Liquid-gas phase transition in finite nuclei

Simulations in Fermionic Molecular Dynamics

The forces between the individual nucleons in a nucleus vary according to distance in a manner similar to those between molecules in a liquid. Thus the interesting question arises, whether with increasing excitation energy a liquid-gas phase transition can be observed in finite nuclei. Generally it is believed that signatures of phase transitions are washed out in systems with few constituents due to finite size effects. Theoretical simulations show, however, that even small systems exhibit all features of a phase transition, provided the total energy of the system can be determined well enough for each member of the statistical ensemble. The results are compared to the caloric curve deduced for finite nuclei by the ALADIN collaboration.

The investigation of the equation of state of nuclear matter, in particular the search for the long predicted liquid-gas phase transition is an experimentally tough problem. Besides the fact that one can manipulate only finite nuclei, the measured information on the system is rather indirect. The difference to macro-physics is not only the smallness of the system, but also that one cannot control the thermodynamic quantities volume or pressure. TIn an experiment one is colliding two nuclei in order to produce excitation energy and compression. But as there is no container, the system begins to expand into the vacuum right after the compression and heating phase. Therefore, one is all the time in a transient state where equilibrium in its original meaning, i.e. a time-independent stationary macro-state, is not reached.

The challenge to study the nuclear equation of state has been accepted not only for astrophysical reasons, like a deeper understanding of supernova explosions or neutron stars, but also because the subject in itself is of interest as one is dealing with a small charged quantum liquid which is self-bound by the strong interaction.

In the following we investigate the liquid-gas phase transition within Fermionic Molecular Dynamics. This model can simulate nucleus-nucleus collisions as well as equilibrium situations. We will, however, concentrate on an experimentally not accessible situation, namely an excited nucleus which is put into an external field. This field plays the role of a container so that evaporated nucleons cannot escape, but

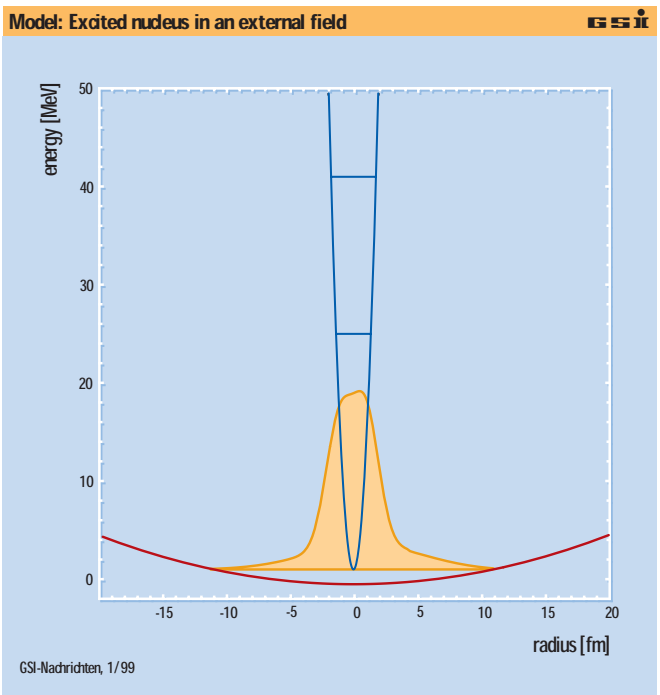


Figure 1: The self-bound excited nuclear system, whose density profile is represented by the yellow area, is enclosed in a broad container potential (red line). For the thermometer, which is coupled to all nucleons, only the oscillator potential (blue line) is displayed together with the lowest eigenstates.

equilibrate with the remaining nucleus (hot liquid).

