Aspects of statistical model for multifragmentation

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We deal with two different aspects of an exactly soluble statistical model of fragmentation. First we show, using zero range force and finite temperature Thomas-Fermi theory, that a common link can be found between finite temperature mean field theory and the statistical fragmentation model. We show the latter naturally arises in the spinodal region. Next we show that although the exact statistical model is a canonical model and uses temperature, microcanonical results which use constant energy rather than constant temperature can also be obtained from the canonical model using saddle-point approximation. The methodology is extremely simple to implement and at least in all the examples studied in this work is very accurate. [S0556-2813(99)06512-7]

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I. INTRODUCTION

Recently we have presented a two-component statistical model of fragmentation to describe features of heavy ion collisions. The first study [1] was a one component model in which no distinction between neutrons and protons was made. In this model, large systems containing as many as 3000 particles could be studied. A first order transition could then be established in the thermodynamic limit. This has been further followed in later studies [2] where equations of state for finite number of particles were obtained, formal extensions to two kinds of particles and preliminary studies to make contact with a microcanonical treatment were made. More recently realistic calculations for ''caloric curves'' for finite nuclei were completed [3]. Calculations for populations of different isotopes seen in heavy ion reactions at the National Superconducting Cyclotron Laboratory at Michigan State University are nearly complete.

The advantage of this soluble statistical model (for brevity, we will call this SSM) is that it is simple to implement. Given the assumptions of the model which we state clearly in the next section, the canonical partition function of the system is calculated exactly (even if numerically). The model is extremely flexible. One can use as inputs experimental binding energies and excitation energies of nuclei. The numerical calculations are, in fact, simpler to carry out than grand canonical calculations which were initiated for Bevalac Physics [4]. Apart from the two practical applications just mentioned we foresee many uses of this model in the future.

The purpose of the present paper is to explore some other features of SSM. It is found that models of multifragmentation predict a peak in the specific heat when the disintegrating nuclear system has a temperature around 5 MeV [5,3]. This can be thought to be the remnant of a first order phase transition [1] as would be seen in a finite system. Indeed studies with a lattice gas model also suggest this [6]. However phase transition in nuclear matter in mean field theories indicated a critical temperature around 17 MeV. Although in finite nuclei this number would come down, signature of a phase transition at about 5 MeV seems too low for comfort (Experimental results do support a 5 MeV temperature [10]). Faced with this, it is pertinent to ask: is there any connection between mean field theory calculations and the SSM? Which one is ''better''?

In Secs. III, IV, and V we explore this question in detail and come up with the answer that it is indeed possible to find a link between the two. This link is most obvious if one uses the Skyrme interaction and finite temperature Thomas-Fermi theory. This link is then exploited to show that under conditions that are deemed to be appropriate for the disintegrating system, SSM is superior to mean field calculation. Free energy consideration will drive the system towards fragmentation, leading to a model very close to the SSM. While this does not explain why the mean field theory gives such a high critical temperature it does show that it is better to put faith in a SSM type of model.

Sections VI, VII, and VIII deal with another aspect of SSM. Since the canonical partition function is known exactly in the SSM, can we not, by suitable manipulations, also obtain results of the microcanonical ensemble, at least, approximately? This question was raised in an earlier paper [2] and the saddle-point approximation was suggested as a potential tool for such problems. Here we explore this in complete detail. We show that calculations are easy and as examples, compute inclusive cross sections for some isotopes and the total yield. The tests which we perform to check the accuracy of the saddle-point approximation suggest that the approximation gives very reliable estimates for a microcanonical calculation. This is extremely gratifying. We want to remind the reader that microcanonical calculations are very long because of two reasons: (1) the microcanonical phase space is difficult to compute for a general partition and (2) the number of partitions is so huge that summing over all possible partitions is impractical. Algorithms have been developed to do samplings of important parts of the phase space [8]. SSM avoids the difficult problem of computing the phase space and sums over all the partitions with the correct weight. The passage back to the microcanonical ensemble will be seen to be neither long nor tortuous.

II. THE SOLUBLE STATISTICAL MODEL

In this section, for completeness and later use, we present the details of the SSM. Assume that at the time of disinte-

gration the system can be characterized by a temperature T and a freeze-out volume $V_{\rm fr}$. The partition function of the system characterized by z protons and n neutrons is given by

$$Z_{z,n}=\sum \prod_{i,j} \frac{\omega_{i,j}^{n_{i,j}}}{n_{i,j}!}. \tag{2.1}$$

Here $n_{i,j}$ is the number of composites with proton number i and neutron number j and $\omega_{i,j}$ is the one particle partition function of this composite. The form of Eq. (2.1) is correct if interactions between different clusters are neglected or can be included in a mean field term. One obvious interaction between different clusters is that they cannot overlap with each other. We hope to take account of this approximately through an average excluded volume [see the discussion following Eq. (2.3)]. This would allow us to adopt the form of Eq. (2.1).

