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Fragment Interactions in Nuclear Disassembly*

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Abstract:

The importance of interfragment forces in nuclear multifragment systems is examined in the hard-sphere idealization. Commonly used approximations for the effective volume and the Coulomb energy are examined, and improved one-body approximations are presented.

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1 Introduction

Multifragment systems are of central importance both for the description of nuclear matter at subsaturation density, since such systems tend to cluster, and for the understanding of medium-energy nuclear collisions, in which many fragments are produced. Until recently, statistical models addressing nuclear multifragmentation did not incorporate the forces acting between the nuclear fragments in the source considered and it was necessary to resort to simple one-body approximations.¹ The recently developed microcanonical simulation model[2] for nuclear multifragmentation presents a significant advance because it allows interfragment forces to be included in a straightforward and formally well-founded manner. With tractable reference calculations available, it is possible to ascertain the quality of the various simple approximations that have been commonly employed. It is also of interest to seek to improve the approximations, without introducing complexity beyond the one-body level. This is necessary because the simulation of interacting fragments is computationally demanding, so that there are practical advantages associated with having reasonably accurate one-body models.

Therefore, in the present paper, we address the role of interfragment forces in a multifragment system. First, in section 2, we consider the effect of the nuclear interaction potential, as idealized in terms of hard spheres, and commonly adopted “excluded-volume” prescriptions are tested; an improved “virial” approximation is also presented. Subsequently, in section 3, the electrostatic (Coulomb) energy is studied and the validity of various popular one-body approximations is assessed; again, an improved formula is proposed. Some concluding remarks are then given.

2 The nuclear interaction

The most important feature of the nuclear component in the interfragment potential arises from the high nuclear incompressibility which acts to prevent fragments from overlapping. To a rough approximation, this effect can be taken into account by representing the nuclear fragments as hard spheres. (Deviations from this idealization are expected to be quantitatively important, but they are considerably harder to address and their inclusion is postponed for later study.[4]) Although somewhat simplistic, the hard-sphere approximation is still quite demanding in terms of computation, since it requires knowledge of all the relative fragment positions. Most models developed so far do not contain this degree of detail and so it has been common to adopt some form of a one-body approximation. In intuitive terms, the presence of the other fragments limits the volume available for a given fragment. It is therefore natural to attempt to approximate the mutual fragment repulsion in terms of a reduced “effective” volume Ω_{eff} , within which the fragments can be

¹The first formulation of nuclear disassembly into complex excitable nuclei was made within the grand canonical approximation for non-interacting fragments,[1] and most later modelings have had an essentially similar basis.

considered as independent. In the present section, we wish to examine such approximations in order to ascertain their quality and in the hope of devising more accurate approximations.

For the present analysis, it is most instructive to consider the level of detail at which the multifragment system is characterized by its *positioning*, or *placing*, $\mathcal{P}$,

$$\mathcal{P} = \{A_n, \mathbf{r}_n, n = 1, \dots, N\} , \quad (1)$$

i.e. by its mass partition $\alpha = \{A_n\}$ together with the positions $\{\mathbf{r}_n\}$ of the fragments. In the canonical approximation,[2] the statistical weight of a given positioning $\mathcal{P}$ is

$$W(\mathcal{P}) = \prod_{n=1}^N \left[\Omega \left(\frac{m A_n \tau}{2\pi \hbar^2} \right)^{3/2} \zeta_n(\tau) e^{B_n/\tau} \right] \delta \left(\sum_n A_n - A \right) e^{-V/\tau} , \quad (2)$$

where B_n is the binding energy of fragment n and its intrinsic partition function is

$$\zeta_n(\tau) = \int \rho_n(\epsilon_n) e^{-\epsilon_n/\tau} d\epsilon_n . \quad (3)$$

Furthermore, A is the total number of nucleons in the system, τ is the imposed temperature, and $V(\mathbf{r}_1, \dots, \mathbf{r}_N)$ is the interaction potential. The combined weight of all positionings $\mathcal{P}$ having the same mass partition α is then

$$\begin{aligned} W(\alpha) &= \prod_{n=1}^N \left[\int \frac{d\mathbf{r}_n}{\Omega} \right] W(\mathcal{P}) \\ &= \delta \left(\sum_n A_n - A \right) \prod_{n=1}^N \left[\Omega \left(\frac{m A_n \tau}{2\pi \hbar^2} \right)^{3/2} \zeta_n(\tau) e^{B_n/\tau} \right] \int \frac{d\mathbf{r}_n}{\Omega} e^{-V/\tau} \\ &= \kappa(\alpha)^N W_0(\alpha) . \end{aligned} \quad (4)$$

