

Particle evaporation from semiclassical dynamics

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Particle evaporation from excited nuclei is calculated with the Boltzmann-Uehling-Uhlenbeck equation, which is solved numerically using the test-particle method. If the collision integral is omitted, the resulting Vlasov dynamics is very sensitive to numerical noise inherent in the test-particle method. With the collision integral included, the numerical error can be reduced to a point where the system reaches a steady state of evaporative decay. The evaporation rate is found to be consistent with the Weisskopf statistical formula.

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One-body transport theory [1–4] has been widely applied in recent years to describe heavy ion collisions in the Fermi energy domain. The theory has been quite successful in treating phenomena such as flow that depend on the initial stages of the collision, but fails on other phenomena such as multifragmentation that depend on a late development. In most collisions the final state is only reached after excited nuclei decay by particle evaporation. So far, this final statistical decay period has appeared to go beyond the scope of one-body transport as well. In principle, neutron evaporation occurs without the necessity of invoking particle-particle correlations, and so should be accessible to one-body transport theories. In this work we will show that the one-body transport theory based on the Boltzmann-Uehling-Uhlenbeck equation (BUU) can be extended into the statistical decay domain, using the usual test-particle method to solve the equation numerically.

The numerical problem in propagating the test-particle method over long time periods is far from trivial. The pure mean-field dynamics described by the Vlasov equation is extremely sensitive to numerical errors of the test-particle method. The natural steady state for Vlasov dynamics is the Maxwell-Boltzmann single-particle distribution rather than the Fermi-Dirac distribution, as discussed in Refs. [5,6]. The Pauli principle is not built into the numerical algorithms for the dynamics, and numerical errors imply a diffusion in phase space which in the long run causes the single-particle distribution function to relax to the Boltzmann distribution. The excitation energy is unphysically high, when measured with respect to the Boltzmann ground state. This results in a high and unphysical evaporation rate once one reaches that dissipative regime. When the Uehling-Uhlenbeck collision integral is added to the mean-field dynamics the system behaves properly and relaxes to a Fermi-Dirac distribution, provided the collision rate is strong enough to overwhelm the artificial dissipation present in the mean-field propagation. This unwanted dissipation can be systematically reduced by

improving the numerical representation through using a sufficiently large number of test particles.

When a nucleus is given some excitation energy that is not too high, it will evolve in two distinct stages. In a first rapid stage, the energy is equilibrated and quantities such as single-particle occupation factors become nearly stationary. In the second stage, the nucleus evaporates particles and loses excitation energy. It is not clear that an exact Vlasov dynamics would be sufficiently dissipative to produce such a behavior. On the other hand, the BUU dynamics has explicit and physical dissipation and the desirable feature that the stationary state is the correct Fermi-Dirac state, even in the presence of numerical noise. Thus we have good reason to expect that the BUU equation could be applied in the statistical evaporation domain.

In the statistical limit, the neutron evaporation rate W is given by the Weisskopf formula [7],

$$W = \frac{2\sigma_{\text{cap}}}{\hbar^3 \pi^2} m T^2 e^{-E_B/T}. \quad (1)$$

Here σ_{cap} is the neutron capture cross section, E_B the neutron separation energy in the nucleus, and T the temperature of the nucleus. The BUU model will provide values for these quantities as well as the evaporation rate itself.

The BUU equation is solved using the same Skyrme energy functional as in the previous studies [5]. The potential energy function is given by

$$E_{\text{pot}}(\rho) = \frac{1}{2} t_0 \rho^2 + \frac{1}{3} t_3 \rho^3, \quad (2)$$

with parameters $t_0 = -926 \text{ MeV fm}^3$ and $t_3 = 4118.9 \text{ MeV fm}^6$. This reproduces typical nuclear saturation properties and yields a compressibility modulus of $K = 380 \text{ MeV}$. The forces are calculated with a smoothed potential obtained by convoluting the density ρ with a Gaussian $\exp[-(r-r')^2/2\sigma^2]$. The BUU equation is solved with the full ensemble of test particles [8] to evaluate the Pauli blocking factor in the collision integral. The cross section for particle scattering is taken to be 50 mb.

