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Mean-field study of the nuclear partition function: application to level density and compound nucleus fission

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Functional integral formulation of the mean-field approximation for many-body systems is used to study the nuclear partition function. Both static and dynamic mean-field solutions with statistical occupations of the single particle wave functions are discussed. These correspond to different physical processes in the nuclear system. In the static case the effect of mean-field fluctuations on the nuclear level density is exhibited. This effect enters consistently along with the usual effects of temperature and chemical potential fluctuations. Together they account for generalized random phase approximation correlations and produce bosonlike terms in the nuclear entropy. Because of the self-consistency of the approach, no overcounting of the collective and single-particle degrees of freedom occurs. The effects of the single particle continuum are included in the discussion. Consequences of a possible multiplicity of static mean-field configurations are briefly discussed. Dynamical mean-field solutions are considered in relation to compound nucleus fission. They provide the extension of the mean-field description of spontaneous fission given recently. A microscopic expression for the energy dependence of the average fission width is presented. It combines both the dynamical and statistical features of the tunneling mean-field solution in the subbarrier region.

NUCLEAR STRUCTURE, FISSION Static and dynamic mean field with statistical occupations, level density, RPA correlations, bosonlike terms in the nuclear entropy, single-particle continuum, mean-field equations for compound nucleus fission.

I. INTRODUCTION

Considerable interest has recently been focused on investigating the capabilities of the dynamical mean-field approximation for the description of large scale nuclear phenomena. This interest is mainly connected with the realization that the functional integral method developed in statistical physics and quantum field theory provides an excellent framework for the discussion of the dynamics of the nuclear many-body system. The flexibility of the method is reflected already in the variety of different functional integral expressions one can select as a suitable starting point.

The possibilities begin with the original Feynman path integral[1] over coordinate trajectories, which is appropriate for the purpose of the conventional semiclassical analysis of problems with few phenomenologically selected degrees of freedom.[2-4] A more general type involves path integrals over field variables, which in the fermion case are anticommuting c numbers. This was first introduced into nuclear physics in relation to the so-called nuclear field theory.[5] Yet another kind of functional integral follows the exact propagation of the many-body system as an integral of propagations in a fluctuating one-body field.[6] Finally, the coherent state formulation of path integrals has recently been extended to the fermion many-body systems in a number of studies[7-9] as a functional integral over determinantal wave functions.

The functional integral method has proved to be a very useful approach in the analysis of dynamical mean-field approximations. In a previous work[6] the

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mean-field equations for a transition amplitude were derived. They were extended in Ref. 10, which represents a first step toward a functional integral mean-field theory of the nuclear S matrix, discussed from a different point of view in Ref. 11. The time dependent Hartree-Fock (TDHF) description of large amplitude nuclear motions in bound states was presented in Refs. 12–14 and finally, the mean-field equations for tunneling and spontaneous fission were derived in Refs. 15 and 16.

The present work is a continuation of the study of the functional integral mean-field approximation based on the fluctuating one-body field representation of Ref. 6. At the moment, this particular form of the functional integral seems to provide the shortest way of getting mean-field results. However, it has a disadvantage in that the exchange terms in the self-consistent potential arise only in a more complicated formulation discussed, for instance, in Ref. 13. Another formulation in which the exchange terms appear in a more natural way is presumably provided by determinantal functional integrals.[7–9] Their understanding, however, is still not entirely clear and further investigation of their properties is now under way.

In these circumstances we use the simple form of Ref. 6 and essentially work with Hartree rather than Hartree-Fock mean fields. Our results, however, in most cases are of such a nature that there is little doubt how they should be modified in order to include the exchange terms. This amounts to replacing the matrix elements of a two-body interaction V_{ijkl} by its antisymmetrized counterpart $V^A_{ijkl} = V_{ijkl} - V_{ijlk}$. A complete exposition of this aspect based on a particularly simple modification of the fluctuating one-body field formulation will be published elsewhere.[17] Eventually, the pairing should also be considered.

The general purpose of this work is to introduce statistical averages in the dynamical mean-field equations, such that the theory will still retain the one-body self-consistent potentials but will not be limited to an evolution of Slater determinants. We are particularly interested in the generalization of the spontaneous fission theory of Ref. 15 to the description of induced fission. By the latter we mean the fission of a compound nucleus, which is characterized by a given excitation energy and total angular momentum. Although it is, in principle, possible to use the theory of Ref. 15 for the calculation of the partial fission widths of all the nuclear states over which the compound nucleus is distributed, this way is not only intractable in practice but is probably conceptually incorrect in view of the average nature of the mean-field description. One needs instead a new type of theory with statistical averaging built into the equations.

For the description of the compound nucleus itself such a theory has been known for some time.[18–21] It is a temperature-dependent generalization of the static Hartree-Fock method. The conventional discussion[19] employs the variational principle for a free energy with the result that the self-consistent potential is determined by the one-body density given as a sum over single-particle states with statistical occupation numbers. The effective temperature is determined by the requirement that the average excitation energy is equal to a given energy of a compound nucleus.

We start in Sec. II by showing that this static theory is contained in the functional integral formulation of the mean field. We do work with the grand-canonical partition function. However, it should be emphasized that this does not imply that we assume that the nuclear system is in actual contact with a heat bath which has a real temperature and chemical potential. As is well known, the partition function is the natural object to study in order to extract average information about various physical quantities from a functional integral. The temperature and chemical potential will be seen as parameters which facilitate the average over the irrelevant degrees of freedom. Their mean values will be fixed by the energy and the particle number (cf. Secs. IV and V). All this is standard and we mention it only in order to avoid a possible misunderstanding.

Discussing the static mean field in Sec. II, we point out that there should be a multiplicity of the mean-field configurations corresponding to different local minima of the nuclear free energy as a function of deformation, and that the contribution of all these minima should be included in the partition function. In our picture these minima do not correspond to Slater determinants of the excited states which become lower in energy than the ground state as the deformation increases.[22] In the mean field with statistical occupations these are all mixed together and their effect is accounted for by the effective temperature. We expect that the higher local minima appearing in the free energy will correspond to a geometry of the mean field which is very different from the ground state.

