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Publication Date
1988-07-01

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July 1988

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Classical Simulation of Nuclear Systems *

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July 24, 1988

Abstract:

With a view towards nuclear collisions at intermediate energies, we develop a microscopic nuclear model based on classical nucleons interacting via a momentum-dependent Pauli repulsion, a modified Lennard-Jones nuclear interaction, and a standard Coulomb repulsion. The ensuing model approximates well the energy per nucleon in nuclear matter over a broad range of temperatures and densities (including the saturation energy and density and the compressibility), as well as the sizes and binding energies of finite nuclei.

1 Introduction

Much effort has been devoted in recent years to the theoretical description of nuclear dynamics at high excitation, such as can be probed in medium-energy nuclear collisions. Particularly promising have been approaches adapted from Nordheim's treatment [1], in which individual nucleons are propagated in a common mean field and are subject to some residual direct scattering. However, further developments are still needed in order to incorporate dynamical fluctuations and fragment formation, aspects of central importance in the processes of interest.

In order to establish a useful supplement to such current models, we seek to develop a quasi-classical model based on the microscopic dynamics of interacting classical particles. This type of model contains the entire many-body matrix and thus automatically incorporates statistical fluctuations and clusterization phenomena.

A first step in this program is the introduction of a momentum-dependent repulsion for the purpose of simulating the Pauli exclusion principle. Such a "Pauli" potential was recently developed [2] and shown to give a satisfactory simulation of the Fermi gas over a broad range of temperatures and densities of interest in medium-energy nuclear collisions. In the present work we take the next step, namely the subsequent inclusion of a real two-body interaction for the purpose of achieving an approximate description of nuclear systems.

First, the development of the model is described (Section 2) and then the results obtained for nuclear matter and finite nuclei are described (Section 3); finally, a concluding discussion is given (Section 4).

2 Development of the model

In the present approach, the nuclear system is modelled as a quasi-classical system of interacting particles (nucleons). The exclusion principle, which acts to prevent identical nucleons with the same spin and isospin components from being close in phase space, is simulated by a momentum-dependent repulsive two-body potential (hence the term "quasi"-classical). In ref. [2] the following Pauli potential was determined,

$$V_P(p_{ij}, r_{ij}) = V_P^0 \left(\frac{\hbar}{p_0 q_0}\right)^3 e^{-(p_{ij}^2/p_0^2 + r_{ij}^2/q_0^2)/2} . \tag{1}$$

Here $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ is the spatial distance between the particles and $p_{ij} = |\mathbf{p}_i - \mathbf{p}_j|$ is their separation in momentum space. For the parameter values V_P^0=34.32 MeV, p_0=2.067 MeV·10^{-22} s/fm, q_0=6.00 fm, a reasonable reproduction of the Fermi gas was obtained for temperatures above a few MeV and densities within a factor of three of the saturation value. This range is relevant for nuclear collisions for beam energies between several tens and several hundreds of MeV per nucleon.

The successful simulation of the Fermi gas invites to further development of the quasi-classical approach. The next natural step is to incorporate a real two-body

interaction potential in an attempt to achieve an approximate description of nuclear matter and finite nuclei. In the present note we report on our success in this regard. Thus, we have arrived at a model in which the interaction potential between two nucleons is given by

$$V(p_{ij}, r_{ij}) = V_P(p_{ij}, r_{ij}) + V_N(r_{ij}) + V_C(r_{ij}) \ . \tag{2}$$

The second term is the nuclear interaction potential, which will discussed in more detail below, and the third term is the Coulomb potential, given by the point-charge repulsion $V_C(r_{ij}) = e^2 Z_i Z_j / r_{ij}$, where Z_i is the charge number of nucleon i and e is the elementary electric charge.

In order to determine a reasonable nuclear interaction potential, we have proceeded as follows. We have first considered a standard Lennard-Jones potential, $V_{LJ}(r) \sim (r_1'/r)^{12} - (r_2'/r)^6$. Such a form is computationally simple and has been employed in numerous theoretical studies. The parameters can be determined by requiring that symmetric nuclear matter saturate at the right density and energy, and that the α-particle has a reasonable binding energy. [This latter system is especially easy to consider, since its four constituent nucleons (which are not subject to mutual exclusion) can be assumed to be arranged in a tetrahedral configuration, so that the only variable is the overall scale.] With this done, both nuclear matter and finite nuclei can be treated.

