Quantum molecular dynamics and multistep-direct analyses of multiple preequilibrium emission

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(Received 20 April 1995)

We study multiple preequilibrium emission in nucleon induced reactions at intermediate energies, and compare quantum molecular dynamics (QMD) calculations with multistep-direct Feshbach-Kerman-Koonin results [M. B. Chadwick, P. G. Young, D. C. George, and Y. Watanabe, Phys. Rev. C **50**, 996 (1994)]. When the theoretical expressions of this reference are reformulated so that the definitions of primary and multiple emission correspond to those used in QMD, the two theories yield similar results for primary and multiple preequilibrium emission. We use QMD as a tool to determine the multiplicities of fast preequilibrium nucleons as a function of incident energy. For fast particle cross sections to exceed 5% of the inclusive preequilibrium emission cross sections we find that two particles should be included in reactions above 50 MeV, three above about 180 MeV, and four are only needed when the incident energy exceeds about 400 MeV.

PACS number(s): 24.60.Gv, 02.70.Ns, 24.60.Dr, 25.40.Ep

A theory for multiple preequilibrium emission (MPE), where more than one fast preequilibrium particle is emitted in a nuclear reaction, was recently presented in Ref. [1] for use in quantum mechanical Feshbach-Kerman-Koonin (FKK) [2] analyses. It was argued that above about 50 MeV incident energy such processes should be included when inclusive proton and neutron emission spectra are analyzed, and equations were presented for their determination. The quantum molecular dynamics (QMD) theory [3], however, automatically includes fast multiparticle emission processes since the time evolution of the degrees of freedom of every nucleon is considered explicitly. Previous deterministic preequilibrium calculations below 200 MeV (using both semiclassical [4,5] and quantum [1] theories) have usually made the simplifying assumption that it is only necessary to include a maximum of two fast particle emissions before a sequential statistical-decay model is used. In this report we study multiple preequilibrium emission with QMD, compare our results with those from FKK analyses to provide a check of the modeling used in Ref. [1], and determine the incident energies at which different numbers of preequilibrium particle emissions become important.

The significance of MPE processes in preequilibrium analyses was first stressed by Blann and Vonach [4], who included them in their semiclassical hybrid model. By studying the $(p,2p)$ excitation function for mercury (where compound emission is strongly suppressed by the large Coulomb barrier), Blann and Vonach showed that without MPE processes the excitation function is underpredicted by orders of magnitude. Similarly, Vonach *et al.* [5] recently showed that the ^{208}Pb$(n,2n)$ excitation function can only be accurately predicted for neutrons with incident energies up to 200 MeV if MPE processes are included. In these cases, MPE provides a mechanism by which two fast particles are emitted, leaving the residual nucleus with a low excitation energy so that it decays to its ground state by γ emission. In Ref. [1] the contribution of MPE processes to inclusive emission spectra was investigated, and since a number of groups are currently studying their importance for interpreting new measurements of continuum inelastic cross sections [6] it is useful to compare our model from Ref. [1] with QMD predictions.

The QMD theory, which was originally formulated for heavy-ion reactions [7], has been recently extended for use in nucleon-induced calculations [8,9] by combining it with a statistical decay model (SDM) from residual nuclei following fast particle emissions [9]. In this theory, the time evolution of every nucleon is traced in event-by-event simulations through Newtonian equations of motion in the self-consistent mean-field and two-body collision processes. The change in the relative importance of the mean-field effects and the two-body collisions naturally gives a transition between equilibrium, preequilibrium, and spallation mechanisms as the projectile energy varies, automatically including fast multiparticle emission. Our implementation of this theory can be used to calculate nuclear reactions with incident energies from approximately several tens of MeV to 3 GeV, using a fixed parameter set, and in Ref. [9] its predictive capabilities were demonstrated. In order to partition the QMD results into contributions from different sequential emissions, we determine the time for the nucleon ejectiles to pass beyond a radial distance of 2 fm beyond the composite nucleus surface. This then allows the partitioning of the inclusive emission spectrum into a time-ordered sequence of primary and multiple emissions. Details of the QMD model used in this work are given in Ref. [9].