Already, in the discussion of the static limit, it becomes clear that dynamical configurations of the mean field should also arise. In the functional integral for the partition function the fluctuating one-body field depends not only on space variables but also on the time parameter. This is a quantum mechanical effect and as a consequence one should expect dynamical mean-field configurations in the situations where quantum fluctuations of the field are important. In Sec. III we discuss the simplest implication of such fluctuations around the static mean-field solution. Working in harmonic limit we calculate appropriate corrections to the zero order partition function. These correspond to so-called one-loop corrections in the loop expansion and in the conventional language of nuclear physics represent the effect of the residual interaction in terms of random-phase approximation (RPA) correlations. One-loop corrections to a mean field were already discussed in Ref. 14, a preprint of which we received when the present work was completed. The difference in our result is that the frequencies of the eigenmodes of the harmonic fluctuations are determined not by ordinary RPA equations but by using a more general form[19] suitable for finite temperatures. This difference is due to the mean-field equations with statistical averages over all Slater determinants as opposed to the separate treatment of each determinant in Ref. 14. Our result is for the averaged free energy, whereas Ref. 14 dealt with corrections to energies of isolated bound states.

In Sec. IV we start the discussion of the microcanonical partition function, i.e., the level density. In order to define this quantity for the compound nucleus one should separate the appropriate mean-field configurations. The additive nature of the saddle point approximation is very useful in this respect. We discuss the role of the single-particle continuum states in relation to the nucleon gas of evaporated nucleons in equilibrium with the compound nucleus. We indicate the proper subtraction procedure which generalizes the treatment of Ref. 23 and provides a physically correct, volume independent level density of a compound nucleus with a given excitation energy and nucleon number. The implementation of the results obtained in Sec. III with respect to the quantum fluctuations of the mean field produce additional terms in the entropy which are of boson nature and can be viewed as a contribution from collective vibrations of the mean field. No overcounting of single-particle and collective degrees of freedom occurs.

Another effect leading to a possible increase of the level density is related to the presence of several local minima in the nuclear free energy as a function of deformation.

In Sec. V we derive, apparently for the first time, mean-field equations which contain both dynamical and statistical effects and are not confined to the evolution of a Slater determinant. We discuss their relevance for the problem of compound nucleus fission and show that the spontaneous fission equations of Ref. 15 arise as their limiting case. We present expressions for the averaged fission width given as a function of the excitation energy of the fissioning compound nucleus.

We will see that the presence of a timelike parameter in our equations is related to a kind of dynamical averaging over the range of deformations from the compound nucleus shape to the scission configuration. The statistical occupations of the single particle wave functions are independent of the "time" parameter. However, they do depend self-consistently on the entire dynamics of the mean field and provide relative weights of particular deformations depending on how rapidly the mean field is changing in the vicinity of these deformations. These self-consistent statistical occupations define the "dynamical" entropy in the expression for the fission width which effectively counts the many nucleon states available to the nuclear system in the fission process.

II. MEAN-FIELD CONTRIBUTIONS TO THE NUCLEAR PARTITION FUNCTION

The grand canonical partition function is

$$Z(\alpha,\beta)=\mathrm{Tr}e^{\alpha\hat{A}-\beta H}\ , \tag{2.1}$$

where $\hat{A}$ is the number operator, β is the inverse temperature, α/β is the chemical potential, and H is the exact Hamiltonian of the system. In a nuclear physics application H is usually replaced by a one body Hamiltonian of the independent particle model and the trace is computed in a standard way.[24,25]

The level density $\rho(E,A)$ is then given by the Laplace transform of $Z(\alpha,\beta)$ over β and α variables which is evaluated using a saddle point approximation (SPA). The SPA conditions define the mean temperature β^{-1} and the mean chemical potential α/β which are given in terms of the excitation energy and the particle number

$$E=\langle H\rangle,\ A=\langle \hat{A}\rangle\ , \tag{2.2}$$

where the brackets denote statistical averages. Further approximations of the resulting expression for $\rho(E,A)$ lead to the well known Bethe formula.[25]

We use the mean-field functional integral method and evaluate $Z(\alpha,\beta)$. We do not make the independent particle assumption but rather define a one-body potential self-consistently and calculate corrections to the result. Our main purpose in this section is to demonstrate how the well known expressions for the temperature dependent mean field[18–21] can be obtained using the functional integral formulation. This will serve as a basis for our discussion in the following sections.

For notational simplicity, in this section we consider H with a two-body interaction which depends on the relative distance only

$$H = K' + \tfrac{1}{2}\int \hat{\rho}(x)V(x-x')\hat{\rho}(x')dx\,dx' ,$$
$$\hat{\rho}(x) = \sum_{i=1}^{A}\delta(x-x_i) , \tag{2.3}$$
$$K' = K - \frac{A}{2}V(0) ,$$

where K is the kinetic energy. A more general form is discussed in the next section together with the corrections to the mean-field result.

Using the functional integral representation of Ref. 6 the trace in (2.1) can be written as

$$Z(\alpha,\beta) = \int D\sigma\, e^{\beta/2(\sigma,V\sigma)}\,\mathrm{Tr}\,e^{\alpha\hat{A}}U_\sigma(\beta) , \tag{2.4}$$

where $\sigma \equiv \sigma(x,\eta)$,

$$U_\sigma(\beta) = T_\eta \exp\{-\beta[(K',\hat{\rho}) + (\hat{\rho},V\sigma)]\} , \tag{2.5a}$$

$$(\hat{\rho},V\sigma) \equiv \int_{-1/2}^{1/2} d\eta \int dx\,dx'\hat{\rho}(x)V(x-x')\sigma(x',\eta) , \tag{2.5b}$$

with similar notations for $(\sigma,V\sigma)$ and $(K',\hat{\rho})$. Here T_η denotes ordering with respect to the "imaginary time" parameter η which is chosen to vary from $\eta = -\frac{1}{2}$ to $\frac{1}{2}$. The integration measure is defined similarly to that in Ref. 6.

As in the standard finite-temperature many-body theories, the introduction of the time $\tau \equiv \beta\eta$ is ultimately a consequence of quantum mechanical ordering effects accounting for noncommutativity of kinetic and potential terms in the Hamiltonian.

We will evaluate the integral in (2.4) by the saddle point approximation. The saddle point condition singles out the most significant mean-field configurations. In general, one should expect that more than one such configuration will result from the saddle point selection. The dependence of the σ field on η also implies that both static η-independent and dynamical η-dependent configurations should be expected. In this section we will concentrate on static saddle points. The role of dynamical σ fields will be discussed in Secs. III and V.