The sum in Eq. (2.1) runs over a huge number of partitions all of which must satisfy two constraints $\Sigma_{i,j} i n_{i,j}=z$ and $\Sigma_{i,j} j n_{i,j}=n$. These constraints would appear to make the computation of $Z_{z,n}$ prohibitively difficult (this is one reason why one works with a grand canonical ensemble), but a recursion relation makes the numerical computation of $Z_{z,n}$ quite easy, even for large z and n. Three equivalent recursion relations exist, any one of which could be used. For example, one such relation [7] is

$$Z_{z,n}=\frac{1}{z}\sum_{i=0}^{z}\sum_{j=0}^{n} i\omega_{i,j}Z_{z-i,n-j}. \tag{2.2}$$

Here $Z_{0,0}=1$. In present day computers the numerical value for typical values of z,n as would be encountered in heavy ion collisions can be computed in seconds.

All nuclear properties are contained in $\omega_{i,j}$. It is given by

$$\omega_{i,j}=\frac{V}{h^3}(2\pi mT)^{3/2}(i+j)^{3/2}\times q_{i,j_{\rm int}}. \tag{2.3}$$

Here V is the free volume within which the particles move; V is related to $V_{\rm fr}$=freeze-out volume. The relationship is through $V=V_{\rm fr}-V_{\rm ex}$ where $V_{\rm ex}$ is the excluded volume due to finite sizes of the composites. In reality, $V_{\rm ex}$ is not constant and depends upon multiplicity as well as sizes of objects (see Ref. [9] for a study of this). In the past the value of $V_{\rm ex}$ has often been taken to be V_0 where V_0 is the normal volume of a nucleus with mass number $(z+n)$. We will use this value but the precise value is quite unimportant for the discussions of what is to follow in latter sections. The quantity $q_{i,j_{\rm int}}$ is the internal partition function of the composite. It is given by

$$q_{i,j_{\rm int}}=\sum_k (2s_k+1)e^{-E_k/T}. \tag{2.4}$$

The average number of particles of a composite is given by

$$\langle n_{i,j}\rangle=\omega_{i,j}\frac{Z_{z-i,n-j}}{Z_{z,n}}. \tag{2.5}$$

The versatility of the model arises from the fact that many choices of $\omega_{i,j}$ in Eq. (2.1) can be made. We designate the simplest model as model 1.

In model 1 no distinction is made between neutrons and protons. A composite is characterized by only the mass number a. The composites have ground state energy $e_0 a+\sigma(T)a^{2/3}$. The first term is the volume energy with $e_0=-16$ MeV. The second term is the surface tension term taken (in keeping with Ref. [5]) to be temperature dependent: $\sigma(T)=\sigma_0[(T_c^2-T^2)/(T_c^2+T^2)]^{5/4}$ with $\sigma_0=18$ MeV and $T_c=18$ MeV. The intrinsic partition function in this model is

$$q_{a_{\rm int}}=\exp\left(\frac{e_0 a}{T}-\frac{\sigma a^{2/3}}{T}+\frac{Ta}{\epsilon_0}\right). \tag{2.6}$$

In Ref. [5] the numerical value of ϵ_0 is taken as 16 MeV and we use the same value here. The last term in the exponential arises from summing over excited states in a low temperature Fermi gas limit.

The generalization of Model 1 to a more realistic model with two kinds of particles is straightforward. The intrinsic partition function above gets modified to

$$q_{i,j_{\rm int}}=\exp\left[\frac{1}{T}\left(e_0(i+j)-\sigma(i+j)^{2/3}-\kappa\frac{i^2}{(i+j)^{1/3}}-s\frac{(j-i)^2}{(j+i)}+\frac{(i+j)T^2}{\epsilon_0}\right)\right], \tag{2.7}$$

where we have added parametrized terms for symmetry and Coulomb energies. Of course instead of this parametrized version of binding energies, one can use experimental binding energies from data tables and we will have occasion to do so in Sec. VIII.

We have described SSM. In the next section we will try to find a connection between SSM and mean field theory. The latter explores thermodynamic properties by assuming an underlying interaction and a uniform density but no fluctuations and hence no clusters. The two models seem very different with no obvious common ground. But a common link can be found.

III. FREE ENERGY IN DIFFERENT MODELS

In making preferences between different models we will compute free energies in different models. If two models have the same underlying Hamiltonian, the one which gives a lower free energy will be the favored one. In the statistical model which we outlined in the beginning, the canonical partition function is directly calculated and hence $F=E-TS=-T\ln Z_N$ (N being the total number of particles) is known. But we also want to consider mean field theories and the ones we will consider directly generate the grand partition function. In such cases we are constrained to calculate $E-TS$ from grand canonical ensemble with a chemical potential so chosen as to give the prescribed number of particles and assume this is indeed the result from a canonical ensemble as well. In the thermodynamic limit this is rigorously correct but since in the nuclear case the number of

nucleons is usually between 100 and 300, one needs to have an estimate of the corrections to relations which are exact only in the thermodynamic limit.