The Fermionic Molecular Dynamics (FMD) model [1] describes the quantum system with a parameterized antisymmetric many-body wave function. In this many-body state each nucleon is represented by a Gaussian wave packet, which is the closest possible quantum analogue to a classical phase-space point. The wave packet is characterized by its mean position, mean momentum and the widths around these mean values, all of which are time-dependent. Their FMD equations of motion are derived from the time-dependent quantum variational principle. Although the derivation is straightforward, the resulting equations are very complex and the numerical effort becomes prohibitive for more than about 80 particles. This is due to the antisymmetrization which is needed to describe properly the fermionic nature of the nucleons . Without this, a nucleus is not a quantum liquid with Fermi-Dirac statistics but a classical system.

In the present investigation the effective two-body nucleon-nucleon interaction in the Hamilton operator consists of a short-range repulsive and a long-range attractive central potential with spin and isospin admixtures and includes the Coulomb potential [2]. The parameters of the interaction have been adjusted to minimize deviations between calculated and measured binding energies for nuclei with mass numbers $4 \leq A \leq 40$.

Besides the kinetic energy of the nucleons and the nucleon-nucleon interaction, the Hamilton operator also includes an external field which serves as a container. The container is an important part of the model because it keeps the evaporated nucleons in the vicinity of the remaining drop of liquid. This facilitates equilibration of liquid and surrounding vapor. The vapor pressure is controlled by the volume which is made available by the external potential.

In our model the nuclear system is quantal and strongly interacting. The quantal nature does not allow to deduce the temperature from the kinetic energy distribution as it is the case for classical systems with momentum-independent forces. The zero-point motion is always present and does not imply a finite temperature.

Therefore, the concept of an external thermometer which is coupled to the nuclear system is used. The thermometer consists of a quantum system of distinguishable particles which move in their own potential (different from the container potential) and interact weakly with the nucleons (see Fig. 1). The time evolution of the whole system is described by the FMD equations of motion.