Here $W_0(\alpha)$ is the statistical weight for the same system if there were no interfragment forces, *i.e.* $V \equiv 0$. The quantity $\kappa(\alpha)$, which expresses the reduction of the available volume due to the fragment interactions V , is then defined by

$$\kappa(\alpha)^N = \prod_{n=1}^N \left[\int \frac{d\mathbf{r}_n}{\Omega} \right] e^{-V/\tau} . \quad (5)$$

Thus, the weight of a particular mass partition α is equal to that associated with noninteracting fragments confined within the smaller *effective* volume $\Omega_\alpha^{\text{eff}} = \kappa(\alpha)\Omega$. When the fragments are hard spheres the interaction potential V vanishes if none of the fragments overlap and is infinite otherwise. Therefore, for any positive temperature τ , $e^{-V/\tau}$ is either one or zero, respectively, and $\kappa(\alpha)^N$ is then simply the number of allowed (*i.e.* non-overlapping) positionings divided by the total number of positionings of the N fragments with the specified masses $\alpha = A_1, \dots, A_N$.

For any fixed mass partition α , the replacement of hard spheres within the volume Ω by non-interacting fragments within the (α -dependent) effective volume $\Omega_\alpha^{\text{eff}}$ is exact, of course, provided that the exact value (5) is employed for $\kappa(\alpha)$. The

aim of any effective-volume approximation is to estimate $\kappa(\alpha)$ without invoking specific information about the fragment positions.

When a one-body model is used, as is most often the case, information about the mass partition is only available in terms of the mean multiplicities of the various fragment species, $\bar{\nu}_A$. The most common approximations therefore employ an effective κ -value that is independent of mass partition, *i.e.* use $\Omega_{\text{eff}} = \kappa_{\text{eff}}\Omega$, for all the different mass partitions α . In order to have a convenient reference value, we define, for a given fragment multiplicity N , the following effective value of κ ,

$$\kappa_{\text{eff}}^N = \langle \kappa(\alpha)^N \rangle_\alpha = \frac{\sum_\alpha W(\alpha) \kappa(\alpha)^N}{\sum_\alpha W(\alpha)}. \quad (6)$$

A number of effective-volume approximations have been devised and employed in studies of nuclear disassembly. In the simplest one the effective volume is taken as the total volume minus the volume taken up by all the fragments combined, $\Omega_{\text{eff}} = \Omega - \Omega_0$, where $\Omega_0 = \sum_n \Omega_n = A/\rho_0$ is the volume of the N hard spheres. This approximation has been employed in particular by Kapusta and coworkers [5]. It follows that the corresponding effective κ -value is

$$\kappa_K = 1 - \frac{\Omega_0}{\Omega} = 1 - \frac{\rho}{\rho_0}. \quad (7)$$

A more refined approach was taken by Fai and Randrup [6], based on the recognition that the (anti)correlated positioning of the N fragments can be viewed as a sequential process, so that progressively less volume is available as the fragments are placed. Clearly, the entire volume Ω is available to the first fragment, and by assuming that each fragment placed blocks an additional volume equal to its own volume, the following approximation was derived,[6]

$$\kappa_{\text{FR}} = \frac{\rho}{\rho_0} \chi = \frac{1}{e} \left(1 - \frac{\rho}{\rho_0}\right)^{1-\rho_0/\rho}. \quad (8)$$

In the dilute limit, $\rho \ll \rho_0$, we have $\kappa_{\text{FR}} \approx 1 - \frac{1}{2} \frac{\rho}{\rho_0}$, whereas $\kappa_{\text{FR}} \approx \frac{1}{e} \frac{\rho}{\rho_0}$ in the dense limit, $\rho \approx \rho_0$. The fact that only the last fragment is blocked by the full amount Ω_0 implies that the value (8) will be closer to unity than (7). However, even though more refined, the consideration employed in deriving (8) does not yet take account of the fact that the volume blocked by a given fragment exceeds that fragment's own volume by a layer of thickness equal to the radius the next fragment placed. Therefore the approximation (8) is expected to underestimate the effect of blocking, and hence to overestimate the value of κ . This feature is most significant for dilute systems, for which the average excluded volume is typically underestimated by a factor of eight, whereas (7) would be off by a factor of four (see below).