This estimate can be obtained by looking at the relation between $Z_{\rm can}$ and $Z_{\rm gr}$ for finite number of particles. Since $Z_{\rm gr}(\lambda)=\Sigma_N \exp(\lambda N) Z_N$, the following exact relationship holds:

$$Z_N = e^{(-\lambda_0 N)} \frac{1}{2\pi} \int_{-\pi}^{+\pi} e^{-i\lambda N} Z_{\rm gr}(\lambda_0 + i\lambda) d\lambda. \qquad (3.1)$$

The exact evaluation of this integral is very difficult so we attempt an approximate evaluation. The relationship implied in Eq. (3.1) is true for any value of λ_0 but we choose λ_0 such that the $-i\lambda N + \ln Z_{\rm gr}(\lambda_0 + i\lambda)$ maximizes at $\lambda = 0$. This means $\partial \ln Z_{\rm gr}(\lambda_0)/\partial \lambda_0 = \langle N \rangle$ where the system we want to study has exactly $\langle N \rangle$ nucleons. Expanding up to second order and assuming that the kernel falls off quickly one obtains the result

$$Z_{\langle N \rangle} = \exp(-\lambda_0 \langle N \rangle) \frac{Z_{\rm gr}(\lambda_0)}{\sqrt{2\pi (\partial^2/\partial^2 \lambda) \ln Z_{\rm gr}}}. \qquad (3.2)$$

This is of course the saddle-point approximation in one dimension. Later we will have occasion to use the saddle-point approximation in four dimensions. The reader will recognize that the second derivative of the log of the grand partition function is just the fluctuation in the number of particles:

$\partial^2 \ln Z_{\rm gr}/\partial^2 \lambda = \langle N^2 \rangle - \langle N \rangle^2$. Taking the logarithm of both the sides and multiplying by the temperature we get the equation

$$F = -T \ln Z_{\rm gr} + \mu \langle N \rangle + T \ln \sqrt{2\pi (\langle N^2 \rangle - \langle N \rangle^2)}, \qquad (3.3)$$

where we have written μN for $T\lambda_0 N$ to conform to the traditional way of writing the thermodynamic relation: $TS - E = pV - \mu N$ which corresponds to the above equation except for the last part which is an estimate of the correction due to finite number of particles.

We have looked at the correction in two models. One is the Fermi-gas model. Here for 140 particles at $\rho = 0.04$ fm^{-3} and 5 MeV temperature the estimate to the correction to free energy per particle is only 0.105 MeV. This has no consequence in the discussion that we will pursue in the next section. At $\rho = 0.1$ fm^{-3} the correction at the same temperature is 0.098 MeV. Let us now consider model 1 of SSM. Here we know the exact value of F/N, but we can also solve the same problem in the grand canonical ensemble, then use Eq. (3.3) to get F/N for 140 particles with or without the estimate of finite number correction. At temperature 5 MeV the exact answer is -15.08 MeV, the thermodynamic answer is -15.22 MeV and including the finite number correction it is -15.01 MeV. We therefore know the limits of the accuracy of our predictions when we try to get the free energy from a grand canonical calculation.

IV. INSTABILITY TOWARDS FRAGMENTATION

Skyrme type of interaction has been used to explore the p-V diagram and to locate the critical point of nuclear matter. The critical point was calculated to be around 17 MeV. Experimentally, interesting features appear to emerge around 5 MeV. Although precise extraction of caloric curves from experiments is very hard, evidence is that interesting things happen around 5 MeV and not beyond. What is also intriguing is that models of fragmentation, although often quite schematic, find that the peak in specific heat should appear around 5 MeV. This, for example, is true in the lattice gas model. What we can readily show is that the Skyrme mean field theory, which predicts a high value of T_c cannot be trusted at low temperature and low density. The system is unstable towards fragmentation in this regime.

We take the potential energy density to be of the form

$$W(\rho) = \frac{A_t}{2} \frac{\rho^2}{\rho_0} + \frac{B_r}{\sigma + 1} \frac{\rho^{\sigma+1}}{\rho_0^\sigma}. \qquad (4.1)$$

The one body potential that a particle feels is

$$U(\rho) = A_t \frac{\rho}{\rho_0} + B_r \left(\frac{\rho}{\rho_0} \right)^\sigma. \qquad (4.2)$$

In the above ρ_0 is a constant taken here to be 0.16 fm^{-3}. The constants A_t, B_r, and σ can be set to give the saturation density, the binding energy per particle and the compressibility. We have chosen two sets of values $A_t = -356.8$ MeV, $B_r = 303.9$ MeV, $\sigma = 7/6$ which give a saturation density of 0.16 fm^{-3}, binding energy per particle of 16 MeV and compressibility $K = 201$ MeV. The other set is $A_t = -123.03$ MeV, $B_r = 70.135$ MeV, and $\sigma = 2$. The second set gives the same saturation density and binding energy but a higher compressibility of $K = 377$ MeV. The first will be referred to as a soft equation of state and the second as a hard equation of state. There is strong evidence that a soft but momentum dependent equation of state is more appropriate but we will not consider this complication here.

Consider now the following scenario. The relevant region is $\rho < \rho_0$. We put $\rho = 0.04$ as a typical freeze-out density. In mean field theory a large nucleus is stretched so that density at every point is ρ. But it may be easier for this large blob to break up instead into two blobs, each with normal density. We ought to compute free energies for the two situations. In the second situation there is also the possibility of relative motion of the two blobs but this is just three degrees of freedom compared to $3N$ so we neglect this. (The inclusion anyway strengthens our argument.) Therefore what we need to consider is free energy per particle in the two situations. Now free energy per particle in the Skyrme interaction is easy to compute. It is given by $e_0 + e^* - Ts$ where $e_0 = \frac{3}{5}\epsilon_F + (A_t/2)(\rho/\rho_0) + [B_r/(\sigma+1)]\rho/\rho_0)^\sigma$; e^* and s are excitation energy and entropy per particle respectively. The quantity $e^* - Ts$ (its approximate value at low temperature is the well-known expression $-\pi^2 T^2/4\epsilon_F$) is easily obtained from numerical integration of Fermi integrals.