In order to calculate the thermostatic properties implied by the model, we employ the Metropolis sampling technique [3], using the canonical weights $W \sim \exp(-H/\tau)$, where H is the Hamiltonian for the nuclear many-particle system under consideration. [H is equal to the kinetic energy of the nucleons, $T = \sum_i p_i^2/2m$, plus the interaction potential V in eq. (2).] For nuclear matter at a specified density and temperature, we can then calculate the mean energy, ϵ, as well as other statistical properties of interest (*e.g.* the cluster structure). The initial ("seed") configurations are constructed by placing the nucleons at random within the basic cell, in a manner that seeks to maximize the spatial separation between nucleons with the same spin-isospin components. For finite nuclei near the ground state, a similar sampling method can be used, since the problem of particle escape by "evaporation" is negligible; thus it is possible to extract the properties of ground-state nuclei, such as their sizes and binding.

As is well known, the strong repulsive core of the Lennard-Jones potential generates a very stiff equation of state, *i.e.* a too high compressibility coefficient. In order to rectify this problem, we have softened the potential by reducing the powers 6 and 12 characteristic of the standard Lennard-Jones potential to approximately half their values. However, while this remedy improves the compressibility considerably, it also renders the range of the potential too long. This problem is then largely removed by introducing a radial truncation factor of the form $1/[1+\exp((r-d)/a)]$, with $a > 0$. Thus, the nuclear interaction potential is taken to be of the form

$$V_N(r) = V_N^0 \ [(\frac{r_1}{r})^{p_1} - (\frac{r_2}{r})^{p_2}] \ \frac{1}{1 + e^{(r-d)/a}} \ . \tag{3}$$

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Using as Metropolis seeds those nuclear configurations that were generated with the standard Lennard-Jones potential, it is then relatively easy to adjust the several parameters in V_N to optimal values for which satisfactory results for both nuclear matter and finite nuclei are obtained. By this procedure, the values determined for the various parameters in V_N were determined to be as follows: The overall strength is $V_N^0 = 25.93$ MeV, the Lennard-Jones powers are $p_1 = 6.2$, $p_2 = 3.0$, and the corresponding charateristic distances are $r_1 = 1.757$ fm, $r_2 = 1.771$ fm; the parameters for the modulation factor are $d = 3.350$ fm, $a = 5/6$.

When comparing this potential with commonly employed nucleon-nucleon interactions, it should be kept in mind that any potential that is usable in a classical treatment will differ significantly from the potentials employed in corresponding quantum-mechanical calculations: the classical interaction would generally be more gentle since classical particles can exploit potential minima better than quantal particles, which are subject to the indeterminacy relation and thus are less sensitive to narrow potential wells.

3   Results

With the model specified as described above, it is now possible to treat various nuclear systems. Below we present the results obtained for (uncharged) nuclear matter at various densities and temperatures, as well as those for finite nuclei near the ground state.

3.1   Nuclear matter

The thermostatic properties resulting from the developed model are conveniently expressed in terms of the mean energy per nucleon, ϵ, as a function of the density and temperature. In the calculation, a periodic system is considered as an approximation to infinite uniform matter, as was done in ref. [2]. Typically, a single cell contains 144 nucleons (36 of each spin-isospin component). Because of the finite range of the interparticle potentials, $V_P(r, p)$ and $V_N(r)$, it is necessary to let a given particle interact with particles from neighboring cells. For the Pauli potential V_P we have included contributions from four layers of neighboring cubic cells, whereas for the shorter-range nuclear interaction V_N a single layer of neighbor cells has proved to be sufficient.

In Figure 1 are shown the results for three temperatures, $\tau = 0.5, 4, 8$ MeV (the first being a good approximation to zero temperature), over a range of densities from about half to nearly twice the standard saturation value of $\rho_0 = 0.17$ fm^{-3}. The zero-temperature curve has a minimum at $\rho \approx 1.1\rho_0$, so that standard nuclear matter emerges as $\approx 10\%$ too dense. At this saturation minimum, the binding energy per nucleon is given by $-\epsilon_0 = 16.7$ MeV, a very satisfactory value. The zero-temperature curve crosses through $\epsilon = 0$ at $\rho \approx 2\rho_0$, which is what would happen for a standard Equation of State with a compressibility coefficient of $K \approx 300$ MeV. It

should be noted, though, that since our model yields a saturation density, that is slightly higher than ρ_0 the actual compressibility *coefficient*, which is proportional to the second derivative of ϵ at saturation, is larger than that value.[1]

