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Microcanonical lattice gas model for nuclear disassembly

C. B. Das,[1] S. Das Gupta,[1] and S. K. Samaddar[2]
[1]*Physics Department, McGill University, 3600 University St., Montréal, Québec, Canada H3A 2T8*
[2]*Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Calcutta 700064, India*
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Microcanonical calculations are no more difficult to implement than canonical calculations in the lattice gas model. We report calculations for a few observables where we compare microcanonical model results with canonical model results.

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The lattice gas model (LGM) is frequently used to compute observables in heavy ion collisions. The applications are numerous; see [1,2] for references. The calculations are normally done for a fixed temperature so that we will also call the usual model canonical lattice gas model CLGM. The temperature is fixed so there will be fluctuations in energy. It is often argued that it might be more appropriate to keep energy fixed. In the following we set up a scheme for doing calculations with fixed energy. We will call this MLGM.

We assume the reader is familiar with the usual LGM model for nuclear disassembly.

In CLGM, N neutrons and Z protons are put in N_s lattice sites using a Metropolis algorithm. Because of bonds between nearest neighbors ($\epsilon_{np}=-5.33$ MeV, $\epsilon_{nn}=\epsilon_{pp}=0$, [1]) and Coulomb interaction between protons, there is a potential energy which we denote by E_{pot}. In Metropolis method, a switch is attempted between occupied sites and unoccupied sites and also between occupied neutrons and protons. If, in the switch, the energy goes down the move is accepted. If the energy goes up, the move is accepted but only with a probability $\exp(-\Delta E/T)$. After many such switches an event is chosen. Once an event is picked, momenta are assigned from Monte Carlo sampling of a Maxwell-Boltzmann distribution at temperature T. We denote the kinetic energy by E_{kin}. The total energy of the system is $E_{tot}=E_{pot}+E_{kin}$ which will fluctuate from event to event.

The change to MLGM can be made in the following way. We start from a given configuration, hence a given E_{pot}. The total energy which will be kept fixed is E_{tot}, so the kinetic energy is $E_{kin}=E_{tot}-E_{pot}$. The available phase space of $A=N+Z$ nucleons having this kinetic energy is known analytically:

$$\int \delta\left(E_{kin}-\sum_1^A p_i^2/2m\right)\Pi d^3p_i = \frac{(\sqrt{\pi})^{3A}}{\Gamma(3A/2)}(2m)^{3A/2}E_{kin}^{(3A/2)-1}. \quad (1)$$

We will call the value of the integral $\Omega_1(E_{kin})$. We now attempt a switch in the configuration space. The potential energy will change to E'_{pot}. To conserve energy the kinetic energy of the system should be fixed at $E_{tot}-E'_{pot}=E'_{kin}$. If $\Omega_1(E'_{kin})/\Omega_1(E_{kin})>1$, the move is accepted. If it is less, the probablity is given by the ratio. Since all configurations have identical weights, this satisfies the principle of detailed balance. After many such switches an event is accepted. We now have to assign momenta to the nucleons so that the total kinetic energy of the A nucleons add up to correct kinetic energy which we denote by $\tilde{E}_{kin}$. The correct way to do this such that the sole criterion is phase space is the following. Choose a sphere of radius P. Do a Monte Carlo sampling on A particles for uniform distribution in this sphere. This means fixing p,θ_p,ϕ_p for each particle from $p=P(x_1)^{1/3}$, $\cos\theta_p=1-2x_2$ and $\phi_p=2\pi x_3$ where x_1, x_2, and x_3 are random numbers. Finally normalize P so that the total energy equals $\tilde{E}_{kin}$. We are now ready to calculate all relevant quantities including cluster decomposition.

In microcanonical simulation observables can be calculated without having to invoke a temperature. But it is useful to extract a temperature in the model. The ''temperature'' will vary from event to event. The event temperature is taken from $\frac{3}{2}(A-1)T\approx\frac{3}{2}AT=E_{kin}$. The ensemble average gives the average temperature for the given microcanonical total energy. This is obviously attractive from an experimental point of view but we can also justify it from more basic principles. Let us write

$$\Omega_T(E_{tot})=\sum \Omega_1(E_{kin})\Omega_2(E_{tot}-E_{kin}). \quad (2)$$

Although we are talking of one system only which has both kinetic and potential energy, formally, the right-hand side is the same as two systems in ''thermal'' contact whose total energy is fixed but each one's individual energy can vary. This is very standard statistical mechanics [4]. For large systems, the sum is dominated by the maximum in the product $\Omega_1(E_{kin})\Omega_2(E_{tot}-E_{kin})$ which is obtained when $[\partial\ln\Omega_1(E_{kin}]/\partial E_{kin}=[\partial\ln\Omega_2(E_{pot}]/\partial E_{pot}$ which then defines the inverse of the average temperature. This of course leads again to the same identification as above and is consistent with Eq. (1). The sharpness of the maximum in the sum depends on the size of the system. For a small system we will then expect the fluctuation in temperature $\langle T^2\rangle-\langle T\rangle^2$ to be larger for the same value of $\langle T\rangle$.