We find that for the soft equation of state at $\rho=0.04$, the free energy for two blobs with normal density has a lower value than the uniform low density situation until temperatures of about 11 MeV. Break up into two blobs of normal density continues to be the preferred situation for the hard equation of state until an even higher temperature: about 13.5 MeV. This is expected. For a hard equation of state it should be harder to stretch nuclei to lower density. It therefore follows that it is better to discard the mean field theory at low temperature and density. This however is the range which is most interesting for experiments.

But then if it is more advantageous to break the system into two blobs with normal density why should it not break up also in three or more blobs? Allowing for all sizes of fragments can only lower the free energy. This of course directly takes us into the statistical model of fragmentation. We will see in the next section that Skyrme type interaction and Thomas-Fermi theory takes us uniquely to a specific model of fragmentation.

V. FRAGMENTATION IN THOMAS-FERMI THEORY WITH ZERO-RANGE FORCES

Thomas-Fermi theory with Skyrme interactions of the above type has the following features for all nuclei, big or small. The density is ρ_0 throughout the volume of the nucleus. The ground state energy is $e_0\times a$ where e_0, with the choices of force parameters of the previous section, is -16 MeV and a is the number of nucleons in the nucleus. There is no surface tension term. Of course if we treat the Skyrme interaction in quantum mechanics, each nucleus needs to be treated separately and this universal feature will disappear. A diffuse surface will appear with the accompaniment of a surface tension like term in the energy. This is also true even in Thomas-Fermi theory if instead of zero range forces a finite range force is used as is usually the case.

Returning however to the Thomas-Fermi approximation for zero range forces, the intrinsic partition function of a composite of a nucleons with Skyrme force of the above type is

$$q_{a_{\rm int}}=\exp\left(\frac{-e_0a+a(Ts-e^*)}{T}\right). \tag{5.1}$$

If we replace $Ts-e^*$ by the low temperature expansion $\pi^2T^2/4\epsilon_F$ we see that we have recovered model 1 of SSM (see Sec. II) for fragmentation except for the surface tension term. Of course the surface tension term is very important and is crucial for interesting features such as the appearance of a maximum in specific heat. We may put it in by hand, as something which is essential for getting the correct physics but for the moment let us follow the Thomas-Fermi prescription with Skyrme interaction and compare the free energies for the two scenarios: (1) soft equation of state and uniformly low density mean field theory and (2) fragmentation model where each fragment appears as a normal density composite with the intrinsic partition function given by Thomas-Fermi theory, namely, that of Eq. (5.1). In the mean field model at temperature 5 MeV, $\rho=0.04$ fm^{-3} the free energy per particle is -11.91 MeV. For 140 particles in the second case at the same temperature, the free energy per particle is -21.55 MeV. If we now add a temperature dependent surface tension as in model 1 the free energy per particle rises to -15.18 MeV. If we keep the surface tension coefficient fixed at 18.0 MeV [$\sigma(T)=\sigma(0)=18.0$ MeV] this number becomes -14.55 MeV.

Model 1 can be regarded as a low temperature expansion of Eq. (5.1) to which a surface tension term has been added. Numerically, $\pi^2T^2/4\epsilon_F$ reduces to $(T^2/14.95)$ MeV for ϵ_F corresponding to normal nuclear density of 0.16 fm^{-3}. The value $(T^2/16)$ MeV is used in model 1. In model 1 free energy per particle at $\rho=0.04$ fm^{-3} and temperature 5 MeV is -15.08 MeV. To summarize, in the spinodal region, Skyrme type of interaction coupled with a finite temperature Thomas-Fermi theory, naturally leads to a model of fragmentation very similar to the statistical model of fragmentation.

VI. CONTACT WITH MICROCANONICAL ENSEMBLE

We now come to the second part of our investigation as posed in the Introduction: since we can calculate the value of the canonical partition function exactly and since the canonical partition function is a Laplace transform of microcanonical phase space, can we also, by suitably manipulating canonical results, obtain results of microcanonical calculation, at least, approximately? One might argue that a constant total energy E rather than constant T describes the heavy ion situation. This need not be completely correct. There is usually pre-equilibrium emission and presumably equilibrium statistical mechanics such as we described above happens after such pre-equilibrium emission. The same amount of energy need not be carried away in pre-equilibrium emission in every event.

