result provided several conditions are respected: (1) The transition-state configuration is the same as the final decision-point configuration for detailed balancing. (2) The transmission factor is assigned for a single exit or reentry attempt.

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