The curves for finite temperature give an impression of the behavior of hot nuclear matter. The overall behavior with increasing temperature is quite satisfactory, although the growth for small values of τ is somewhat too rapid, as is generally the case in a classical model.[2] However, the anticipated regime of application for the model is to systems with equivalent temperatures of at least several MeV, so the failures in thermal properties for fairly cold systems should not cause major concern. [It might also be noted that the too large heat capacity at low temperature is somewhat counteracted by the lack of shell effects: due to shell effects, ground-state nuclei tend to have extra binding which disappears as the temperature is raised above a few MeV.]

3.2 Finite nuclei

As already shown by Abraham *et al.* [4] for studies of molecular drops, the statistical properties of finite clusters can also be calculated by the Metropolis sampling method, provided that appropriate care is taken to avoid spurious particle losses. The seed configurations are constructed by placing the nucleons at random inside a sphere of a size expected for the nucleus considered. In our treatment, a nuclear cluster C is defined by the demand that each of its constituent nucleons have a negative energy, $\forall i \in C : \ \epsilon_i < 0$, where

$$\epsilon_i = T_i^C + \sum_{j \in C} V_{ij} \tag{4}$$

is the single-particle energy of nucleon i, referred to the CM frame of the cluster C.

In Table 1 are listed the calculated values for the root-mean-square radius of the matter distribution in nuclei in the light mass region, together with the corresponding experimental values. The same information is displayed graphically in Figure 2. The overall trend is quite good but, as expected from the fact that our calculated nuclear matter equilibrium density is too high, the calculated nuclear radii are somewhat too small. The effect is approximately 20% through the mass region shown.

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[1] In fact, the second derivative at saturation is not well suited as a measure of the actual compressional energy at higher densities, since a given model usually contains additional parameters (*e.g.* the effective mass) whose values affect the compressional energy significantly. A less ambiguous indication of the response of the system to compression can be obtained in terms of an *effective* compressibility coefficient K_{eff} which invokes information about the behavior at densities above saturation. Specifically, exploiting the relationship $\epsilon(\rho) - \epsilon_0 = (K/18)(\rho/\rho_0 - 1)^2$, we suggest defining $K_{\text{eff}} = 18(\epsilon(2\rho_0) - \epsilon_0)$. In words, K_{eff} is that compressibility coefficient which, in the parabolic idealization, yields the actual compressional energy at double density.

[2] In a classical model, the specific heat is linear in the temperature near the ground state, whereas it is quadratic in a quantal system. This principal difference arises from the fact that in a quantized system there is a certain minimum energy required for making an elementary excitation whereas infinitesimal excitations are possible in a classical system.

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The measured and calculated binding energies are listed in Table 2 and displayed in Figure 3, up to medium-mass nuclei. Again, the overall trend is quite good. The nuclei tend to be somewhat overbound, typically by less than one MeV per nucleon. For the very lightest nuclei the calculation agrees well with the average trend of the experimental values.

As mentioned earlier, these results are obtained for $\tau = 0.5$ MeV, since it is technically difficult to treat $\tau = 0$. However, neither the radii nor the binding energies are expected to vary significantly with temperature at such small values, so the calculated results can be assumed to correspond to the true ground state of the perticular clusters considered.

4   Discussion

In the preceding, we have presented a novel quasi-classical model for nuclear systems. The model describes the nucleons as classical point particles subject to a momentum-dependent Pauli repulsion and a modified Lennard-Jones nuclear interaction, in addition to a standard Coulomb repulsion between the protons.

The major advantanges of the model are as follows. First, as was already shown in ref. [2], the non-interacting Fermi gas is simulated rather well in terms of the Pauli potential, over an interesting range of temperatures and densities. For interacting nuclear matter, the behavior of the energy with density and temperature is also quite satisfactory. In particular, reasonable values result for both the saturation energy and the saturation density (although the latter value is around 10% too high). The effective compressibility, as indicated by the energy of cold matter at double density, is also close to that produced by standard nuclear models. For finite nuclei, a satisfactory global behavior is achieved for both binding energies and radii, with these quantitites being typically 10% and 20% too large, respectively.