The multistep-direct (MSD) FKK theory for primary particle emission expands the transition amplitude into a series of scattering terms to describe one-step and multistep processes. Statistical arguments are then applied—notably, the phases of different matrix elements describing transitions between different continuum momenta directions are assumed to be random, and an on-shell approximation is made. This results in a particularly simple form for the multistep scattering cross section which is expressed as a convolution of one-step scattering cross sections [10]. Our MSD calculational procedure using the FKK-GNASH code (which includes sequential compound nucleus decay with Hauser-Feshbach theory following preequilibrium emission) was described in Ref. [1], to which we refer the reader, rather than repeating the equations here. Multiple preequilibrium emission in FKK analyses is calculated in the following way. The usual MSD theory is used to determine primary particle emission, and the primary particle can have an emission energy ranging from the maximum kinematically allowed value down to zero. This leaves particle-hole states in the residual nucleus, and in some cases the excited particles are at a high excitation energy in the continuum and may be emitted. In Ref. [1] we presented formulas for determining MPE once the primary emission has been calculated, with the approximation of including a maximum of two preequilibrium ejectiles. That work considered incident energies up to 160 MeV, where the importance of a third fast emission particle was considered to be small.

The ordering of particles considered to be "primary" and "multiple" using the above calculational approach differs in some cases from the QMD definition described above. The differences in definition can be most clearly seen by considering the one-step scattering in which the projectile collides with a target nucleon, with both particles being immediately ejected. In the FKK calculation of this process it is possible for the primary particle to be of a low energy, with the second particle emitted to be of a high energy, whereas the time ordering in the QMD calculations results in the higher energy ejectile being emitted first. While such definition questions have no bearing on the underlying physics involved, it is necessary to use consistent definitions to compare the predictions of these two theories.

We have, therefore, reformulated the FKK equations in Ref. [1] to be consistent with the above QMD counting scheme. This was done by first calculating the primary and multiple FKK contributions as before, but then exchanging emission cross sections between primary and multiple events according to the ejectile's energy—the ejectile with the higher emission energy was always considered as the primary emitted particle. Although the FKK theory does not use a time-dependent formalism, we can assume that the time ordering of the ejectiles can be obtained from the ordering of their kinetic energies. In Fig. 1 we show for comparison the FKK primary and multiple contributions to the inclusive proton spectrum in the 160 MeV ^{90}Zr(p,xp) reaction, for the two types of definitions. In the time-ordered definition the primary spectrum is significantly harder than before, while the multiple emission is softer, and is zero above an emission energy of just under half the incident energy. This can be easily understood: if a particle is considered as a multiple emission event it must have an energy lower than the primary ejectile, and the limiting energy occurs when the two particles are ejected with approximately the same energy, which is then reduced by the extra separation energy expended by the second particle. As described above, the differences between primary and multiple contributions in Fig. 1 for the two counting schemes arise because low energy primary emission events often become multiple events, and vice-versa, when changing between the usual FKK and the time-ordered schemes. Since this is just a question of definitions, the full inclusive emission spectra are identical in the two cases.

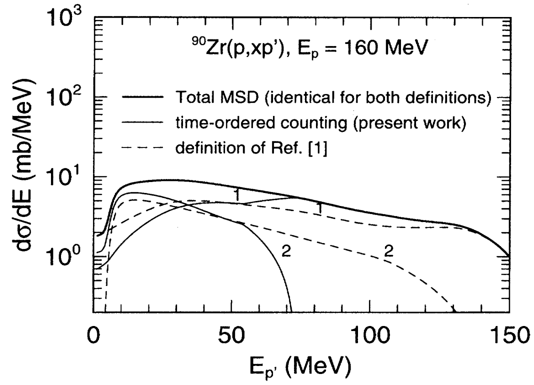

FIG. 1. Calculated primary and multiple (two particles) FKK emission in the 160 MeV ^{90}Zr(p,xp) reaction, comparing the results using the definition in Ref. [1] with the time-ordered definition in this work. The total inclusive spectrum is identical in the two cases.

In Fig. 2 we show our angle-integrated results for primary and MPE for the 160 MeV ^{90}Zr(p,xp) inclusive reaction, compared with Richter *et al.*'s recent measurements [11]. Both FKK and QMD results are shown, and in the case of QMD we give the contributions from emissions of up to five

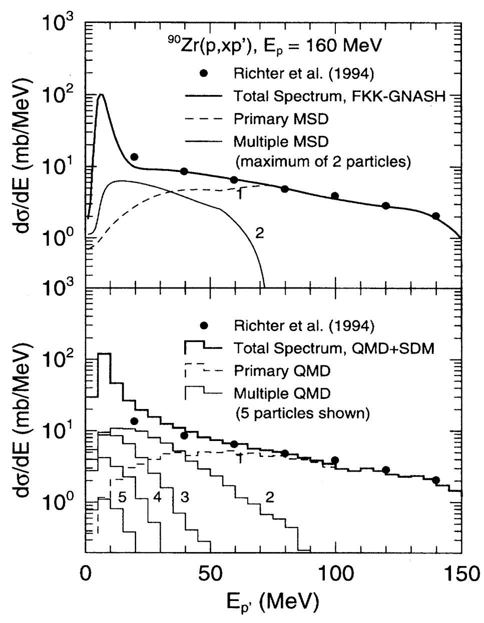

FIG. 2. Primary and multiple preequilibrium emission compared against 160 MeV ^{90}Zr(p,xp) measurements [11], using the time-ordered definition of MPE. The upper figure shows the FKK-GNASH calculation for a maximum of two preequilibrium particles. The lower figure shows the QMD results with statistical decay model (SDM) contributions at low energies.