The above two approximations depend only on the relative density, ρ/ρ_0 , and thus give the same value of κ for all multiplicities. A simple comparison can be made for two fragments having the same volume, $\Omega_1 = \Omega_2 = \frac{1}{2}\Omega_0$. The exact effective volume parameter is then $\kappa^2 = 1 - 4\Omega_0/\Omega$, since the first fragment blocks

a volume equal to $\frac{4\pi}{3}(R_1 + R_2)^3 = 4\Omega_0$. By contrast, the approximation (7) gives $\kappa_K = 1 - \Omega_0/\Omega$, whereas (8) would give $\kappa_{FR}^2 = 1 - \frac{1}{2}\Omega_0/\Omega$ in the dilute limit.

We now discuss a more refined approximation that we have developed in the course of the present study. It is based on the assumption of independent pairwise correlations between the fragments, and we shall denote it the virial approximation, because our considerations are rather similar to the virial treatment of interacting particles in a gas. Thus, for a given mass partition α , we assume that each fragment pair ij contributes a factor P_{ij} to κ^N , *i.e.*

$$\kappa_V(\alpha)^N = \prod_{i<j} P_{ij} = \exp\left(-\sum_{i<j} \omega_{ij}\right). \quad (9)$$

While we have explored several different forms of the “pair correlation” $P_{ij} = \exp(-\omega_{ij})$, we shall here focus on the simple but quite useful approximation in which

$$\omega_{ij} = \frac{4\pi}{3}(C_i + C_j)^3 \frac{1}{\Omega} = \frac{\Omega_{ij}}{\Omega}. \quad (10)$$

Here C_i and C_j are the (central) radii of the two nuclear fragments. Because $\Omega_{ij} \equiv \frac{4\pi}{3}(C_i + C_j)^3$ is the size of the volume that fragment i blocks for fragment j , or vice versa, and since $P_{ij} \approx 1 - \omega_{ij}$ for dilute systems, it follows that P_{ij} is approximately equal to that value of κ^N that would have resulted if only the two fragments i and j were present. The virial value (9) of κ is also displayed in fig. 1.²

The virial approximation is amenable to a one-body treatment. It follows from the definition (9) that the virial value of κ associated with a given mass partition α can be written in the form

$$\kappa_V(\alpha)^N \equiv \prod_{i<j} P_{ij} = \prod_{i=1}^n \left[\prod_{j(\neq i)} P_{ij} \right]^{1/2} = \prod_{i=1}^N \kappa_i(\alpha), \quad (11)$$

i.e. as a product of contributions from each of the individual fragments. The value κ_i associated with a given fragment i can be calculated as

$$\ln \kappa_i(\alpha) = -\frac{1}{2} \left[\sum_{j=1}^N \omega_{ij} - \omega_{ii} \right] = -\frac{1}{2} \left[\sum_A \nu_A \omega_{iA} - \omega_{ii} \right]. \quad (12)$$

In the last relation, the summation has been reorganized so that all fragments with the same mass number A are grouped together, and ν_A is the multiplicity of such

²The standard textbook treatment of interacting particles is by way of a virial expansion.[3] When carried to first order, this procedure would yield a result of the form (9), with the suppression factor from a given pair given in terms of their interaction potential V_{ij} ,

$$P_{ij} = 1 - \int \frac{d\mathbf{r}_{ij}}{\Omega} (1 - e^{-V_{ij}/\tau}) = 1 - \omega_{ij}$$

The last relation holds for hard spheres, for which the integrand is unity inside the blocked volume Ω_{ij} and vanishes outside. We have replaced $1 - \omega_{ij}$ by $e^{-\omega_{ij}}$ in order to avoid problems when $\omega_{ij} > 1$, as may happen at high densities. (For equal fragments, this happens when $\rho > \rho_0/4$.)