There are also certain drawbacks in the model, of course. As already pointed out, it is a general property of classical systems that the specific heat is linear in the temperature near the ground state, contrary to the quadratic behavior of quantal systems. In our model, this difference is insignificant for temperatures above a few MeV and thus of minor concern for the anticipated applications to medium-energy heavy-ion collisions. Another deficiency is that there is no zero-point motion for the nucleons. This is particularly apparent in the α-particle whose four nucleons are at relative rest (since their different spin-isospin components render them insensitive to the Pauli exclusion). Even so, the binding energies of light nuclei are quite acceptable. For heavy nuclei, the zero-point motion is small in comparison with the Fermi motion, which is well reproduced by the Pauli potential.

Having thus established that the model accounts reasonably well for the general thermostatic nuclear properties, we are in a solid position to address dynamical problems; our progress in this regard will be reported in due course. Over the past decade or so, there have been several studies of nuclear dynamics within the framework of classical molecular dynamics. One of the first such studies was by

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Bodmer *et al.*[7], who made extensive investigations of nuclear collisions at a few hundred MeV per nucleon. Among other aspects, they studied the sensitivity to the variation of the two-body interaction subject to the constraint of scattering equivalence and they also incorporated relativistic effects to first order by way of a momentum-dependent interaction. However, no attempt was made to incorporate the Pauli exclusion principle and so the quantitative applicability to actual nuclear problems was limited. An explicit inclusion of a Pauli potential was first made by Wilets *et al.* [8]. However, at that time it was not investigated to which extent a reasonable simulation of the Fermi gas can actually be achieved; our preceding work [2] accomplishes this task. Relatively recently, Pandharipande *et al.* have studied the dynamics of argon droplets on the basis of classical molecular dynamics.[9] While these latter studies have yielded interesting insight into the dynamics of small many-body systems, their implications for nuclear systems are limited by the fact that the characteristic parameters for argon differ substantially from those of nuclei. Remaining within the framework of classical equations of motion, our present model approximates nuclear systems much better and should thus be of more direct utility for the exploration of nuclear dynamics.

Our present work is motivated by the need for developing useful models for nuclear dynamical processes. As a minimum requirement, any model employed for the study of energetic nuclear collisions ought to give a reasonable reproduction of general thermostatic nuclear properties, in order that its results for dynamical processes be interpretable and informative. Although there are presently several molecular-dynamics models in use, none of them have yet been demonstrated to actually approximate nuclear properties to the extent exhibited by our present model. The lack of a built-in mechanism for simulating the Pauli exclusion principle is a particularly serious weakness of ordinary classical models, since their ground-state "nuclei" are devoid of Fermi motion and thus substantially different from real nuclei. It is a major strength of the model presented here that it overcomes this long-standing problem by the incorporation of a Pauli potential.[3]

As a final remark, we feel that the present model, having passed the minimum requirement outlined above, presents a useful supplementary tool for theoretical studies of nuclear dynamical processes. It may well be possible (in fact, it would be desirable) to develop different combinations of Pauli potential and nuclear interaction that yield comparable correspondence with the thermostatic properties of infinite matter and finite nuclei. If that were to occur it would be instructive to study the possible differences arising when specific dynamical problems are addressed.

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[3]While completing this work, we have become aware of an approach being developed by Boal *et al.*[10]; also incorporating a Pauli potential, that model yields fairly reasonable nuclear radii and binding energies, while the properties of infinite matter have yet to be assessed.

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Table 1: Nuclear radii

Element	Experiment	Calculation	Deviation
He	1.63	1.40	-14%
Li	2.54	1.66	-35%
C	2.50	2.01	-20%
O	2.65	2.21	-17%
Si	3.04	2.67	-12%
Ca	3.52	2.95	-16%

Measured [5] and calculated rms radii of nuclei up to $A=40$, averaged over isotopes.