Microcanonical calculations require evaluation of phase spaces. We will require two types of phase space integrals. Let us introduce some abbreviations. A composite is characterized by two indices: $i=$number of protons in the composite and $j=$number of neutrons in the composite. Let us write $a=(i,j)$. Then the basic integral of microcanonical ensemble (in which interactions between different particles are neglected although the particles are allowed to be in intrinsic excited states) is

$$\mathcal{D}=\sum_{n_a}\left(\frac{V}{h^3}\right)^M\Pi_a\frac{(2s_a+1)^{n_a}}{n_a!}\int\delta\left[E-\sum_{j=1}^{M}\epsilon_j(p_j)\right]\times\delta\left(\vec{P}-\sum_{j=1}^{M}\vec{p}_j\right)\times\delta_{z,\Sigma in_a}\delta_{n,\Sigma jn_a}\prod_{j=1}^{M}d^3p_j. \tag{6.1}$$

Here $\Sigma_a n_a=M$ is the multiplicity. We will call this $\mathcal{D}=g(E,\vec{P},z,n)$ meaning it is related to the phase space for a system which has z protons, n neutrons, total energy E and total momentum $\vec{P}$. For a general case it is extremely difficult to calculate $g(E,\vec{P},z,n)$. The reason is $\epsilon_j=-(B\cdot E)_j+p_j^2/2m_j$ and m_j is different for each composite. Here $(B\cdot E)_j$ stands for the binding energy of the jth particle. Analytic solutions when there are only two different masses

were obtained in Ref. [11]. Without an analytic solution where contributions from different composites factor out, the huge sum in the above equation is impractical to carry out.

We do the following trick to evaluate the phase-space integral. We use the Laplace transform on $E,\vec{P}$ with the transformed variables $\beta,\vec{q}$. This gives us the canonical partition function which we know how to evaluate exactly (even if it is numerical). The Laplace inversion problem is then done by the saddle-point method. Generating an approximate microcanonical result from a grand canonical calculation was done in Ref. [12]. There, the objective was to estimate the error introduced by the use of the grand canonical ensemble to study systems which had finite number of particles.

Writing then

$$Z_{z,n}(\beta,\vec{q})=\int dE\int d^3P g(E,\vec{P},z,n)e^{-\beta E-\vec{q}\cdot\vec{P}},$$

we get

$$Z_{z,n}(\beta,\vec{q})=\sum_{n_a}\prod\left(\frac{V}{h^3}\right)^{n_a}\frac{(2s_a+1)^{n_a}}{n_a!}\times\prod_{j=1}^{M}\int\exp\left(-\beta\sum\epsilon_j-\vec{q}\cdot\sum\vec{p}_j\right)d^3p_j. \tag{6.2}$$

The reader will recognize that except for the term $\vec{q}\cdot\Sigma\vec{p}_j$ the above equation defines the usual partition function. Indeed, the relationship is very simple: $Z_{z,n}(\beta,\vec{q})=Z_{z,n}(\beta)e^{m_A q^2/(2\beta)}$ where m_A is the mass of the whole system.

The relationship between $g(E,\vec{P},z,n)$ and $Z(\beta,\vec{q})$ is given by

$$g(E,\vec{P},z,n)=\exp(\beta_0 E+\vec{q}_0\cdot\vec{P})\frac{1}{(2\pi)^4}\int e^{i\beta E+i\vec{P}\cdot\vec{q}}\times Z_{z,n}(\beta_0+i\beta,\vec{q}_0+i\vec{q})d\beta d^3q. \tag{6.3}$$

This is an exact relationship valid for any β_0 and $\vec{q}_0$ but in order to evaluate the integral in the saddle-point approximation we will choose particular values. We rewrite the kernel of the above equation as $\exp[i\beta E+i\vec{P}\cdot\vec{q}+\ln Z_{z,n}(\beta_0+i\beta,\vec{q}_0+i\vec{q})]$, choose the value of β_0 and $\vec{q}_0$ such that the argument in the exponential maximizes at $\beta=0$ and $\vec{q}=0$. This leads to

$$E=-\frac{\partial\ln Z_{z,n}(\beta_0,\vec{q}_0)}{\partial\beta_0}. \tag{6.4}$$

Given E this determines β_0. The other quantity $\vec{q}_0$ is determined by

$$\vec{P}=-\vec{\nabla}_{q_0}\ln Z_{z,n}(\beta_0,\vec{q}_0). \tag{6.5}$$

This last equation is particularly simple and leads to $\vec{q}_0=-\beta\vec{P}/m_A$. The argument in the exponential is now expanded to second order in a Taylor series about the saddle point. Once the Taylor expansion is truncated at second order, the integrations can be done analytically since they involve only Gaussians. Thus, $g(E,\vec{P},z,n)$ in the saddle-point approximation is given by

$$g_{\rm sp}(E,\vec{P},z,n)=\frac{Z_{z,n}(\beta_0)}{(\sqrt{2\pi})^4|\det|^{1/2}}e^{\beta_0 E-\beta_0 P^2/2m_A}. \tag{6.6}$$

The value of the determinant is $(m_A/\beta)^3(\partial^2/\partial^2\beta)\ln Z$. For completeness the matrix is explicitly given in the Appendix.