Key numerical parameters are the number of test particles per nucleon, N/A , and the width of the Gaussian σ . The

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numerical relaxation of the Vlasov dynamics to a Boltzmann distribution is characterized by the time scale that varies with σ and N/A as [6,9]

$$\tau \sim \sigma^4 \frac{N}{A}. \quad (3)$$

A typical case for which calculations can still be done conveniently on a work station would have parameters $N/A = 400$ and $\sigma = 1 \text{ fm}/\sqrt{2\ln(2)} = 0.85 \text{ fm}$. This value of the width is uncomfortably large to treat the nuclear surface in detail, but it can only be reduced with difficulty. The numerical error scales as the fourth power of σ and it would require more than an order of magnitude increase in the number of test particles to improve the spatial resolution by a factor of 2. With the given choice of numerical parameters, we have pushed the relaxation time above 1000 fm/c which leaves us sufficient time for studying evaporation. Our numerical study will be for a midmass nucleus, $A = 64$. This is large enough to show typical evaporation behavior, but the computation is still reasonably fast.

In either the BUU or the Vlasov theory, the ground state of the system has a phase space distribution function of the Thomas-Fermi form

$$f(\mathbf{r}, \mathbf{p}) = 4 \theta(\epsilon_F - h(\mathbf{r}, \mathbf{p})). \quad (4)$$

Here h is the mean-field Hamiltonian corresponding to f and the factor 4 accounts for the spin-isospin multiplicity of nucleons. We find that ground state binding energy of $A = 64$ is about 10.4 MeV/nucleon with the energy function in Eq. (2) and numerical parameters $N/A = 400$ and $\sigma = 0.85 \text{ fm}$.

To produce an excited state, we initialize the nucleus as follows. We start with a uniform distribution in phase space, within spheres of the momentum and position coordinates,

$$f(\mathbf{r}, \mathbf{p}) = 4 \theta(R_0 - r) \theta(k_F - p). \quad (5)$$

The two parameters in this distribution are the Fermi momentum k_F and the radius of the initial nucleus R_0 . We typically produce the excitation by increasing R_0 (and decreasing k_F correspondingly) from the bulk equilibrium values. The BUU dynamics is then evolved in time, and the evaporation is measured by the number of test particles passing outside of a large radius, which we take to be 10 fm.

Figure 1 shows the evaporation under a variety of conditions. The dashed curve shows the evolution starting from the Thomas-Fermi ground state. Less than half a nucleon is lost over a time period of 1000 fm/c. Thus we expect our numerical evaporation rates to be meaningful down to rates of a few times 10^{-3} nucleons per fm/c. The solid curve shows the evaporation rate starting from a state having excitation energy $E^*/A = 2.2 \text{ MeV}$ and using the BUU dynamics. Note that there is no evaporation for the first 100 fm/c, and then it starts with an initial burst of test particles. This is a result of the initialization method: The nucleus starts out expanded, and it contracts and undergoes a cycle of radial oscillation before any particles come out. The (collective) radial oscillations are damped quickly and we deduce from the decay of its amplitude that the nucleus has thermalized by 200 fm/c, and the particle emission thereafter can be com-

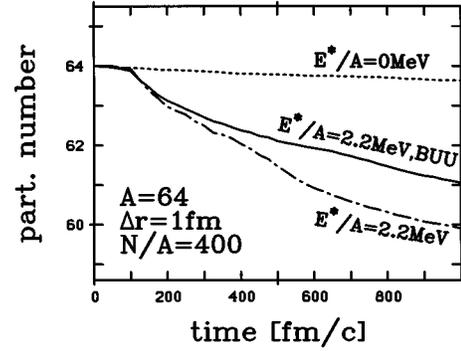


FIG. 1. The number of particles remaining in the bound nucleus as function of time for the standard test case, $A = 64$, $N/A = 400$, $\sigma = 0.85 \text{ fm}$, for three different dynamical situations: Vlasov propagation of the Thomas-Fermi ground state (dotted line), BUU propagation starting from an initial excitation of 2.2 MeV/nucleus (solid line), and Vlasov propagation starting from an initial excitation energy of 2.2 MeV/nucleus (dot-dashed line).