Table 2: Nuclear Binding Energies

Nucleus	Experiment	Calculation	Deviation
^{4}He	28.30	18.8	-34%
^{6}Li	31.993	34.5	7.8%
^{8}Be	56.50	48.4	-14%
^{12}C	92.16	88.92	-3.5%
^{16}O	127.62	124.48	-2.4%
^{20}Ne	160.65	163.8	2.0%
^{28}Si	236.63	247.8	4.7%
^{40}Ca	342.06	375.2	9.7%
^{50}Ti	437.79	473.5	8.2%
^{64}Zn	559.01	611.2	9.3%
^{82}Kr	714.28	738.4	3.4%

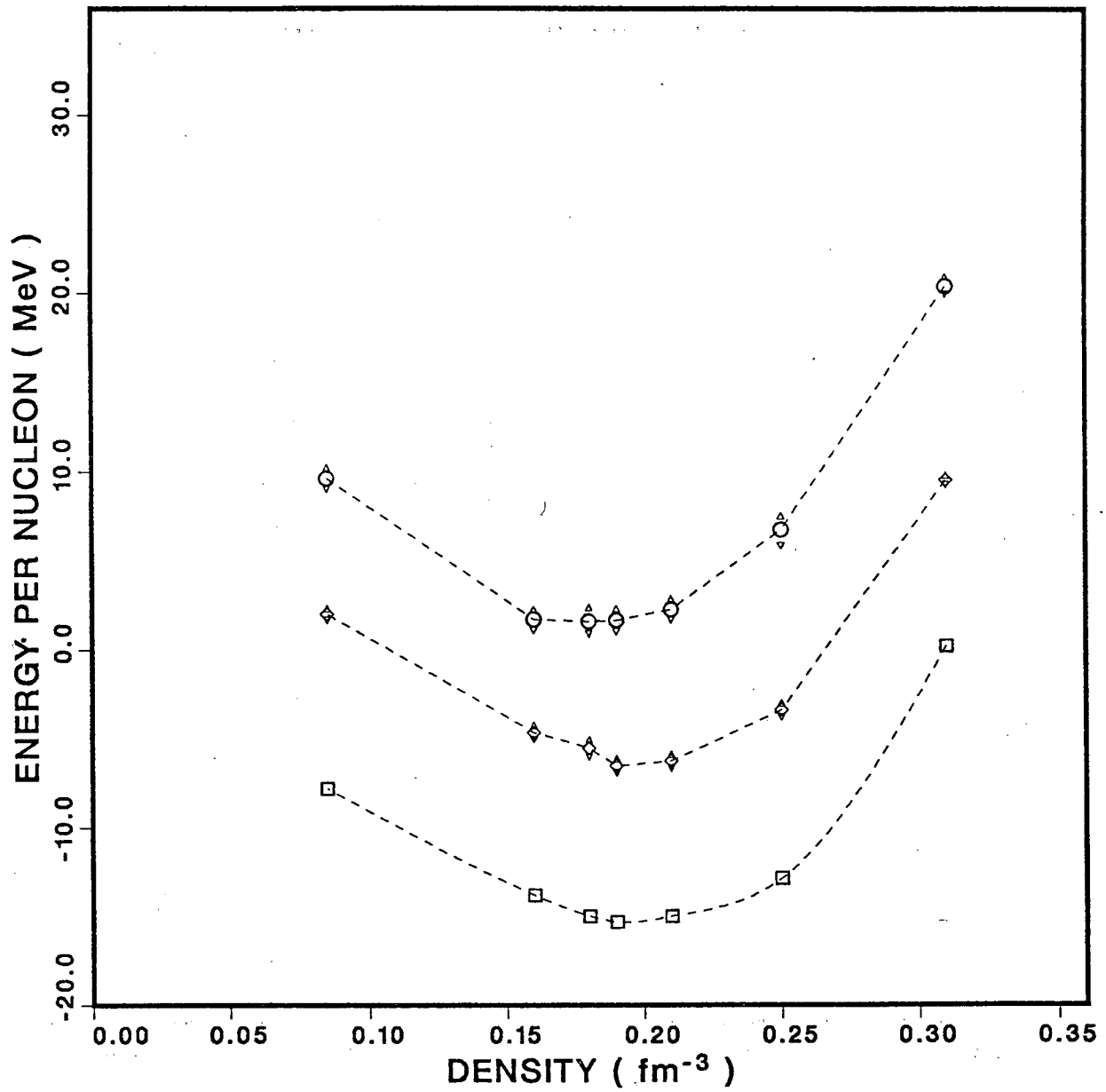Measured [6] and calculated binding energies for light and medium-heavy nuclei.