VII. INCLUSIVE CROSS SECTION

As the simplest example we will consider the inclusive cross section of a given species b where b stands for proton and neutron labels k,l. In the canonical description the inclusive cross section must turn out to be Maxwellian but nonetheless to show correspondence with microcanonical procedure we will derive this as a ratio of two partition functions. Thus

$$\frac{d^3n_a}{d^3p_b}(\vec{p}_b)=\frac{Z_{z,n}(\beta,\vec{p}_b)}{Z_{z,n}(\beta)}, \tag{7.1}$$

where $Z_{z,n}(\beta)$ is the standard canonical partition function and $Z_{z,n}(\beta,\vec{p}_b)$ is given by

$$Z_{z,n}(\beta,\vec{p}_b)=\sum n_b\frac{1}{n_b!}\left[\frac{V}{h^3}(2s_b+1)e^{-\beta p_b^2/2m_b}q_{b_{\rm int}}\right]\times\left[\frac{V}{h^3}(2s_b+1)(2\pi m_a T)^{3/2}q_{b_{\rm int}}\right]^{n_b-1}\prod_{k\neq b}\frac{\omega_k^{n_k}}{n_k!}. \tag{7.2}$$

The various terms in Eq. (7.2) arise because in a partition which has n_b particles of type b, any one of them could be in the infinitesimal volume d^3p_b around $\vec{p}_b$. With slight manipulation Eq. (7.1) can be recast to the form

$$\frac{d^3n_b}{d^3p_b}(\vec{p}_b)=\langle n_b\rangle\frac{\exp^{-\beta p_b^2/2m_b}}{(2\pi m_b T)^{3/2}}, \tag{7.3}$$

which is indeed the form one would have expected *a priori*.

The corresponding inclusive cross section in the microcanonical ensemble is also a ratio, the denominator being the quantity $\mathcal{D}$ of Eq. (6.1) with $\vec{P}=0$. (The calculation is done in the c.m. frame.) The numerator is given by

TABLE I. $T_{\rm eff}$ for ^{6}Li and ^{20}Ne calculated for different combinations of incident protons and neutrons.The energy was chosen such that Eq. (6.4) would give a temperature of 6 MeV.

z	n	^{6}Li	^{20}Ne
39	46	5.50940	4.97317
54	68	5.65563	5.26758
77	100	5.76246	5.49141

$$\mathcal{N}=\sum n_b\left(\frac{V}{h^3}\right)^M\prod\frac{(2s_i+1)^{n_i}}{n_i!}\int\delta\Bigg(E-\epsilon_b(p_b)-\sum_{j=1}^{M-1}\epsilon_j(p_j)\Bigg)\delta\Bigg(\vec{p}_b+\sum_{j=1}^{M-1}\vec{p}_j\Bigg)\delta_{z,\Sigma in_i}\delta_{n,\Sigma jn_i}\prod_{j=1}^{M-1}d^3p_j. \tag{7.4}$$

The numerator can be written as

$$\mathcal{N}=\frac{V}{h^3}(2s_b+1)g(E-\epsilon_b,-\vec{p}_b,z-k,n-l). \tag{7.5}$$

The phase-space factor indicated above can also be calculated by saddle-point approximation as before. We can write down by inspection of Eq. (6.6).

$$g_{\rm sp}(E-\epsilon_b,-\vec{p}_b,z-k,n-l)=\frac{Z_{z-k,n-l}(\beta_0')}{(\sqrt{2\pi})^4|\det'|^{1/2}}\exp\{\beta_0'[(E-\epsilon_b)-p_b^2/2m_{(A-b)}]\}. \tag{7.6}$$

Of course the corresponding changes to Eqs. (6.4) and (6.5) need to be implemented: for example, Eq. (6.4) leads to

$$E-\epsilon_b=-\frac{\partial\ln Z_{z-k,n-l}(\beta_0',\vec{q}_0')}{\partial\beta_0'}. \tag{7.7}$$

It is interesting to write this out in detail: putting in the appropriate factors one obtains

$$E-\epsilon_b=-\frac{\partial\ln Z_{z-k,n-l}(\beta_0')}{\partial\beta_0'}+p_b^2/2m_{A-b}. \tag{7.8}$$

The left hand side of the above equation shows that the system with proton number $z-k$ and neutron number $n-l$ has energy $E-\epsilon_b$ because a particle left with energy ϵ_b. The right hand side of this equation shows that part of this energy is taken by the recoil of the system.

Let us consider under what circumstances the ratio $\mathcal{N}/\mathcal{D}$ can approximate Eq. (7.3). Assume that the difference in the values of β_0 and β_0' is negligible. Remembering that ϵ_b contains both the binding energy and the kinetic energy $p_b^2/2m_b$ the ratio becomes the right hand side of Eq. (7.3) except for an attenuating factor $e^{-\beta_0'p_b^2/2m_{A-b}}$. Unless p_b is very large, this attenuating factor is simply unity. This attenuating factor is very reasonable and will cut down on the inclusive cross-section at very high momentum causing a deviation from Maxwell-Boltzmann distribution.