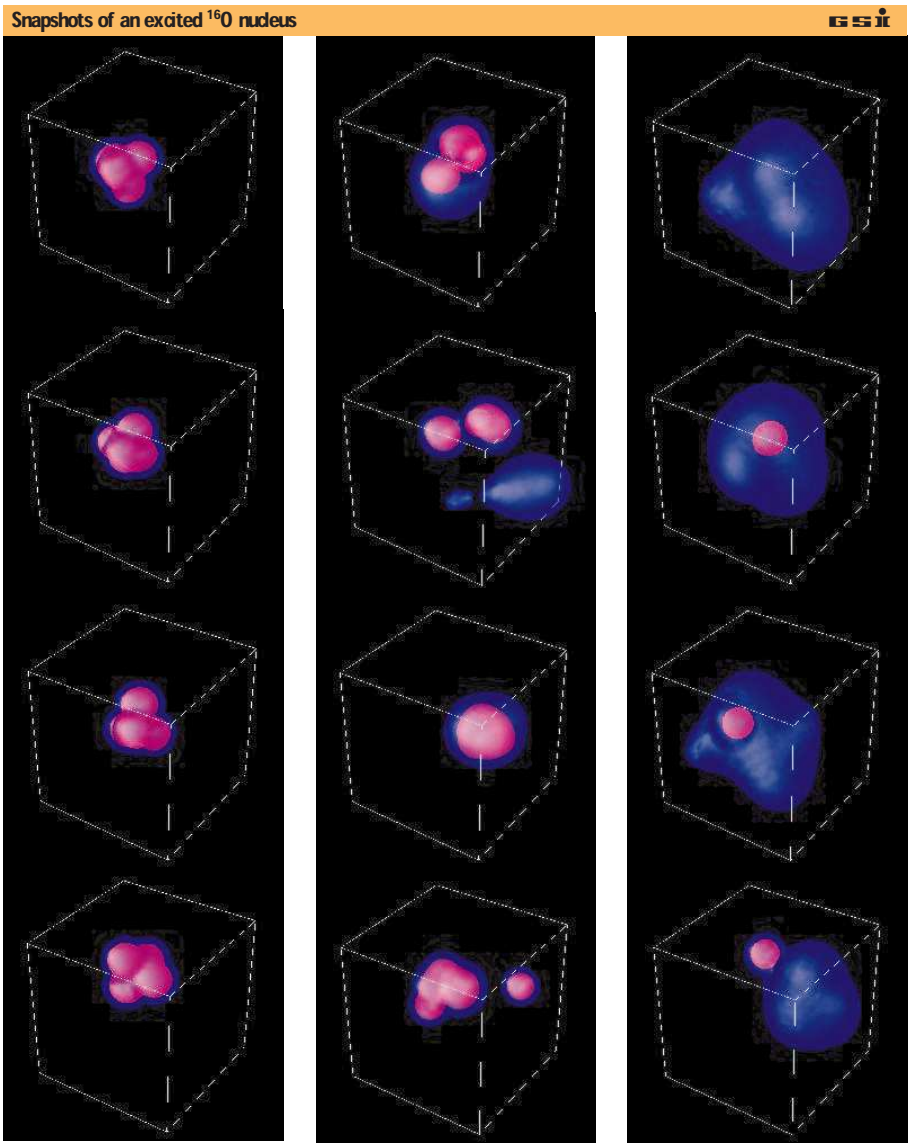


Figure 2: Snapshots of an excited ^{16}O endosed in a shallow harmonic container potential with level spacing $\hbar\omega$ = 1MeV and excitation energy per particle of 3.5 MeV (left), 7MeV (center) and 11MeV (right). Bright surfaces enclose densities above $\rho_0/10$ i.e. liquid, darker surfaces $\rho_0/100$ i.e. gas (saturation density ρ_0 = 0.16 fm^{-3}). The cube which is drawn to help visualizing three dimensions has an edge length of 20 fm.

PHASE TRANSITION AND DENSITY OF STATES

In a macroscopic system, where the particle number N is very large (e.g. N = 10^{20}), the number of microstates, $\rho_N(E)\Delta E$, in an energy interval of width ΔE around E is huge so that the density of states, $\rho_N(E)$, is smooth enough to allow the definition of a first and second derivative.

If, in an experiment, a system is prepared such that its energy is given by E within a resolution ΔE, one calls it a microcanonical ensemble and attributes an entropy

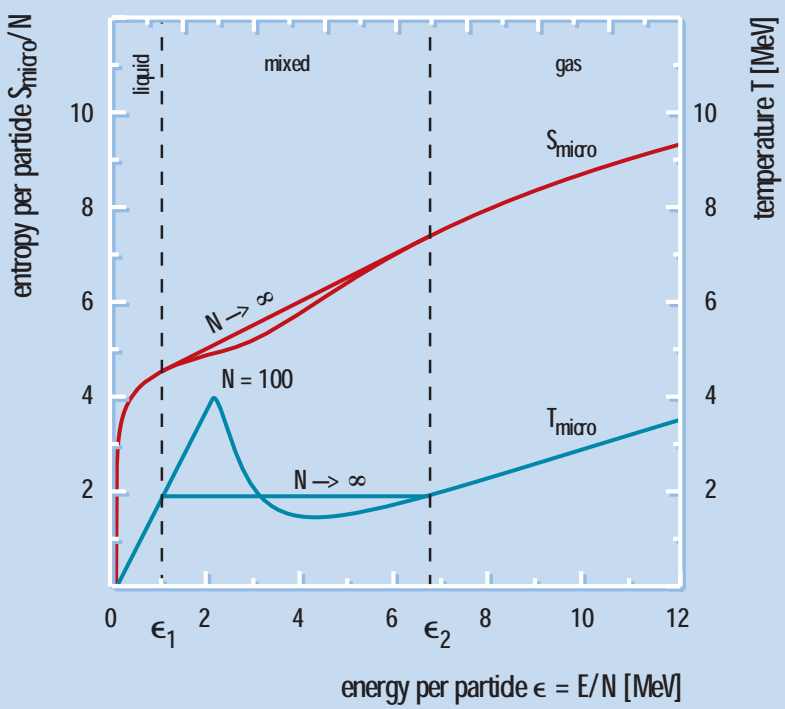
$$S_{micro}(E) = \ln(\rho_N(E)\Delta E),$$

to it, which may be used in conventional thermodynamic relations as long as the energy E is not too close to the ground-state energy where the spectrum is not dense.