It is convenient to write the integrand in (2.4) in the form $\exp\{-\beta\Omega[\alpha,\beta,\sigma]\}$ with the effective grand canonical free energy

$$\Omega[\alpha,\beta,\sigma] = -\tfrac{1}{2}(\sigma,V\sigma) - \beta^{-1}\ln \mathrm{Tr}\,e^{\alpha\hat{A}}U_\sigma(\beta) . \tag{2.6}$$

The saddle point condition $\delta\Omega/\delta\sigma = 0$ gives the following equation for σ:

$$\sigma_0(x,\eta) = \langle \hat{\rho}(x,\eta)\rangle_{\sigma_0} , \tag{2.7a}$$

with the notation

$$\langle \hat{\rho}(x,\eta)\rangle_\sigma = \frac{\mathrm{Tr}\,e^{\alpha\hat{A}}U_\sigma(\beta/2,\beta\eta)\hat{\rho}(x)U_\sigma(\beta\eta,-\beta/2)}{\mathrm{Tr}\,e^{\alpha\hat{A}}U_\sigma(\beta)} . \tag{2.7b}$$

The appearance of the two operators U_σ in the right-hand side of (2.7b) is similar to Eq. (3.6) of Ref. 6 and is due to the effect of the time-ordering operator T_η in our definition [Eq. (2.5a)]. To cast Eq. (2.7a) in a more transparent form we consider η-independent σ's and evaluate the trace in (2.6) in a basis of eigenfunctions of $U_\sigma(\beta)$. For the purpose of this evaluation consider a single particle equation

$$\left[\frac{p^2}{2m} - \tfrac{1}{2}V(0) + \int V(x-x')\sigma(x')dx'\right]\psi_i(x) = \epsilon_i\psi_i(x) . \tag{2.8}$$

Slater determinants built from the solutions of (2.8) represent eigenfunctions of U_σ with η-independent σ. The eigenvalues are

$$\exp\sum_{i=1}^{\infty}(-\beta n_i\epsilon_i) ,$$

where $n_i = 0$ or 1 and $\sum_{i=1}^{\infty} n_i = A$. All the values of A should be included in evaluating the trace in (2.6) and one obtains

$$\mathrm{Tr}\, e^{\alpha\hat{A}} U_\sigma(\beta) = \sum_{A=0}^{\infty} \sum_{\{n_i\}} e^{\sum_{i=1}^{\infty} n_i(\alpha-\beta\epsilon_i)} . \qquad (2.9)$$

In a standard way this is transformed as

$$\mathrm{Tr}\, e^{\alpha\hat{A}} U_\sigma(\beta) = \prod_{i=1}^{\infty} (1 + e^{\alpha-\beta\epsilon_i}) \qquad (2.10)$$

and the free energy of Eq. (2.6) becomes

$$\Omega[\alpha,\beta,\sigma] = -\tfrac{1}{2}(\sigma,V\sigma) - \beta^{-1} \sum_{i=1}^{\infty} \ln[1 + e^{\alpha-\beta\epsilon_i}] . \qquad (2.11)$$

Note that ϵ_i's in the second term are functionals of σ.

Using perturbation theory in Eq. (2.8) to calculate $\delta\epsilon_i/\delta\sigma$, one finds from the SPA condition $\delta\Omega/\delta\sigma = 0$ an explicit equation for $\sigma(x)$ in this static case

$$\sigma_0(x) = \sum_{i=1}^{\infty} f_i \psi_i^2(x) , \qquad (2.12a)$$

where we defined the Fermi occupation numbers

$$f_i = (1 + e^{\beta\epsilon_i - \alpha})^{-1} . \qquad (2.12b)$$

Not surprisingly, the resulting mean field is a statistical average of the single particle densities and coincides with the expressions obtained using a variational principle[18–21] or standard finite temperature perturbation theory.[26] Although the approximation is formulated in terms of a one body potential and single particle wave functions, it is clearly not confined to a single Slater determinant. Rather, the sum over determinants present in (2.9) is contained in the mean-field expression through the occupation numbers for single particle states.

One should observe that working in the grand canonical representation was only a matter of convenience. In canonical representation, for instance, the mean-field expression (2.12) would be replaced by

$$\sigma_0(x) = \frac{\sum_{i=1}^{\infty} \psi_i^2(x) e^{-\beta\epsilon_i}}{\sum_{i=1}^{\infty} e^{-\beta\epsilon_i}} . \qquad (2.13)$$

As was indicated earlier there are, in principle, many solutions to the mean-field Eq. (2.8). The simplest way to see this is perhaps in realizing that a partition function describing a nuclear system with the average number of nucleons A should contain contributions from a bound state of A nucleons, two bound states of $A/2$ nucleons, and so on. Obviously, these contributions are described by different solutions of Eq. (2.8) with different spatial localization.

Apart from this trivial multiplicity of solutions one should also expect different solutions corresponding to different shapes of the mean potential for the same nucleus. Analogous to the ground state energy, the free energy as a function of deformation exhibits several minima.[21] However, in contrast to the ground state where only the lowest minimum is considered, one must in principle account for all the minima in computing the finite temperature partition function. Formally, this follows from the prescription of the SPA by which the contributions from all the saddle points should be included in the evaluation of the functional integral (2.4). The relative importance of various contributions is, of course, determined by the relative energies of the corresponding minima.

In the lowest order SPA the partition function is thus seen to have the form

$$Z(\alpha,\beta) \cong \sum_{\sigma_0} e^{-\beta\Omega_p[\alpha,\beta,\sigma_0] - \beta\Omega_c[\alpha,\beta,\sigma_0]} , \qquad (2.14)$$

with the single-particle free energy $\Omega_p[\alpha,\beta,\sigma_0]$ defined in (2.6) or (2.11) and σ_0 calculated from Eqs. (2.8) and (2.12). The sum runs over all mean-field solutions σ_0 and the additional term $-\beta\Omega_c[\alpha,\beta,\sigma_0]$ in the exponent of (2.14) represents the log of the functional integral (2.4) with the integrand expanded around σ_0. This integral is usually evaluated in a quadratic approximation and will be discussed in the next section. It will be shown there that it includes the effects of collective motion and hence the subscript in $\Omega_c[\alpha,\beta,\sigma_0]$.

The two terms in expression (2.11) for the single-particle part $\Omega_p[\alpha,\beta,\sigma_0]$ of the free energy have an obvious interpretation. The second term is simply the free energy of independent nucleons in a self-consistent one body potential determined by σ_0. The first term is the finite temperature generalization of the usual correction for overcounting of the potential energy in the sum of the single-particle energies.