Figure 1: Specific Energy of Nuclear Matter

The mean energy per nucleon ϵ of infinite nuclear matter at a given temperature τ=0.5 MeV (squares), 4.0 MeV (diamonds), and 8.0 MeV (circles), as a function of the mean density of nucleons ρ.
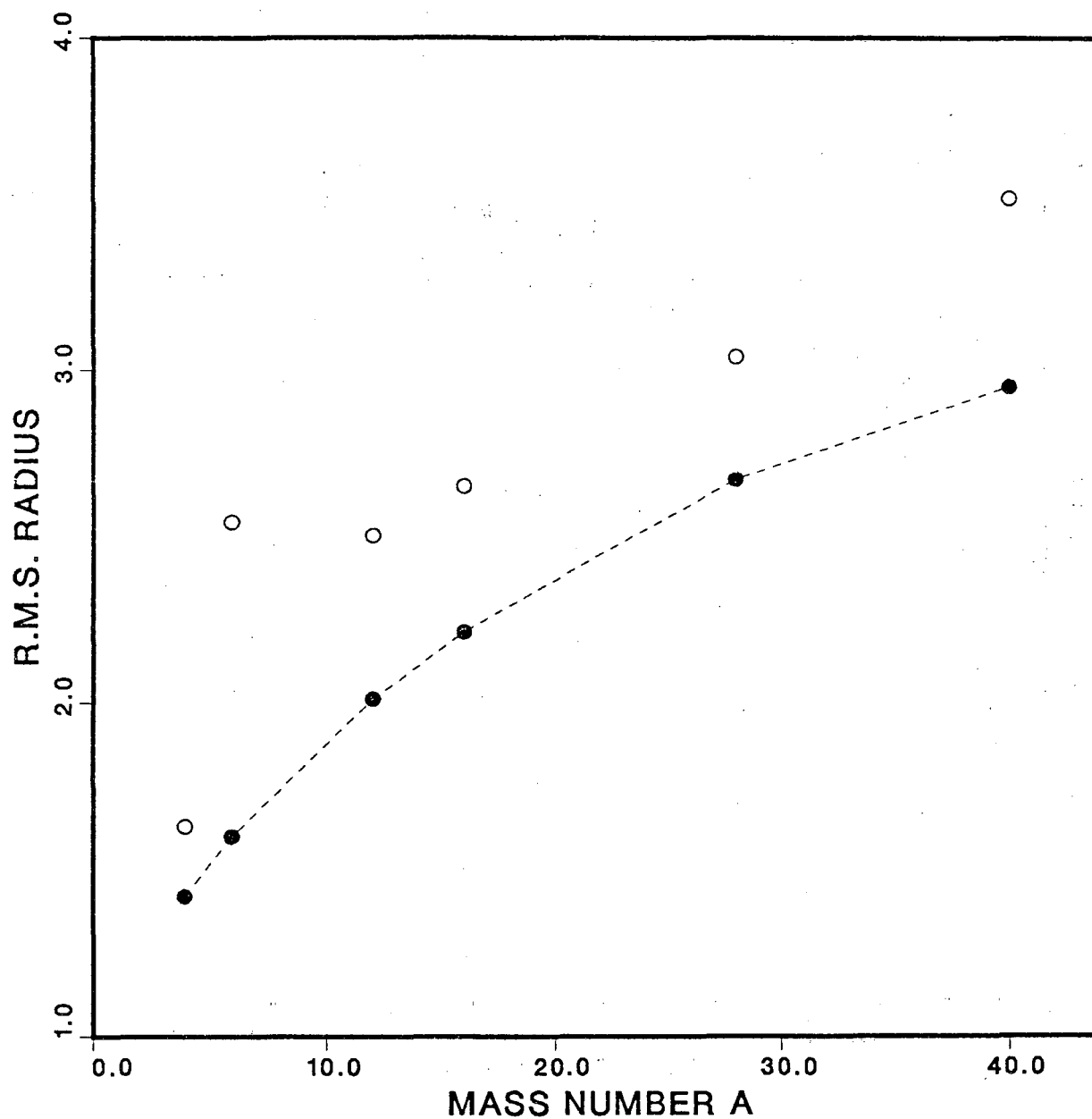
Figure 2: Nuclear radii
The root-mean-square radius of a nuclear cluster containing A nucleons and having a temperature of $\tau=0.5$ MeV. The open circles indicate the experimental values for ground-state