Finally although the starting point of the Metropolis algorithm can be fairly arbitrary, it is helpful computationally to start from close to equilibrium. The method of generating the starting point followed the scheme given in [3] which was

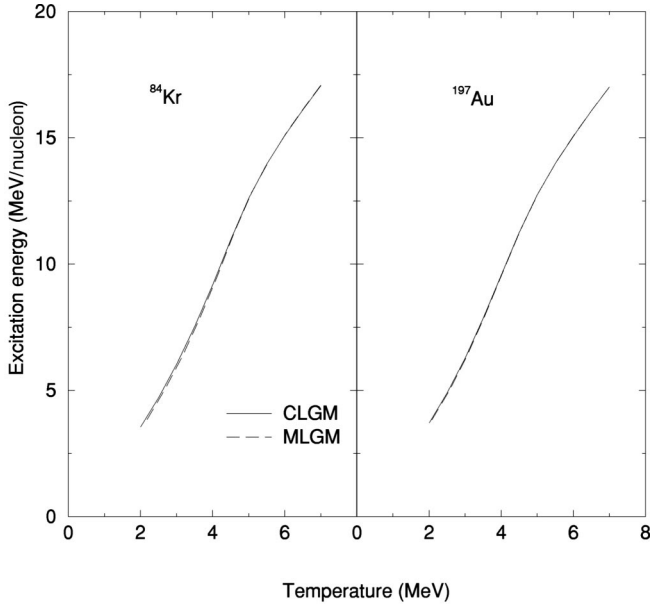

FIG. 1. Caloric curves for ^{84}Kr and ^{197}Au systems in the two models.

modified to take into account that there are two kinds of bonds and the Coulomb force between protons.

Below we consider a few applications. Many more can be made.

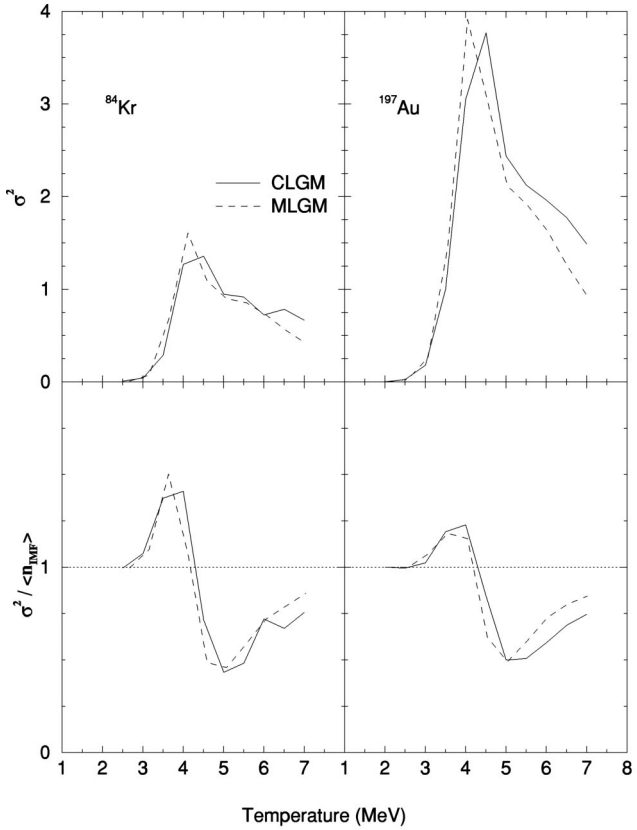

FIG. 2. $\sigma^2 \equiv \langle n_{IMF}^2 \rangle - \langle n_{IMF} \rangle^2$ (upper panel) and $\sigma^2/\langle n_{IMF} \rangle$ (lower panel) at different temperatures, as obtained in the two models. The left panels are for ^{84}Kr and the right ones are for ^{197}Au.