The simple summation (2.14) over the saddle point configurations may appear to involve an "overcounting" error due to the nonorthogonality of the many particle states built upon different configurations. This error is, however, expected to be small when all the saddle points are well separated since then the states are approximately orthogonal. The error is, in fact, consistent with the saddle point approximation which breaks down when some of the saddle points are too close by an appropriate measure. In the latter case a more complicated uniform expression derived in Ref. 27 should replace the sum (2.14). We will not discuss such situations here.

III. FLUCTUATIONS AROUND THE MEAN FIELD

We will now discuss the term $\Omega_c[\alpha,\beta,\sigma_0]$ in (2.14). This is given by the functional integral over the fluctuations around the mean-field configuration σ_0. It can be calculated approximately and thus provide corrections to the mean-field result $\Omega_p[\alpha,\beta,\sigma_0]$. For the purpose of this calculation it will be more appropriate to work with the many-body Hamiltonian in a second quantized form for which we use the notation

$$H=\sum_{i,j}K_{ij}a_i^+a_j+\tfrac{1}{2}\sum_{i,j,k,l}V_{ijkl}a_i^+a_j^+a_l a_k\ . \tag{3.1}$$

Introducing

$$\hat{\rho}_{ik}=a_i^+a_k \tag{3.2}$$

this becomes

$$H=\sum_{i,j}K'_{ij}\hat{\rho}_{ij}+\tfrac{1}{2}\sum_{i,j,k,l}V_{ijkl}\hat{\rho}_{ik}\hat{\rho}_{jl}\ , \tag{3.3}$$

where K' includes the self-energy term $-\frac{1}{2}AV(0)$ as in Eq. (2.30). Repeating the steps at the beginning of Sec. II, one obtains the same representation [Eq. (2.4)] for the partition function, with the only difference that σ is now $\sigma_{ik}(\eta)$ and Eqs. (2.5) are appropriately changed.

Our estimate of the functional integral representing $\exp(-\beta\Omega_c[\alpha,\beta,\sigma_0])$ is given as the Gaussian functional integral which is obtained by expanding $\Omega[\alpha,\beta,\sigma]$ in (2.6) around σ_0 and retaining only quadratic terms. In this approximation

$$e^{-\beta\Omega_c}=\int D\xi\, e^{-\beta/2[\xi,(\delta^2\Omega/\delta\sigma\delta\sigma)\xi]}\ , \tag{3.4}$$

where $\xi\equiv\xi_{ik}(\eta)=\sigma_{ik}(\eta)-\sigma_{ik}^0$ in the general representation defined by (3.1).

Using Eq. (2.6) we calculate the second variation of Ω and obtain

$$\frac{\delta^2\Omega}{\delta\sigma_{ik}(\eta)\delta\sigma_{lm}(\eta')}=-V_{ilkm}\delta(\eta-\eta')-\beta V_{ipkn}D_{pn,rs}(\eta,\eta')V_{lrms}\ , \tag{3.5}$$

where

$$D_{pn,rs}(\eta,\eta')=\langle\hat{\rho}_{pn}(\eta)\hat{\rho}_{rs}(\eta')\rangle_{\sigma_0}-\langle\hat{\rho}_{pn}(\eta)\rangle_{\sigma_0}\langle\hat{\rho}_{rs}(\eta')\rangle_{\sigma_0} \tag{3.6}$$

and we have used the summation convention over repeated indices and the notation of Eq. (2.7b) to define quantitites like $\langle\hat{\rho}(\eta)\rangle$.

When differentiating (2.6) one should take account of the time ordering operator T_η in the definition (2.5a) so that the densities $\hat{\rho}$ in (3.6) are placed between the operators U_σ as in (2.7b).

In Eq. (3.6), $D(\eta,\eta')$ is the standard finite temperature density-density correlation function. Its explicit expression is conveniently found by differentiating both sides of (3.6) with respect to η. Using the equation of motion for $\hat{\rho}_{ik}(\eta)$ in the single-particle representation specified by the mean field equations (2.8) and (2.12), one finds

$$\frac{dD_{pn,rs}}{d\eta}-\beta(\epsilon_p-\epsilon_n)D_{pn,rs}=\delta_{nr}\delta_{ps}(f_p-f_n)\delta(\eta-\eta')\ . \tag{3.7}$$

The inhomogeneous term arises from the difference in the values of $D(\eta,\eta')$ when $\eta\to\eta'$ above or below η'.

A formal solution of Eq. (3.7) is

$$D=-FG\ , \tag{3.8a}$$

with

$$G=\left[\frac{d}{d\eta}-\beta\Delta\epsilon\right]^{-1}\ , \tag{3.8b}$$

where we have defined matrices

$$\Delta\epsilon_{pn,rs} = \delta_{pr}\delta_{ns}(\epsilon_n - \epsilon_p) , \tag{3.9a}$$

$$F_{pn,rs} = \delta_{ps}\delta_{rn}(f_n - f_p) . \tag{3.9b}$$

As is well known,[26] D can be interpreted as the finite temperature generalization of the particle-hole propagator. It can be written in the equivalent form

$$\begin{aligned} D_{pn,rs}(\eta,\eta') &= f_p(1-f_r)\delta_{ps}\delta_{rn}e^{\beta(\epsilon_p-\epsilon_r)(\eta-\eta')}, \text{ for } \eta > \eta' \\ &= f_r(1-f_p)\delta_{ps}\delta_{rn}e^{\beta(\epsilon_p-\epsilon_r)(\eta-\eta')}, \text{ for } \eta < \eta' , \end{aligned} \tag{3.10}$$

which can also be obtained using Wick's theorem for finite temperature[26] in Eq. (3.6).

We now proceed to evaluate the Gaussian integral (3.4). It is expressed via the determinant of the second variation (3.5)

$$e^{-\beta\Omega_c} = \left[\frac{\det(\beta V)}{\det(\beta V + \beta^2 VDV)}\right]^{1/2} = [\det(1+\beta VD)]^{-1/2} . \tag{3.11}$$

One should recall[6] that the functional integral measures $D\sigma$ in (2.4) and $D\xi$ in (3.4) contain the determinant of βV which is written explicitly in the numerator of (3.11). The determinants in (3.11) are taken with respect to both space and time η.