nuclei [5], while the solid circles are those calculated with our quasi-classical model.
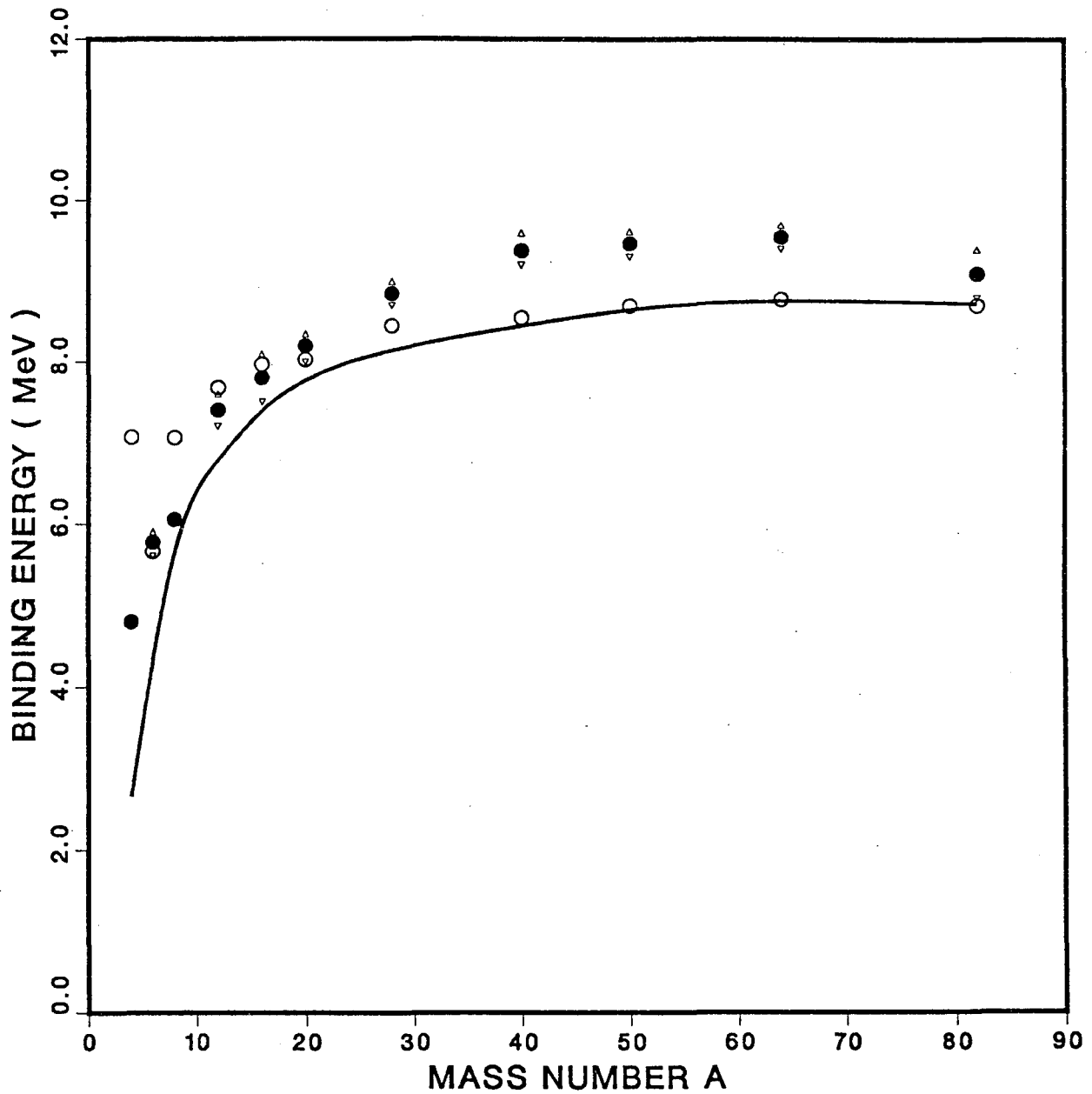
Figure 3: Nuclear binding energies
The binding energy of a nuclear cluster containing A nucleons and having a temperature of τ=0.5 MeV. The open circles indicate the experimental values for nuclear ground states [5], while the solid circles are those calculated with our quasi-classical model. The curve gives the results of a simple mass formula.[6]