With increasing energy E new degrees of freedom may open up and cause a phase transition, for example, from a neutral gas of atoms to ions and electrons or from a liquid with high density to a gas with low density. This coincides with an increase in steepness of the density of states $\rho_N(E)$.

A typical situation is sketched in the figure, where a first order phase transition occurs between ϵ_1 and ϵ_2. The red lines show the entropy of the microcanonical ensemble divided by the particle number N as function of the energy per particle ϵ = E/N. The reason for this representation is that, for systems with short-range interactions, the shape of the graph depends only weakly upon N. In particular, the energies ϵ_1 and ϵ_2 which separate the liquid, mixed, and gas phase do not change much with N, once N is large enough.

In the thermodynamic limit where N → ∞ the density of states grows



exponentially with E in the mixed phase such that the microcanonical temperature (blue lines)

$$T_{micro} = \left(\frac{\partial S_{micro}}{\partial E}\right)^{-1}$$

stays constant and the specific heat diverges. For a finite particle number (e.g. N =100) the density of states exhibits a depression in this region. The deviation from the envelope (N → ∞) then is the surface entropy per particle, which is proportional to $1/N^{1/3}$ due to the non-negligible surfaces of the bubbles or drops in the coexistence region.

The most promising way to identify a phase transition in a finite system is to prepare a microcanonical situation, measure the density of states and estimate the energies ϵ_1 and ϵ_2 by fitting the double-tangent to $\ln(\rho_N(N\epsilon)\Delta E)$. The density of states can be measured by looking at a small subsystem acting as a thermometer. Assuming weak coupling and equilibrium with the rest of the sytem which is characterized by a density of states ρ_{rest}, the states of the subsystem with energy $e_n \ll E$ are occupied with Boltzmann weight factors $e^{-\beta e_n}$, where

$$\beta = \frac{\partial \ln(\rho_{rest}(E)\Delta E)}{\partial E}$$

and where

$$\ln(\rho_{rest}(E)\Delta E) \approx \ln(\rho_N(E)\Delta E).$$

In the nuclear case the subsystem may be, for example, the kinetic degrees of freedom of protons, the intrinsic excitations of a fragment, or the multiplicities of small clusters.

In a heavy-ion collision, however, it is unclear whether global equilibrium between these degrees of freedom is achieved. ■

The determination of the caloric curve is done in the following way. The nucleus is excited by displacing all wave packets from their ground-state positions randomly. Both, center of mass momentum and total angular momentum are kept fixed at zero. To allow a first equilibration between the wave packets of the nucleus and those of the thermometer, the system is evolved over a long time, about 10000 fm/c (a typical time for a nucleon to cross the hot nucleus is 30 fm/c). After that, a time-averaging of the energy of the nucleonic system as well as of the thermometer is performed over a time interval of 10000 fm/c. During this time period the average of the nucleonic excitation energy is evaluated. The time-averaged energy of the thermometer, which is calculated during the same time interval, determines the temperature through the relation for an ideal gas of distinguishable particles in a common oscillator potential.

In Figure 2, several snapshots of the one-body density of a hot nuclear system with 8 neutrons and 8 protons are shown. On the left hand side, the ^{16}O nucleus has been given an excitation energy per nucleon E*/A of 3.5 MeV by randomly displacing the wave packets of the ground state. After equilibration this corresponds to a temperature of about 4 MeV. It can be seen that the two-body interaction used here creates an alpha-particle substructure in ^{16}O. There is no gas around the vibrating nucleus because the excitation energy is not high enough to evaporate particles.