Using the explicit form (3.8) of the correlation function D, we transform

$$1+\beta VD = 1-\beta VFG = [(\beta G)^{-1} - VF]\beta G = \left[\frac{1}{\beta}\frac{d}{d\eta} - \Delta\epsilon - VF\right]\left[\frac{1}{\beta}\frac{d}{d\eta} - \Delta\epsilon\right]^{-1} . \tag{3.12}$$

Consider now an eigenvalue equation

$$(\Delta\epsilon + VF)\xi^\nu = \omega_\nu \xi^\nu . \tag{3.13}$$

As discussed in Ref. 19 this is a finite temperature generalization of the RPA equations. The main distinction of these equations from their zero temperature counterpart is that all the single particle energy differences $\epsilon_i - \epsilon_k$ appear in (3.13) while the sharp particle-hole separation is replaced by the presence of the Fermi occupations contained in F. Some general properties of (3.13) are reviewed in Appendix A, where we also show how the ordinary zero temperature RPA is recovered as a limiting case.

The determinant in (3.11) can be expressed in terms of the RPA eigenfrequencies ω_ν. Using (3.12) and the definition [Eq. (3.9)] of $\Delta\epsilon$ we obtain

$$\det(1+\beta VD) = \frac{\det\left[\frac{1}{\beta}\frac{d}{d\eta} - \Delta\epsilon - VF\right]}{\det\left[\frac{1}{\beta}\frac{d}{d\eta} - \Delta\epsilon\right]} = \frac{\prod_{n=-\infty}^{\infty}\prod_\nu \left[\frac{2\pi i N}{\beta} - \omega_\nu\right]}{\prod_{N=-\infty}^{\infty}\prod_{k,j}\left[\frac{2\pi i N}{\beta} - \Delta\epsilon_{kj}\right]}, \quad \Delta\epsilon_{kj} = \epsilon_k - \epsilon_j . \tag{3.14}$$

Note that the operators here are diagonalized in the interval $-\frac{1}{2} \le \eta \le \frac{1}{2}$.

The ratio of products (3.14) can be evaluated by using Euler's formula. Thus we obtain (see Appendix A for details)

$$e^{-\beta\Omega_c} = \frac{\prod_{j>k} 2\sinh(\beta\Delta\epsilon_{jk}/2)}{\prod_{\omega_\nu>0} 2\sinh(\beta\omega_\nu/2)}, \quad \Delta\epsilon_{jk} = \epsilon_j - \epsilon_k . \tag{3.15}$$

This expression has a clear physical meaning. The Gaussian contribution to the free energy amounts to accounting for the small quantum fluctuations of the system around its stationary configuration defined by the temperature dependent mean-field Eq. (2.8) and (2.12). The eigenmodes of these fluctuations are determined by the solutions of the temperature dependent RPA equation (3.13). In this approximation each eigenmode is essentially an independent quantum oscillator, the partition of which is

$$\sum_{n=0}^{\infty} e^{-\beta\omega_\nu(n+1/2)} = \frac{1}{2\sinh(\beta\omega_\nu/2)} .$$

The product of these expressions enters the denominator of (3.15). If alone, it would contain at least two incorrect features. First, the number of RPA eigenmodes is infinite and the product diverges. Second, the bosonlike RPA modes are not independent but are built of the fermion particle-hole excitations already accounted for in the single-particle free energy $\Omega_p[\alpha,\beta,\sigma_0]$ in Eq. (2.14). Clearly, the numerator of (3.15) not only renders the ratio finite but also handles the overcounting of the degrees of freedom by canceling out the effects of those modes ω_ν which are not significantly shifted from the unperturbed energies $\Delta\epsilon_{ik}$ as, for example, in the high frequency continuum. In other words, collective modes produce the largest effect, being mostly influenced and shifted by the residual interaction.

The result of Eq. (3.15) represents a correction to the mean field expression (2.14) for the nuclear free energy. A similar correction has been discussed in condensed matter physics by summing the ring diagrams of the temperature dependent perturbation theory[26] around a translationally invariant mean field with plane wave basis. This summation presumably can also be carried out for finite nuclear systems. We regard the relative simplicity of our derivation, the transparent physical interpretation of our result (3.15), and the natural relation to the temperature dependent RPA equation (3.13) as advantages of the functional integral approach.

The single-particle free energy $\Omega_p[\alpha,\beta,\sigma_0]$ in expression (2.14) has an obvious zero temperature limit

$$\lim_{\beta\to\infty} \Omega_p[\alpha,\beta,\sigma_0] = \sum_{i=1}^{A} (\epsilon_i - \epsilon_f) - \tfrac{1}{2}(\sigma_0, V\sigma_0) , \tag{3.16}$$

where the fixed Fermi energy $\epsilon_f = \alpha/\beta$ defines the particle number A. The σ_0 in the second term is given by Eq. (2.12a) with the occupations f_i replaced by step functions $\theta(\epsilon_i - \epsilon_f)$. Apart from the Fermi energy term, expression (3.16) is the Hartree-Fock energy of the A particle ground state. The Gaussian correction becomes in this limit

$$\lim_{\beta\to\infty} \Omega_c[\alpha,\beta,\sigma_0] = \sum_{\nu} \omega_\nu/2 - \sum_{p,h} (\epsilon_p - \epsilon_h)/2 \tag{3.17}$$

and the quantity in brackets is the RPA correlation energy correction to the Hartree-Fock result. As is explained in Appendix A the particle-hole components in Eq. (3.13) become decoupled from the particle-particle and hole-hole subspace in the limit of zero temperature. Moreover, the eigenfrequencies ω_ν corresponding to this subspace cancel the terms $\Delta\epsilon_{pp'}$ and $\Delta\epsilon_{hh'}$ in the numerator of (3.15), and only the usual zero temperature RPA frequencies and particle-hole energy differences are left in the expression (3.17).

We now comment on the zero eigenfrequencies of the RPA equation (3.13). They arise because various symmetries of the exact Hamiltonian are broken by the mean field solution. The simplest such symmetry is translational invariance. The corresponding zero eigenfrequency can in principle be treated by the general methods of Ref. 28. We simply observe that for Gaussian corrections this treatment will amount to the inclusion in the partition function of a contribution from the translational motion of a nucleus. Since this motion is decoupled from the internal excitations and we are interested only in the latter, we should simply omit the corresponding modes in the Gaussian corrections. Therefore, only nonzero frequencies are included in expression (3.15).