As examples, we calculated inclusive spectra of ^{6}Li and ^{20}Ne using the saddle-point approximation where the disintegrating systems have total proton and total neutron numbers (39,46), (54,68), and (77,100) (Table I). These numbers are somewhat arbitrary but they approximate typical target + projectile combinations. The binding energies have been taken from data tables. The other input is the total energy E of Eqs. (6.1) and (7.4) which was chosen such that the temperature in a canonical calculation would be exactly 6 MeV. We can now ask if the microcanonical calculation of inclusive spectrum (as obtained in the saddle-point approximation) gives an approximate Maxwell-Boltzmann distribution with a temperature and if so what these values are for the two isotopes. We find that for both the isotopes, for $p_b^2/2m$ up to about 50 MeV, the slopes are remarkably Maxwellian. But the deduced temperatures are different for the two isotopes. The difference between the two temperatures decreases as the size of the disintegrating system increases. For the system (39,46) the apparent temperature of Ne is about 0.5 MeV lower than that of Li. This difference is not large enough to be readily recognized in experiments. For kinetic energy bigger than 50 MeV the inclusive spectrum begins to fall off faster than Maxwell-Boltzmann: one is exploring the edges of the phase space. By integrating over d^3n_b/d^3p_b we can obtain the total inclusive cross section. This can then be compared vis-a-vis the canonical predictions (Table II). For ^{6}Li the answers are basically indistinguishable between the two predictions for all the three systems. The differences are bigger for the case of ^{20}Ne. Once again, the differences between the predictions of the two models diminish as the system size grows. So we can conclude here that the canonical approximation of the yields is a reasonable one, provided the nucleus being considered is small compared to the system size.

TABLE II. Yields of ^{6}Li and ^{20}Ne calculated for different combinations of incident protons and neutrons using both canonical and microcanonical ensembles.

		^{6}Li		^{20}Ne	
z	n	Microcanonical	Canonical	Microcanonical	Canonical
39	46	0.106049	0.105507	2.98717×10^{-5}	4.89115×10^{-5}
54	68	0.134853	0.134352	3.74479×10^{-5}	4.87270×10^{-5}
77	100	0.182369	0.182158	5.07698×10^{-5}	5.93936×10^{-5}

VIII. ACCURACY OF THE SADDLE-POINT APPROXIMATION

In this section we quantitatively estimate the accuracy of the saddle-point approximation for inclusive cross sections for soluble cases where the exact microcanonical answer is formally easily calculable. We require the ratio of two integrals given by Eqs. (7.4) and (6.1). Consider the phase space integral of Eq. (6.1) for $\vec{P}=0$. We consider two kinds of particles with masses M and M/α (These could be nucleons and deuterons with $\alpha=1/2$.) For brevity only, we suppress the V/h^3 term, the factorials and the spin factors. Instead of summing over all possible partitions implied in Eq. (6.1) we consider only one partition: n_1 particles of mass M and n_2 particles of mass M/α. All binding energy factors can then be reabsorbed into E. The value of the integral $\int \delta[E-\Sigma_{i=1}^{n_1} p_i^2/2m-\Sigma_{i=1}^{n_2}\alpha p_i^2/2m]\Pi_{j=1}^{n} d^3p_j$ (here $n=n_1+n_2$) can be found in the appendix of [11]. It is given by

$$I_{\rm exact}^{\rm den}=\frac{1}{[\alpha^{n_2-1}(n_1\alpha+n_2)]^{3/2}}\ \frac{(2\pi M)^{3/2}(n-1)}{\Gamma[3/2(n-1)]}\ E^{(3n-5)/2}. \tag{8.1}$$

The same integral in saddle-point approximation gives

$$I_{\rm sp}^{\rm den}=\frac{9}{4\sqrt{2\pi}}\ \frac{\exp[(3/2)n]n^2}{[(\alpha^{n_2-1}(n_1\alpha+n_2)]^{3/2}}\left(\frac{2}{3n}\right)^{(3/2)/n} \times(2\pi M)^{(3/2)(n-1)}\ E^{(3n-5)/2}. \tag{8.2}$$

Notice that the E dependence in both the equations are identical and Eq. (8.2) is related to Eq. (8.1) by Stirling type approximation. For $n_1+n_2=141$ we found $I_{\rm exact}/I_{\rm sp}=0.991$. As we will see below, calculation of observables require ratios of two phase spaces which then is likely to be even more accurate.

To compare the inclusive spectra of the nucleus of mass M/α, we need to calculate the integral appearing in Eq. (7.4) for this specific case. The exact result is given by (again using the appendix of Ref. [11])

$$I_{\rm exact}^{\rm num}=\frac{1}{[\alpha^{n_2-2}(n_1\alpha+n_2-1)]^{3/2}}\ \frac{(2\pi M)^{(3/2)(n-2)}}{\Gamma[3/2(n-2)]} \times E'^{(3n/2)-4}\left(1-\frac{1}{(n_1\alpha+n_2-1)}\ \frac{\alpha p^2}{2ME'}\right)^{(3n/2)-4}, \tag{8.3}$$

where $E'=E-\alpha p^2/2M$. The saddle-point approximation gives

$$I_{\rm sp}^{\rm num}=\frac{9}{4\sqrt{2\pi}}\ \frac{\exp[(3/2)(n-1)](n-1)^2}{[\alpha^{n_2-2}(n_1\alpha+n_2-1)]^{(3/2)}}\left(\frac{2}{3(n-1)}\right)^{(3/2)(n-1)} \times(2\pi M)^{(3/2)(n-2)}\ E'^{(3n/2)-4} \times\exp\left(-\frac{3}{2}\ \frac{n-1}{n_1\alpha+n_2-1}\ \frac{\alpha p^2}{2ME'}\right). \tag{8.4}$$