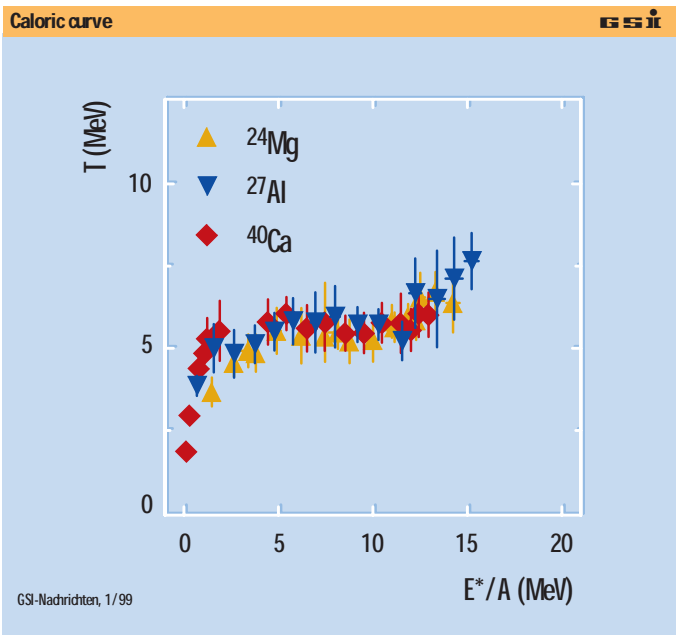


Figure 3: Caloric curve of ^{24}Mg, ^{27}Al and ^{40}Ca at $\hbar\omega$=1 MeV.

In the center column of Figure 2, the excitation energy per nucleon is 7 MeV. Bright areas which indicate the liquid are surrounded by a cloud of gas (for details see the figure caption). Moreover, the nuclear system very often falls apart into several smaller drops which are embedded in vapor.

The right hand side displays the same system but for an excitation energy per nucleon of 11 MeV. Here, half of the time no high density areas are visible (first and third frame) and when a drop is formed it is rather small.

As we shall see later, the two higher E*/A values at 7 and 11 MeV correspond both to a temperature around 5 – 6 MeV in the coexistence region. It is quite obvious that the additional excitation energy of 4 MeV per particle is used to transform liquid to vapor so that we see a clear first order liquid-gas phase transition. This is remarkable as we are dealing with only 16 nucleons and the dynamical model converges to a pure state with a very limited number