More interesting is the breaking of the rotational invariance which occurs when the mean field potential is deformed. For the case of axial symmetry around the z axis, a more suitable partition function to use is[24]

$$Z(\alpha,\beta,\Omega_x) = \mathrm{Tr} e^{\alpha\hat{A} - \beta H + \beta\Omega_x J_x} .$$

The level density at fixed A, E, and J_x will then arise by appropriate Laplace integration over α, β, and Ω_x. In the next section we discuss the projections for A and E. Treatment of angular momentum is deferred to a future work.

IV. COMPOUND NUCLEUS LEVEL DENSITY

Introduction of a physical temperature and chemical potential in nuclear physics problems is probably relevant only for applications in astrophysics.[29] A more appropriate quantity is the level density

$$\rho(E,A) = \mathrm{Tr}\delta(E - H)\delta(A - \hat{A}) . \tag{4.1}$$

This is related to the partition function $Z(\alpha,\beta)$ by the standard Laplace transform.[24]

$$\rho(E,A)=\frac{1}{(2\pi i)^2}\int\int_{-i\infty}^{i\infty} d\alpha\, d\beta\, e^{-\alpha A+\beta E} Z(\alpha,\beta)\,. \tag{4.2}$$

In the mean-field approximation, $Z(\alpha,\beta)$ is given by the sum (2.14), where each term corresponds to a different mean-field configuration. In the present section we are interested in the *part* of the total level density (4.2) which corresponds to an A particle compound nucleus. Accordingly, we use in (4.2) only contributions to $Z(\alpha,\beta)$ with mean-field configurations in which all the nucleons move in *one* localized self-consistent potential well.

The single-particle continuum states in this potential require special attention. The population of these states at finite temperature leads to a constant particle density (2.12a) at distances that are large compared to the extent of the potential well. This reflects the fact that the finite temperature partition function does not describe a definite number of particles. On the contrary, it necessarily describes a self-bound nuclear system in equilibrium with an exterior nucleon gas consisting of evaporated nucleons. As usual the average particle number and energy of this system are proportional to the volume of the system. This implies that in order to use a relation such as (4.2) for the definition of the level density of a compound nucleus with a given *finite* number of nucleons and *finite* energy, it is not sufficient to separate the relevant terms in expression (2.14). In addition, one must subtract the contribution of the exterior nucleon gas present in the grand canonical free energy $\Omega[\alpha,\beta,\sigma_0]=\Omega_p[\alpha,\beta,\sigma_0]+\Omega_c[\alpha,\beta,\sigma_0]$.

This procedure is analogous to that used in Ref. 25, where the contribution of a noninteracting nucleon gas was subtracted when the nuclear free energy was calculated in the framework of the independent particle model. In our case, the free energy of the nucleon gas should be taken as $\Omega[\alpha,\beta,\sigma_\infty]=\Omega_p[\alpha,\beta,\sigma_\infty]+\Omega_c[\alpha,\beta,\sigma_\infty]$, where σ_∞ is a constant mean-field solution which coincides with the mean-field σ_0 of Eq. (2.12a) at large distances.

The explicit expressions for $\Omega_p[\alpha,\beta,\sigma_\infty]$ and $\Omega_c[\alpha,\beta,\sigma_\infty]$ are given by Eqs. (2.11) and (3.15) calculated for a constant $\sigma=\sigma_\infty$. We discuss these expressions in some detail in Appendix B and show that their subtraction from the free energy $\Omega_p[\alpha,\beta,\sigma_0]+\Omega_c[\alpha,\beta,\sigma_0]$ renders the difference $\overline{\Omega}(\alpha,\beta)$ independent of the volume of the system and thus leads to a finite average energy and particle number. This subtraction procedure is necessary for the appropriate definition of the volume independent compound nucleus level density. In order to avoid unnecessary repetition we will always denote subtracted quantities like $\overline{\Omega}(\alpha,\beta)$ with a bar.

Thus we use $\overline{Z}(\alpha,\beta)\equiv\exp[-\beta\overline{\Omega}(\alpha,\beta)]$ in relation (4.2). The integrand then has the form $\exp\overline{S}$, where the entropy $\overline{S}$ is

$$\overline{S}=-\alpha A+\beta E-\beta\overline{\Omega}(\alpha,\beta) \tag{4.3a}$$

and as defined above

$$\begin{aligned}\overline{\Omega}(\alpha,\beta)&\equiv\Omega[\alpha,\beta,\sigma_0]-\Omega[\alpha,\beta,\sigma_\infty]\\ &=\overline{\Omega}_p[\alpha,\beta,\sigma_0]+\overline{\Omega}_c[\alpha,\beta,\sigma_0]\end{aligned} \tag{4.3b}$$

is given in terms of the subtracted single-particle and collective parts of the free energy,

$$\overline{\Omega}_p[\alpha,\beta,\sigma_0]=\left\{-\tfrac{1}{2}(\sigma_0,V\sigma_0)-\frac{1}{\beta}\sum_{i=1}^{\infty}\ln(1+e^{\alpha-\beta\epsilon_i})\right\}-\{\,\infty\,\}\,, \tag{4.3c}$$

$$\overline{\Omega}_c[\alpha,\beta,\sigma_0]=\left\{\sum_{\nu>0}\frac{1}{\beta}\ln\sinh(\beta\omega_\nu/2)-\sum_{i>k}\frac{1}{\beta}\ln\sinh(\beta\Delta\epsilon_{ik}/2)\right\}-\{\,\infty\,\}\,, \tag{4.3d}$$

where $\{\,\infty\,\}$ denotes the subtraction of the same expression corresponding to σ_∞. This is to be calculated as the infinite nucleon gas quantity at the same α and β. We note that expression (4.3d) does not explicitly depend on α as is usual with phononlike excitations.