pared with the statistical evaporation formula. The last curve in the figure shows the results for the same initial excited state, but evolving the nucleus with Vlasov dynamics. As discussed in [5,6], the Vlasov dynamics is very sensitive to numerical error, which drives the phase space distribution to the Boltzmann form. The evaporation rate is seen to be larger in this case.

We now address the question of how well the BUU results have converged numerically. According to Eq. (3), the numerical relaxation time is proportional to N/A , and we might expect observables to scale linearly with this quantity. We have examined the evaporation rate as a function of N/A , with results shown in Fig. 2. The total number of particles evaporated between 200 and 1000 fm/c is shown by the circles, for test-particle numbers ranging from $A/N = 40$ to 400. There is a numerical scatter in the points of the order of a half a particle, but there is a clear linear trend. Extrapolating to an infinite number of test particles, the number evaporated is about 2.

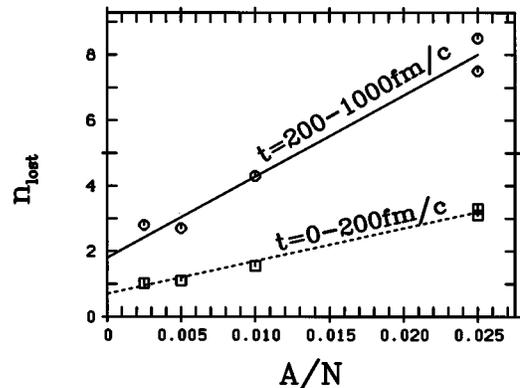


FIG. 2. The number of particles lost in two time intervals, for the nucleus $A = 64$ initialized with an excitation energy $E^* = 2.2 \text{ MeV}$. The circles and squares show the results of the simulations for different values of A/N , the reciprocal number of test particles per nucleon. The double sets of results for $A/N = 1/40$ were from runs with different random number seeds, showing the typical numerical uncertainty in the results.

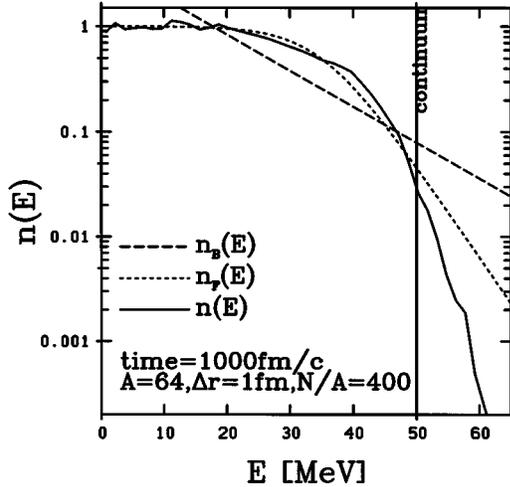


FIG. 3. Phase space occupancy for the test particles as a function of the energy of the particles, at time $t=1000$ fm/c. The different lines show results for the BUU simulation (solid line), the Fermi function of temperature $T=5.0$ MeV (dashed line), and the Boltzmann distribution corresponding to a temperature of $T=11$ MeV (dotted line).