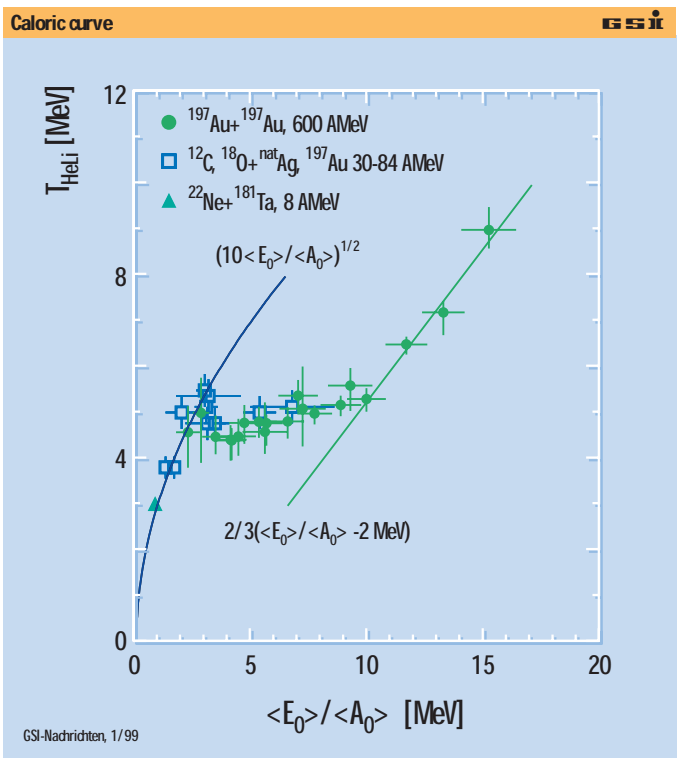


Figure 4: Caloric curve determined by the ALADIN group from the decay of spectator nuclei. The temperature T_{HeLi} is derived from the yield ratios ^{3}He to ^{4}He and ^{6}Li to ^{7}Li and provides a common scale in the liquid, fragmentation and vapor regimes.

of degrees of freedom, actually only eight per particle, three for mean position, three for mean momentum and two for the widths of the corresponding distributions. Furthermore, we have a fermionic system in which due to antisymmetrization the level density is much smaller than in classical mechanics.

The harmonic oscillator container, displayed in Figure 1, is very wide so that the vapor pressure is rather small. Estimates yield 10^{-4} to 10^{-2} MeV/fm^3 which should be compared to a critical pressure of about 0.5 MeV/fm^3. At the surface of the cubes indicated in Figure 2, the container potential itself is only 1.2 MeV higher than in the center.

The relations between the excitation energy and the temperature for ^{24}Mg, ^{27}Al and ^{40}Ca using the same container potential with a level spacing of $\hbar\omega$ = 1MeV is depicted in Figure 3. In order to put the results on the same scale, the respective ground state energies were subtracted from the averaged energy.

All caloric curves clearly exhibit three different parts. Beginning at small excitation energies the temperature rises steeply with increasing energy as expected for the shell model. The nucleons remain bound in the excited nucleus which behaves like a drop of liquid. At an excitation energy of 3 MeV per nucleon the curve flattens and stays almost constant up to about 11 MeV. This coexistence plateau at T $\approx$ 5 to 6 MeV extends from E*/A $\approx$ 3 MeV to about E*/A $\approx$ 11 MeV where all nucleons are unbound and the system has reached the vapor phase. The latent heat at pressure close to zero is hence about 8 MeV.

One has to keep in mind that the plateau is not the result of a Maxwell construction as in nuclear matter calculations. In the excitation energy range between 3 and 11 MeV per particle, an increasing number of nucleons is found in the vapor phase outside the liquid phase. This has been shown in Figure 2. The caloric curve shown in Figure 3 has a striking similarity with the caloric curve determined by the ALADIN group [4] which is displayed in Figure 4. The position and the extension of the plateau agree with the FMD calculation using a containing oscillator potential with $\hbar\omega$ = 1MeV. Nevertheless, there are important differences. The measurement addresses an expanding non-equilibrium system, but the calculation deals with a contained equilibrium system. In addition, the used thermometers are different; the experiment employs an isotope thermometer based on chemical equilibrium and the calculation uses an ideal gas thermometer. One explanation why the thermodynamic description of the experimental situation works and compares nicely to the equilibrium result might be that in the coexistence region, the excited spectator matter equilibrates faster than it expands and cools. ■

REFERENCES

[1] H. Feldmeier, Nucl.Phys. A515, 147 (1990); H Feldmeier, K. Bieler, J. Schnack, Nucl.Phys. A586, 493 (1995); H.Feldmeier, J. Schnack, Nucl.Phys. A583, 347 (1995); H.Feldmeier, J. Schnack, Prog. Part. Nucl. Phys. 39 (1997)

[2] J. Schnack, PhD thesis, TH Darmstadt (1996)

[3] J. Schnack, H. Feldmeier, Nucl. Phys. A601, 181 (1996)

[4] J. Pochodzalla et al.; Phys. Rev. Lett. 75, 1040 (1995); Prog. Part. Nucl. Phys. 39, 443 (1997)