fragments in the particular mass partition α considered. A one-body approximation, $\bar{\kappa}(\alpha)$, is then obtained by replacing the actual multiplicity ν_A by its ensemble average, $\bar{\nu}_A$. Writing $\bar{\kappa}(\alpha)^N = \prod_i \bar{\kappa}_i(\alpha)$, in analogy with (11), we thus have

$$\ln \bar{\kappa}_i(\alpha) = -\frac{1}{2} \left[\sum_A \bar{\nu}_A \omega_{iA} - \omega_{ii} \right]. \quad (13)$$

This one-body approximation yields a κ -value for any given mass partition α , provided that the one-fragment multiplicity distribution $\bar{\nu}_A$ is known for the system. An overall effective value for the entire system can then be obtained by averaging over the mass partitions α , as in (6), $\bar{\kappa} = \langle \bar{\kappa}_\alpha \rangle_\alpha$.

In order to achieve an impression of the quality of the various approximations, we consider idealized systems consisting of N uncharged hard spheres, each with a radius equal to the equivalent sharp fragment radius, $R_n \approx r_0 A_n^{1/3}$, $r_0 = 1.15$ fm. The fragment masses are either all equal, $A_n = A/N$, or chosen randomly. [The random mass distribution is generated by first selecting N random masses from an exponential distribution having the mean value A/N (*i.e.* $A_n = -\frac{A}{N} \ln \eta$ where $\eta \in (0, 1)$ is random) and then renormalizing these masses by a common factor to ensure that $\sum_n A_n = A$. Thus the mass distribution is approximately of Poisson form.]

Figure 1 displays results for both a dilute system ($\rho = \rho_0/16$) and a dense one ($\rho = \rho_0/4$). It is seen that the variation of κ with the fragment multiplicity N is substantial. This casts serious doubt upon the use of multiplicity-independent approximations, such as (7) and (8). The virial approximation exhibits a quantitatively good correspondence with the exact κ -value at low densities, and remains a reasonable approximation at high densities, although far from perfect.

While the above schematic studies are instructive in judging the relative quality of the various approximations, they give little information on the effect on observable quantities, such as the mass distribution or the pressure. Therefore, it is important to also consider more realistic scenarios. For this task, we have employed the simulation model developed in [2]. As an illustration of these results, figure 2 shows the mean fragment mass and the pressure as functions of the density ρ for the temperature $\tau=8$ MeV. Again the virial approximation is generally superior to the simple excluded-volume approximations, and in fact it follows the exact results fairly well. (The near-perfect agreement of the virial approximation for the pressure is probably somewhat fortuitous, since the results have some statistical error, as indicated by the wiggles in the P -curves.) It should also be noted that κ_K happens to produce fairly good values for the mean mass number $\bar{A}$ in the particular example shown. However, as is evident from the behavior of the corresponding pressure P , such agreement for a single observable can be misleading, and it is important to consider several observables when assessing the quality of the approximations.

3 The Coulomb energy

The Coulomb force has a long range and thus acts between all the fragment pairs. The associated interaction energy is typically several MeV/N, so when the temperature is of this order, or less, it is quantitatively important to treat the Coulomb energy accurately. We therefore wish to study the Coulomb energy of multifragment systems.

Real nuclear fragments have non-trivial charge distributions, even when isolated, and they are polarizable as well. However, to a reasonable approximation, they can be considered as sharp spheres with uniform charge distributions. Accordingly, we shall consider an idealized scenario consisting of non-overlapping hard uniform spheres. The exact Coulomb energy of N such fragments is

$$V_C^{\text{exact}} = \sum_n \frac{3}{5} e^2 \frac{Z_n^2}{R_n} + \frac{1}{2} \sum_n \sum_{n' (\neq n)} e^2 \frac{Z_n Z_{n'}}{r_{nn'}}. \quad (14)$$

where e is the elementary electric charge. The first term represents the self-energies of homogeneously charged spheres, having charge numbers Z_n and radii $R_n = r_0 A^{1/3}$. The second term is the interaction energy between these (non-overlapping) spheres, with $r_{nn'} = |\mathbf{r}_n - \mathbf{r}_{n'}|$ being their center separations.

As already mentioned in connection with the discussion of the nuclear interaction potential in the preceding section, the double sum in the energy expression is computationally demanding since it requires the knowledge of all the fragment positions $\mathbf{r}_n$. So it is desirable to approximate the electrostatic energy in a manner that only involves a single sum over the fragments.