We are now almost ready to compare with the statistical evaporation formula, Eq. (1). It requires knowledge of the temperature of the nucleus T , which we may estimate simply using the Fermi gas model. The relation between energy and temperature in the Fermi gas model is

$$E^*/A = \pi^2 T^2 / (4\epsilon_F), \quad (6)$$

where ϵ_F is the Fermi energy. Putting in the initial excitation of $E^*/A=2.2$ MeV, the Fermi gas temperature is $T=5.5$ MeV. We can also look at the distribution of particles in phase space after the nucleus has equilibrated. This is shown in Fig. 3, with the solid curve showing the phase space occupancy as a function of the energy of the nucleons, evaluated at $t=1000$ fm/c. The dot-dashed line shows the Fermi function corresponding to a chemical potential of $\epsilon_F=35$ MeV and a temperature of $T=5$ MeV. The agreement with the numerical distribution is fairly good for the bound particles. The distribution in the continuum falls off more rapidly; these particles obviously are not in local equilibrium because they escape. In Fig. 4 we show the distribution in kinetic energy of the evaporated particles. These should follow a Boltzmann distribution, which has the form $E^{1/2}\exp(-E/T)$. The dotted line shows a fit; it corresponds to a temperature of $T=3.5$, significantly lower than the nucleus itself. A reason for this will be presented shortly.

The final ingredient to evaluate the statistical evaporation rate is the cross section for the inverse capture reaction. Let us assume for the moment that the nucleus is completely absorbing, giving the geometric capture cross section $\sigma = \pi R^2$. For the nucleus $A=64$ the radius may be estimated as $R \approx 5$ fm. Inserting this cross section, the temperature $T=5$ MeV, and the binding energy $E_B=10.4$ MeV in Eq. (1), we find a neutron evaporation rate of 0.006 neutrons per fm/c. This should be doubled to compare with the rate of nucleons emitted in our simulation, since we do not

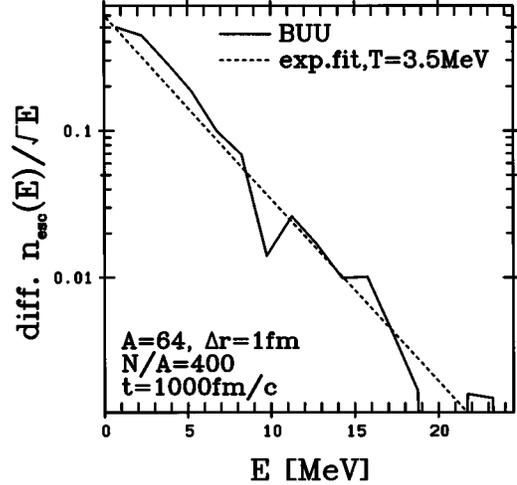


FIG. 4. Distribution of kinetic energies of the emitted particles for the BUU simulation at $E^*/A=2.2$ MeV. The dotted line is the thermal distribution at a temperature $T=3.5$ MeV.

distinguish neutrons and protons. The statistical formula thus gives a rate of about a factor of 5 larger than the simulation.

After obtaining this result, we examined more carefully our assumption that the nucleus is black. In the BUU model, the interaction of the nucleus with nucleons in the continuum may be weaker, because the BUU theory lacks the quantum coupling to collective excitations. We therefore made a special study of the inverse capture cross section. We reinitialize the nucleus with 50 extra test particles impinging with a given momentum and impact parameter but with stochastically chosen directions from the outside, and follow their history. This has been done for a variety of momenta and impact parameters. We found in doing this that the capture probability depends rather strongly on kinetic energy, with a lower capture rate for higher energy particles. This is a qualitative explanation of how the apparent temperature of the evaporated particles can differ from the actual temperature of the source. The source is viewed through the albedo of its surface, which can shift the spectrum. We found an average capture rate of 30–50 % of the black nucleus limit. This brings the statistical rate down to 0.005 nucleons per fm/c which is within a factor of 2 or so of the magnitude found in the BUU calculation. The remaining discrepancy can perhaps be ascribed to cooling during the course of the evolution. We conclude that it is possible to use the BUU calculation to follow nuclear dynamics into the evaporation phase of final nuclei.

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