In a standard way we evaluate the Laplace transform (4.2) over α and β by the saddle-point approximation. The saddle-point conditions $\partial\overline{S}/\partial\beta=0$ and $\partial\overline{S}/\partial\alpha=0$ yield the following equations:

$$\begin{aligned}E=\partial/\partial\beta(\beta\overline{\Omega})=&\left\{\sum_{i=1}^{\infty}f_i\epsilon_i-\tfrac{1}{2}(\sigma_0,V\sigma_0)\right\}-\{\,\infty\,\}\\ &+\tfrac{1}{2}\left\{\sum_{\nu>0}\frac{\partial(\beta\omega_\nu)}{\partial\beta}\coth(\beta\omega_\nu/2)-\sum_{i>k}\frac{\partial(\beta\Delta\epsilon_{ik})}{\partial\beta}\coth(\beta\Delta\epsilon_{ik}/2)\right\}-\tfrac{1}{2}\{\,\infty\,\}\,,\end{aligned} \tag{4.4a}$$

$$A=-(\partial/\partial\alpha)\bar{\Omega}=\left\{\sum_{i=1}^{\infty}f_i\right\}-\{\ \infty\ \}$$
$$+\beta/2\left\{\sum_{\nu>0}\frac{\partial\,\omega_\nu}{\partial\,\alpha}\coth(\beta\omega_\nu/2)-\sum_{i>k}\frac{\partial\,\Delta\epsilon_{ik}}{\partial\,\alpha}\coth(\beta\Delta\epsilon_{ik}/2)\right\}-\beta/2\{\ \infty\ \}\ , \tag{4.4b}$$

where, as in Eq. (4.3), the notation $\{\ \infty\ \}$ always stands for the subtracted quantity. The solutions α_0 and β_0 of Eqs. (4.4) fix the *mean* temperature and chemical potential so that the level density is given at the correct excitation energy and particle number

$$E=\bar{E}_p+\bar{E}_c\ ,$$
$$A=\bar{A}_p+\bar{A}_c\ .$$

We denote by $\bar{E}_p$ and $\bar{A}_p$ the single particle part given by the first two terms of (4.4a) and (4.4b), respectively. The remaining terms denoted as $\bar{E}_c$ and $\bar{A}_c$ represent contributions from the collective degrees of freedom in the sense defined in the preceding section.

In Eqs. (4.4) we have accounted for the fact that ω_ν and $\Delta\epsilon_{ik}$ have implicit dependence on β and α through the mean-field potential. This appears only in the collective terms since the single particle part of $\bar{S}$, Eq. (4.3), is already stationary with respect to the changes of the mean field.

It is expected that for heavy enough nuclei and not too high excitation energies, the implicit dependence of ω_ν and $\Delta\epsilon_{ik}$ on the variables α and β is slow and can be neglected. In this case one can replace the derivatives $\partial(\beta\omega_\nu)/\partial\beta$ and $\partial(\beta\Delta\epsilon_{ik})/\partial\beta$ in (4.4a) by ω_ν and $\Delta\epsilon_{ik}$, respectively, and completely neglect the last two terms in (4.4b). In this approximation the entropy (4.3a) can be written in a transparent form

$$\bar{S}=\bar{S}_p+\bar{S}_c\ , \tag{4.5}$$

where

$$\bar{S}_p=-\left\{\sum_{i=1}^{\infty}[f_i\ln f_i+(1-f_i)\ln(1-f_i)]\right\}+\{\ \infty\ \}\ , \tag{4.6}$$

$$\bar{S}_c=\left\{\sum_{\nu>0}[(1+b_\nu)\ln(1+b_\nu)-b_\nu\ln b_\nu]-\sum_{i>k}[(1+b_{ik})\ln(1+b_{ik})-b_{ik}\ln b_{ik}]\right\}-\{\ \infty\ \}\ . \tag{4.7}$$

Here, in analogy with fermion occupations f_i, we have introduced "boson" occupation numbers

$$b_\nu=(e^{\beta\omega_\nu}-1)^{-1}\ , \tag{4.8}$$
$$b_{ik}=(e^{\beta\Delta\epsilon_{ik}}-1)^{-1}\ . \tag{4.9}$$

The entropy $\bar{S}$ is thus given in terms of the usual expressions for fermion and boson entropies. The collective part consists of the *difference* between the entropy associated with the RPA bosons and the "particle-hole" bosons.

Evaluation of (4.2) by the saddle-point approximation yields

$$\rho(E,A)=\sum_{\sigma_0}\frac{e^{\bar{S}(E,A,\sigma_0)}}{2\pi\sqrt{D}}\ , \tag{4.10}$$

where $\bar{S}(E,A,\sigma_0)$ is given by Eq. (4.5) and D is the usual determinant of second derivatives of $\bar{S}$ with respect to α and β. Using Eq. (4.4) it is written as

$$D=\begin{vmatrix}\partial A/\partial\alpha & \partial A/\partial\beta\\ \partial E/\partial\alpha & \partial E/\partial\beta\end{vmatrix} \tag{4.11}$$

and accounts for the fluctuations of α and β around their mean values α_0 and β_0.

The sum in (4.10) is of the same origin as the sum in Eq. (2.14) and runs over all mean-field configurations

σ_0, which consist of a single potential well at the given energy E and particle number A. As was discussed in the Introduction and in Sec. II, mean-field configurations with geometrical shapes very different from the ground state may produce local minima in the nuclear free energy, as can be seen from the numerical examples of Ref. 21. When the excitation energy E becomes higher than these minima, additional terms appear in expression (4.10) and should lead to the increase of the level density over the value given by the ground state configuration of the mean-field potential. If this effect is significant one should also expect to observe a kink-like structure in the energy dependence of $\rho(E,A)$ appearing at the energies of higher minima. It is obvious that for given values of E and A the mean temperature $\beta_0{}^{-1}$ and chemical potential α_0/β_0 associated with different terms in (4.10) are, in general, different. This is not surprising in the present context, where the concepts of temperature and chemical potential play only an auxiliary role.

V. COMPOUND NUCLEUS FISSION

As was discussed earlier the saddle-point equations for the functional integral (2.4) will, in general, have many mean-field solutions. Let us qualitatively discuss various possible solutions in a system of A nucleons with A large enough to contain a fissioning nucleus. Consider a microcanonical partition function $\mathrm{Tr}\delta(E-H)\delta(A-\hat{A})$. For a given energy E above the ground state this function contains a contribution from an ensemble of excited states with a given energy E, i.e., the compound nucleus. Clearly, this ensemble is not the only contribution to the partition function. Various possible groups of fission fragments with different internal and kinetic energy, consistent with the given total energy, also contribute to the partition function. Owing to volume effects these contributions are actually overwhelmingly large in comparison to the compound state.