The simplest such approximation is often denoted the *mean-field approximation*. In this approximation the interaction of a given fragment with the remaining fragments is replaced by its interaction with the electrostatic field arising if the charge of the entire multifragment system were distributed uniformly throughout the confining volume Ω . Thus

$$V_C^{\text{mf}} = \frac{3}{5} e^2 \sum_n \frac{Z_n^2}{R_n} + \frac{1}{2} \sum_n e Z_n \phi_Z(\mathbf{r}_n). \quad (15)$$

Here the electrostatic field inside the uniformly charged sphere is given by $\phi_Z(r) = (\frac{3}{2} - \frac{1}{2}(\frac{r}{R})^2) \frac{eZ}{R}$, and the factor of one half accounts for the fact that the field is self-generated by two-body forces. Since usually the purpose of making the approximation is to eliminate the need for tracking the fragment positions, one normally uses only the average value of the mean field, $\bar{\phi}_Z = \frac{6}{5} \frac{eZ}{R}$, as is appropriate if the fragments are situated at random within the confining volume. (This is generally not the case, though, because different positionings have different statistical weights.) Then the averaged mean-field approximation reads

$$\begin{aligned} \bar{V}_C^{\text{mf}} &= \frac{3}{5} e^2 \sum_n \frac{Z_n^2}{R_n} + \frac{3}{5} e^2 \sum_n \frac{Z}{R} Z_n \\ &= \frac{3}{5} e^2 \frac{Z^2}{R} + \frac{3}{5} e^2 \sum_n \frac{Z_n^2}{R_n}. \end{aligned} \quad (16)$$

In the second line the sum over the fragments has been carried out, using $\sum_n Z_n = Z$, and the order of the terms has been interchanged. The fragment interaction term is then recognized as the selfenergy of the equivalent uniformly charged sphere, $V_C^0 = \frac{3}{5}e^2 \frac{Z^2}{R}$. This term is a constant for a given system, i.e. it is independent of the particular mass partition, and it can therefore be eliminated by a corresponding redefinition of the total energy of the system. The mean-field approximation was first formulated for nuclear disassembly by Koonin and Randrup[1] and has been employed in most of the subsequent work along that line.

It was first noted by Gross [7] that the above mean-field approximation is relatively inaccurate for configurations having only a few fragments, because the mean field ϕ is calculated on the basis of *all* the charge, rather than only the charge associated with the residual $N-1$ fragments. Therefore, we shall also consider the following *refined mean-field approximation*, in which this shortcoming is remedied,

$$V_C^{\text{rmf}} = \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n} + \frac{1}{2} \sum_n e Z_n \phi_{Z-Z_n}(\mathbf{r}_n). \quad (17)$$

Here ϕ_{Z-Z_n} is the electrostatic field from a uniform sphere containing the residual charge $e(Z-Z_n)$. Again, it is natural to average over the fragment positions, leading to

$$\begin{aligned} \bar{V}_C^{\text{rmf}} &= \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n} - \frac{3}{5}e^2 \sum_n \frac{Z-Z_n}{R} Z_n \\ &= \frac{3}{5}e^2 \frac{Z^2}{R} + \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n} - \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R}. \end{aligned} \quad (18)$$

The incorporation of the last term leads to a substantial lowering of the Coulomb energy of configurations with a low fragment multiplicity. This effect has been discussed in detail by Gross.[7]

A commonly employed approximation in condensed-matter problems was introduced in 1934 by Wigner and Seitz.[8] It is based on the fact that the Coulomb energy can be considered as composed of two terms, one associated with a primordial uniform charge distribution and another associated with the condensation of the individual fragments. The first term is simply the quantity V_C^0 introduced above. The approximation consist in replacing the exact condensation energy, or redistribution energy, by a sum of independent contributions from the individual fragments. Then, for each fragment separately, it is calculated how much the energy is increased when the charge in the neighborhood of the fragment is condensed to form the actual fragment. This redistribution process is considered as the shrinking of a uniform sphere from an original radius of R_n^0 to the actual fragment radius R_n . Since R_n^0 is the radius required to spread out the fragment charge to the primordial uniform density, it is given by $R_n^0 = (A_n/A)^{1/3}R$. Consequently, the Wigner-Seitz approximation can be written as

$$V_C^{\text{ws}} = \frac{3}{5}e^2 \frac{Z^2}{R} + \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n} - \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n^0}. \quad (19)$$