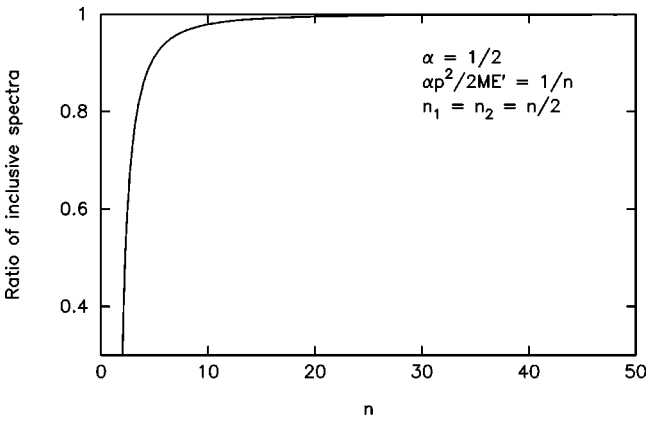

FIG. 1. We plot the ratio of inclusive cross sections calculated exactly to that calculated by the saddle-point approximation. The particle has mass M/α (see text). The value of the kinetic energy of the particle is approximately the average energy of the disintegrating system, i.e., $\alpha p^2/(2ME')=1/n$. We study the value of the ratio as the total number of particle $n=n_1+n_2$ varies. Here $n_1=n_2$ and $\alpha=1/2$.

The ratio of the inclusive spectra for the two cases can then be calculated using Eqs. (8.1), (8.2), (8.3), and (8.4). The value of the same is computed assuming $n_1=n_2=n/2$ and $\alpha=1/2$. Figure 1 shows the variation in this ratio with n for $\alpha p^2/2ME'=1/n$ which is approximately the average system energy. Figure 2 shows the variation in the ratio of the two spectra with varying $\alpha p^2/2ME'$ for $n=122$. In both cases the ratio is close to one thereby showing that the saddle-point approximation is a very reliable one.

IX. SUMMARY AND DISCUSSION

We investigated two aspects of the statistical model of fragmentation in this work. One was to try to establish a contact with a model where the thermodynamic properties are investigated in a finite temperature mean field theory. A contact can be established in finite temperature Thomas-Fermi theory if the underlying interaction is a zero range

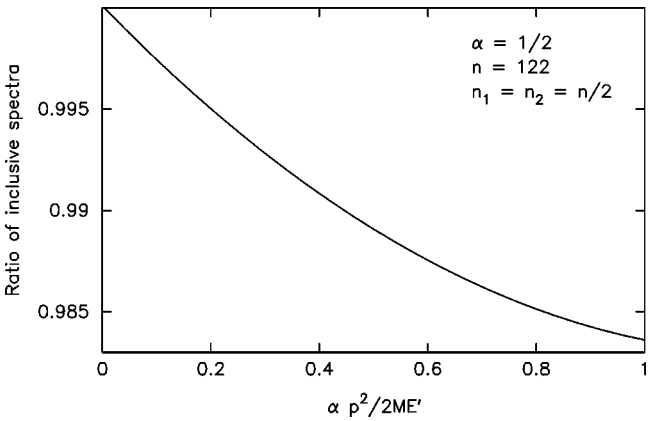

FIG. 2. Here we plot the same ratio as in Fig. 1 but as a function of the ratio of the kinetic energy of the emitted particle to that of the residual system. The total number of particles $n=122$. $n_1=n_2$ and $\alpha=1/2$ (see text).

force. In Skyrme force at densities and temperature thought to be pertinent to disassembly of hot nuclei, the statistical model has a free energy lower than the mean field theory model. Hence, it is the favored model.

We then investigated another aspect. Since the canonical partition function is known exactly in the statistical model we tried the saddle-point approximation to calculate observables in the microcanonical ensemble. Direct calculations in the microcanonical ensemble are very long. Saddle-point approximation is simple and quick and where we could compare saddle-point results with exact phase space calculations, the agreements were remarkably close. It is possible that the approximation fails at true phase transitions. However, because in the nuclear case the number of particles is not too large we do not think this can cause a problem. Some differences between canonical and microcanonical (as seen by the saddle-point approximation) were noticed, specially when very energetic particles are emitted or when the emitting systems are small. But for most purposes the difference between canonical and microcanonical ensemble results are small, often too small to be detected. A very comprehensive study of microcanonical ensembles for nuclear disassembly can be found in Ref. [13], and references therein.

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APPENDIX

We use rectangular coordinates. The elements of the 4×4 determinant can be denoted by $a_{i,j}$. For brevity, we drop the subscripts in β_0 and $\vec{q}_0$. Without loss of generality we take the direction of $\vec{q}$ to be the x direction. Then $a_{1,1}=\partial^2 \ln Z(\beta,\vec{q})/\partial^2\beta+m_A q^2/\beta^3$. Other nonzero elements are $a_{1,2}=a_{2,1}=-m_A q_x/\beta^2; a_{2,2}=a_{3,3}=a_{4,4}=m_A/\beta$.

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