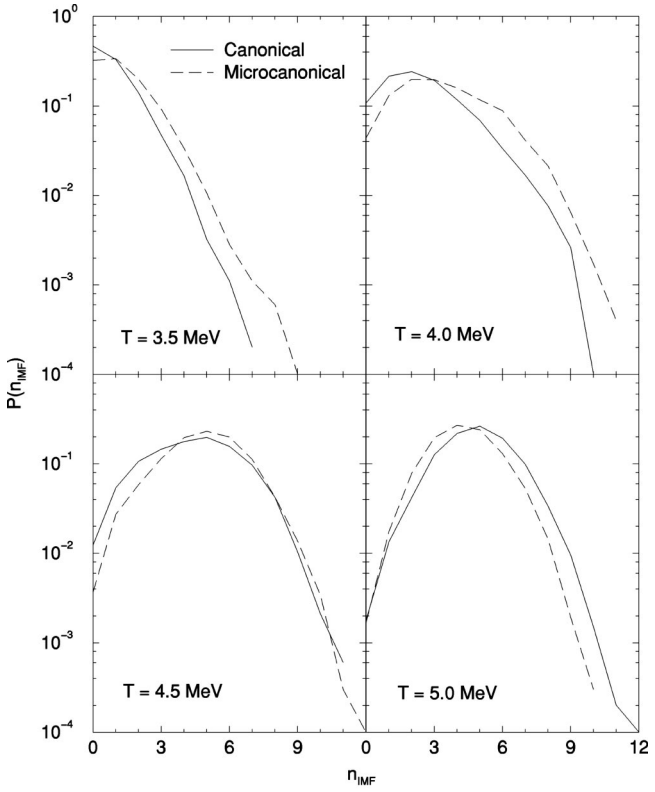

FIG. 3. $P(n_{IMF})$ distributions for ^{197}Au at $T=3.5$, 4.0, 4.5, and 5.0 MeV in the two models.

As the first application, we show in Fig. 1, the caloric curve, E^*/A against temperature T, for ^{84}Kr (an intermediate mass disintegrating system) and for ^{197}Au (a heavy system). All calculations are done in fixed volume. For the microcanonical model, $\langle T \rangle$ is used for T and for the canonical one, $\langle E^*/A \rangle$ is used for E^*/A. Even though the fluctuation $\langle T^2 \rangle - \langle T \rangle^2$ is more than four times in the case of Kr (6.59 MeV^2 at $\langle T \rangle = 5.0$ MeV as compared to 1.1 MeV^2 for Au at the same average temperature) there is almost no difference in the E^*/A vs T curves. We should point out, all calculations use two kinds of bonds and include the Coulomb interaction. For ^{84}Kr we used a cubic lattice of size 6^3; for ^{197}Au, we used 8^3.

One might expect that while average quantities will be nearly the same in both the models, there would be larger differences in fluctuations of observables. With this in view, we have investigated intermediate mass fragment (IMF, Z between 3 and 20) emissions. We show in Fig. 2, the plots of $\sigma^2 \equiv \langle n_{IMF}^2 \rangle - \langle n_{IMF} \rangle^2$ (upper panel) and $\sigma^2/\langle n_{IMF} \rangle$ (lower panel) at different temperatures. Not a great deal of difference is found between CLGM and MLGM calculations for intermediate or heavy masses. Since the fluctuation in temperature for the intermediate case is much larger (more than a factor of 4) this calls for an explanation. We think this is the reason. Referring to Eq. (2) we see that when the temperaure is low, E_{pot} is high. That means in the particular configuration the number of attractive bonds is less. However, the probability of an attractive bond being able to bind two nucleons is much higher since the temperature is low

(the energy of relative motion $p_r^2/2\mu$ has a lesser chance of exceeding the bond energy $-\epsilon_{np}$, see [1]). Similar arguments hold when the temperature is high. This means E_{pot} is low, so that there are many more attractive bonds. However, higher temperature will be able to break these bonds more easily. The two effects seem to cancel each other quite efficiently.

In Fig. 3 we compare $P(n_{IMF})$, the probability of emitting n IMF's, in the two models for the case of ^{197}Au for four different temperatures. Again, the results are quite close.

We verified that in Fig. 3, for temperatures 4.5 MeV and 5 MeV both the microcanonical and canonical probabilities are fitted quite well by a binomial distribution: $P(n) = [m!/n!(m-n)!]p^n(1-p)^{m-n}$, where m and p are obtained from $\langle n\rangle = mp$ and $\sigma^2/\langle n\rangle = 1-p$. This is a topic that has been discussed thoroughly in recent times [5]. This parametrization does not work for temperatures 3.5 MeV and 4 MeV where $(\sigma^2/\langle n\rangle) > 1$. Here our calculated points are fitted quite well by a negative binomial distribution: $P(n) = [\Gamma(N+n)/\Gamma(N)n!]p^n(1-p)^N$. The increase of σ^2 at 4 MeV is not unnatural in LGM. This is happening because at this temperature the system is crossing the co-existence curve [6] with the accompaniment of a maximum in the fluctuation. The value of m stays fairly constant with temperature beyond 5 MeV and m/A is approximately the same for mass 84 and 197. But we do not ascribe much importance to this since the low temperature behavior of fluctuation predicted in the model is not reflected in experimental data so far.

To summarize, microcanonical calculations in LGM are no harder to do than canonical calculations. The lowest mass number that we used was 84. Down to this size at least there are no serious departures from canonical results.

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