Although the Wigner-Seitz approximation is formally very similar to the refined mean-field approximation, the last term in the Wigner-Seitz formula is always larger, since the denominator contains R_n^0 rather than R , and, moreover, it has an additional $A_n^{1/3}$ dependence on the fragment size A_n . The Wigner-Seitz approximation has the advantage, relative to all other approximations we have investigated, that it readily can be applied to an infinite, or periodic, system, since its expression for the redistribution energy makes no reference to the overall size of the system.

After having defined the various approximations of particular interest, we turn now to the analysis of their validity. The results are best presented in a simple schematic model similar to the one considered in section 2. Thus, we consider N spherical fragments whose centers are randomly positioned within a sphere. It is convenient to write its radius as $R = \xi R_0$, where $R_0 = r_0 A^{1/3}$ is the radius of the corresponding compound nucleus. In order to gain some familiarity with the different expressions for the Coulomb energy, we first consider the simplest situation when all the N fragments in the system are equal. Then each fragment has mass $A_n = A/N$, charge $Z_n = eZ/N$, and radius $R_n = \xi^{-1} N^{-1/3} R$, and, moreover, $R_n^0 = N^{-1/3} R$. If the energies are expressed in units of V_C^0 , the entire problem is dimensionless, and we then readily find that the various approximations can be written as follows,

$$\begin{aligned}\bar{V}_C^{\text{mf}}/V_C^0 &= 1 + \xi N^{-2/3}, \\ \bar{V}_C^{\text{rmf}}/V_C^0 &= 1 + \xi N^{-2/3} - N^{-1}, \\ V_C^{\text{WS}}/V_C^0 &= 1 + \xi N^{-2/3} - N^{-2/3}.\end{aligned}\tag{20}$$

Figure 3 shows the resulting values as functions of the fragment multiplicity N , and for two different relative densities, ρ/ρ_0 .

In realistic situations the fragments are not all equal, and we therefore wish to test the approximations in systems with varying fragment sizes. The results for the random-mass system are included in figure 3. While the absolute values differ, the quality of the approximations is very similar to the case of equal masses.

The position-dependent approximate energies V_C^{mf} and V_C^{rmf} have also been calculated. In all cases they are quite close to their respective idealized mean values $\bar{V}_C^{\text{mf}}$ and $\bar{V}_C^{\text{rmf}}$.

Actual nuclei are not sharp spheres but have a finite surface diffuseness. Diffuse nuclei can be packed to the point where their central radii C touch, rather than their equivalent sharp radii R , before the nuclear incompressibility begins to manifest itself. For small nuclei the difference between R and C is larger, and so they can be packed closer than large nuclei. To investigate the quality of the approximations in such a scenario, we have reduced the hard-sphere radius from R_n to the central radius $C_n \approx R_n - b^2/R_n$. This change is of significance at high densities. It should also be noted, that equal hard spheres can only be packed up to a density of around half the saturation value. When the spheres have variable sizes they may be packed to a higher density, essentially by filling the gaps between the large fragments by smaller fragments. This feature is important for densities close to saturation.

These tests, and others, can be summarized as follows. As expected, the simple mean-field approximation (16) overestimates the energy considerably. Since the excess depends on the multiplicity, the discrepancy can not be removed by a simple redefinition of the energy, so in cases where the Coulomb energy is important this approximation is inadequate, as has been noted by Gross repeatedly.[7] The refined mean-field approximation is much better, particularly for small multiplicities. However, for intermediate multiplicities it can be significantly off, and it has a wrong multiplicity dependence at high densities. Therefore, caution should also be exercised when using this approximation.

The Wigner-Seitz approximation is generally superior to the above two, although it fails quantitatively at high densities, $\rho \sim \rho_0/2$, as might perhaps have been expected. For such densities there is a need for devising a better approximation.