particles. As an example, the fifth emitted proton will have had four previous fast particles emitted before it, which could have consisted of any combination of neutrons and protons. Our angle-integrated results for the (p,xn) reaction at the same energy and for the 80 MeV reactions (where measurements also exist) show similar features to those seen in Fig. 2. When comparing the QMD and FKK results, it is evident that the primary and the secondary multiple emission are very similar for the two theories. Given their very different formulations of the scattering process, it is satisfying that these two theories agree so well for the spectral shapes of these contributions. As described above, kinematical considerations prevent secondary multiple emission events from exceeding just under half the incident energy. This feature is seen in the FKK results, but is not strictly obeyed by the QMD theory, due to the difficulty of obtaining the exact nuclear ground-state masses in QMD [9].

The QMD calculations provide a useful way to determine the importance of MPE beyond the second particle. The contributions from the third to fifth emissions shown in Fig. 2 are seen to be important at rather low emission energies. Therefore the assumption of including just two emissions in the FKK calculations is quite reasonable at 160 MeV since subsequent low energy particle emissions are included in the FKK-GNASH code as compound nucleus decays. There is a suggestion, though, that the small underprediction seen for the lowest energy data point would be removed if third particle MPE were included. Only if the multi-particle emissions extend into the "preequilibrium region" (emission energies above about 25 MeV here) need they be explicitly included in preequilibrium reaction analyses. In order to determine the incident energies at which various numbers of MPE particles are important, we show in Fig. 3 the QMD results for the percentages of the total inclusive proton emission contributed by the various particles. The upper figure shows the fractions when all emission energies are considered, while the lower figure includes only those emissions above 25 MeV. Since many of the emissions from MPE events occur at low energies the relative importance of the MPE processes is smaller in the lower figure. Indeed, it is the lower figure which should be used to assess the number of MPE particles that should be explicitly included. If we adopt a criterion that the percentage of particles in the preequilibrium regime should exceed 5% for them to be explicitly included, Fig. 3 suggests that it is necessary to include two preequilibrium particles above 50 MeV and three particles above 180 MeV. A further calculation shows that four particles are only needed when the incident energy exceeds about 400 MeV. We emphasize, though, that these estimates have been obtained specifically for emission spectra considerations, and it is possible that the impact of MPE on activation cross sections of residual nuclei following multiparticle emission may be greater.

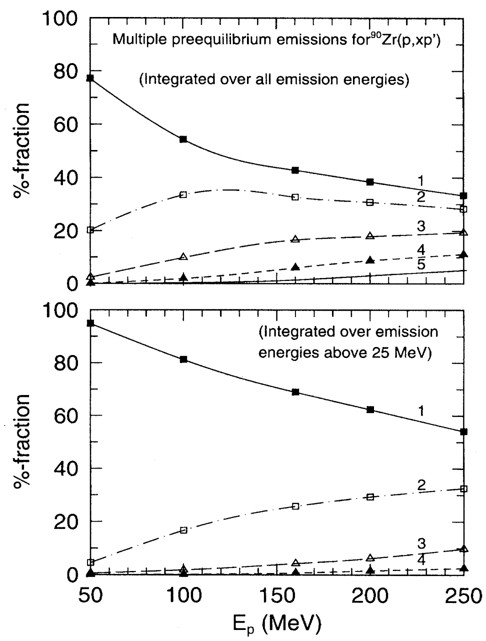

FIG. 3. Relative contributions of multiparticle emissions as a function of the incident energy calculated by the QMD. The upper figure includes all emission energies, whereas the lower figure considers only emission energies above 25 MeV (the preequilibrium regime).

In summary, we have shown that the QMD multiple preequilibrium calculations support the results of Ref. [1] for FKK analyses, when the ordering of primary and multiple emission events is defined in the same way. Our numerical results for the multiplicities of fast particle emission are useful when developing deterministic preequilibrium models. Since such models generally do not include pion physics, they cannot be reliably used beyond about 250 MeV, and our results indicate that for energies above about 180 MeV they should be adapted to include a third-particle preequilibrium emission.

We wish to thank M. Blann, P. G. Young, and Y. Watanabe for useful discussions, and M.B.C. is very grateful to JAERI for its hospitality. This work was performed in part under the auspices of the U.S. Department of Energy under Contract No. W-7405-Eng-36.

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