A particularly simple, but generally quite useful approximation is the following

$$\bar{V}_C^* = \frac{3}{5}e^2 \sum_n \frac{Z_n^2}{R_n} - \frac{1}{2}e^2 \sum_n \frac{Z - Z_n}{\frac{5}{6}R + R_n} Z_n. \quad (21)$$

Relative to the refined mean-field approximation (18), the denominator in the second term has been modified. The first term of the denominator, $\frac{5}{6}R$, is the mean separation between two random points inside a sphere and leads to (18). (Strictly, $\frac{5}{6}R = 1 / \langle 1/r_{ij} \rangle$.) The second term, the fragment radius R_n , is the minimum distance from the considered fragment n to any other fragment. Thus the modified formula has more appealing limits and, consequently, it is somewhat more robust. The results of this approximation are included in figure 3.

It is possible to further refine the formula (21), for example to take account of the facts that the mean charge density generated by the fragments is diffuse and that the spatial distribution of the fragments depends on the temperature. We shall not discuss such additional refinements here.

4 Concluding remarks

In this paper, we have examined some commonly used approximations for the inclusion of interfragment forces in nuclear multifragment systems. The mutual exclusion of fragments brought about by the high nuclear incompressibility was approximated in terms of hard spheres and popular effective-volume approximations were tested. They were generally found to be fairly poor, and so a refined approximation was devised, based on the notion of independent fragment pairs. This “virial” approximation presents a considerable improvement which, moreover, is well represented by the corresponding one-body approximation (13). Therefore, we suggest that this approximation be adopted in one-body calculations of nuclear multifragment systems.

We also studied the Coulomb energy of multifragment systems confined within a sphere and tested the quality of various commonly used approximations. Generally, the simple mean-field approximation is fairly poor, and its refinement (replacing the

total charge by the residual charge) is considerably better. However, the Wigner-Seitz approximation, which is equally simple, is significantly better. We also devised a modified approximation (21), which is generally rather good, and in fact is superior to the Wigner-Seitz approximation for relatively dense configurations. It may therefore be preferable to employ this new approximation.

The work reported here establishes a firmer ground for employing one-body statistical models for nuclear multifragmentation, since we have demonstrated how the most important features of the interfragment forces can be approximated at this level. Our studies also show that unless such one-body approximations are made with care, the calculated results can be in significant error. It should also be remembered, that the nuclear interaction has been considered only in the hard-sphere idealization, which ignores all attraction and thus is expected to be inadequate for studies of phase transitions in subsaturation nuclear matter. Studies aimed at incorporating finite-range fragment interactions in one-body treatments are presently underway.[4]

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Figure 1: Effective volume for hard spheres

The effective κ -values as functions of the fragment multiplicity N , for equal or random hard spheres confined within a periodic cube, and for both a dilute ($\rho = \rho_0/16$) and a dense ($\rho = \rho_0/4$) scenario. The solid curve is the “exact” value κ_{eff}^N of eq. (6). Also shown are the results for the following approximations: κ_K (7) (— —), κ_{FR} (8) (— · —), the virial approximation (9) (— — —), and its one-body approximation $\bar{\kappa}$ based on (13) (· · · · ·). The multiplicity N is shown on a logarithmic scale. For large values of N , the effective volume approaches a limiting value, so in order to assess the quality of the approximations it is not necessary to consider systems with large N , which is a computational advantage.

Figure 2: Results in a “realistic” scenario

Results calculated with the simulation model developed in [2]. Shown is the mean fragment mass number $\bar{A}$ and the pressure P for $\tau = 8$ MeV, both as functions of the considered mean nucleon density ρ . The results were calculated on the basis of 4000 multifragment configurations sampled from periodic cubes containing 100 nucleons. The wiggles in the curves for P are indicative of the statistical error associated with these results. For higher temperatures, the fragment masses remain small up to higher densities and the different approximations therefore differ less from each other with regard to the mean fragment size. Moreover, for lower temperatures the system very quickly prefers to coalesce into large fragments and comparisons would be less informative.

Figure 3: Coulomb energy for uniformly charged spheres

This figure shows the Coulomb energy of N uniformly charged spheres of either equal or random masses; their centers are confined within a sphere of specified size. The solid curve is the exact result (3). Also shown are the following approximations: mean-field (16) (— -), refined mean-field (18) (— —), Wigner-Seitz (19) (- - -), and our improved approximation (21) (— - -).

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