In order to define a separate compound state contribution in the *exact* partition function one should, in principle, use appropriate projection operators which isolate different parts of the many-nucleon Hilbert space. However, in the mean-field approach a separation is performed automatically by means of different configurations of the mean field. The partition function is then approximated by a sum over contributions of these configurations. A configuration of the mean field in which all the nucleons are bound together should be identified with the compound state of the fissioning nucleus. Mean-field configurations which consist of widely separated parts with the nucleons divided between the parts produce contributions in the partition function which should be attributed to various fission fragments and so on. This projection property of the mean-field description is a considerable advantage which allows us to separate different physical processes in an A nucleon system without the necessity to construct explicit projection operators.

The existence of static or uniformly moving mean-field configurations associated with excited fission fragments is clear. In this section we will show that in addition there exists a mean-field solution with nontrivial dynamical behavior which should be attributed to the fission process from the compound nucleus. Such a process contains both statistical and quantum mechanical elements. The former arises because of the averaging over the many nucleon states in a compound system. The latter arises because of the quantum-mechanical tunneling which is essential in subbarrier fission.

In Sec. II it was seen how the statistical averaging is performed in the mean-field expression with statistical occupations of single particle states. On the other hand, the mean-field description of quantum tunneling in many-nucleon systems was introduced in Refs. 15 and 16. There, however, it was limited to spontaneous fission from a single well defined state—the ground state of the fissioning nucleus. Our purpose in this section will be to generalize this description to energies above the ground state with appropriate averaging over compound nuclear states.

We start again with Eqs. (4.2) and (2.4):

$$\rho(E,A)=\frac{1}{(2\pi i)^2}\int\int_{-i\infty}^{i\infty}d\alpha\,d\beta\int D\sigma\,e^{\mathscr{S}[\alpha,\beta,\sigma]}\,, \tag{5.1}$$

where the "action" $\mathscr{S}$ is defined as

$$\mathscr{S}=-\alpha A+\beta E+\beta/2(\sigma,V\sigma)+\ln\mathrm{Tr}e^{\alpha A}U_\sigma(\beta)\,. \tag{5.2}$$

The saddle-point condition for the σ integral is given by the general equation (2.7). We consider σ solutions of this equation with dynamical dependence on the imaginary time parameter η. For this purpose we introduce an η-dependent single-particle equation

$$[\partial/\partial\eta+\beta h_\sigma(\eta)]u_k(x,\eta)=\lambda_k u_k(x,\eta)\ , \tag{5.3a}$$

where

$$h_\sigma(\eta)=p^2/2m-\tfrac{1}{2}V(0)+\int V(x-x')\sigma(x',\eta)dx'\ , \tag{5.3b}$$

with the periodic boundary conditions on the η interval

$$u_k(x,\eta=\tfrac{1}{2})=u_k(x,\eta=-\tfrac{1}{2})\ . \tag{5.3c}$$

The solutions of (5.3) represent a convenient basis for the evaluation of the trace in (5.2) and subsequent application of the condition $\delta\mathscr{S}/\delta\sigma=0$, because the corresponding Slater determinants diagonalize $U_\sigma(\beta)$. The procedure is similar to the static case discussed in Sec. II with the appropriate replacement of the dimensionless single particle energies $\beta\epsilon_k$ by the eigenvalues λ_k of Eq. (5.3a). We defer the details to Appendix C and quote the result.

The expression for the η-dependent mean field is

$$\widetilde{\sigma}_0(x,\eta)=\sum_{k=1}^{\infty}\widetilde{f}_k u_k(x,\eta)u_k(x,-\eta)\ , \tag{5.3d}$$

with the "occupation" numbers defined as

$$\widetilde{f}_k=(1+e^{\lambda_k-\alpha})^{-1}\ . \tag{5.3e}$$

The mean values of β and α are fixed by the energy E and particle number A when the integral over α and β in (5.1) is evaluated by the saddle-point approximation, using the same exterior nucleon gas subtraction procedure as defined in Sec. IV. In the static case discussed in the previous section we have included the contribution from the Gaussian integral around the mean-field configuration σ_0. This gives rise to collective terms in the Eqs. (4.4). Using the general method of Sec. III it is possible, in principle, to evaluate the Gaussian correction for the η-dependent $\widetilde{\sigma}_0$ of Eq. (5.3d). The result will be of the form (3.15) with $\beta\Delta\epsilon_{jk}$ replaced by $\lambda_j-\lambda_k$ and the RPA frequencies ω_ν determined from the appropriate generalization of (3.13) defining the eigenmodes of small oscillations around $\widetilde{\sigma}_0$. The η-dependent solution $\sigma_0(x,\eta)$ breaks the invariance of the exact partition function with respect to translations of the imaginary time parameter η. As usual, this leads to the existence of a corresponding zero eigenfrequency. The standard treatment[30] of this problem should be applicable in the present case.

We will not discuss the Gaussian correction factor for η-dependent $\widetilde{\sigma}_0$ in detail. We apply the saddle-point conditions for the α and β integrals only to the single-particle part of the action given by Eq. (5.2) with $\sigma=\widetilde{\sigma}_0$. Using the results of Appendix C, the equations $\partial\mathscr{S}/\partial\beta=0$ and $\partial\mathscr{S}/\partial\alpha=0$ yield

$$E=\left\{\sum_{k=1}^{\infty}\widetilde{f}_k\langle h_{\widetilde{\sigma}_0}\rangle_k-\tfrac{1}{2}(\widetilde{\sigma}_0,V\widetilde{\sigma}_0)\right\}-\{\,\infty\,\}\ , \tag{5.4a}$$

$$A=\left\{\sum_{k=1}^{\infty}\widetilde{f}_k\right\}-\{\,\infty\,\}\ , \tag{5.4b}$$

where

$$\langle h_\sigma\rangle_k=\int_{-1/2}^{1/2}d\eta\int dx\, u_k(x,-\eta)h_\sigma(\eta)u_k(x,\eta) \tag{5.4c}$$

and h_σ is defined in (5.3b). The solutions of (5.4) are denoted in the following as $\widetilde{\alpha}_0$ and $\widetilde{\beta}_0$. Their values are, of course, generally different from α_0 and β_0 of the static solution of the previous section. We now show that the set of Eqs. (5.3) and (5.4) represent the proposed generalization of the spontaneous fission equations and describe in a statistically averaged way the fission of an equilibrated compound state with energy E.

In our notation the spontaneous fission equations of Ref. 15 are written as

$$\lim_{\beta\to\infty}\left\{\partial/\partial\eta+\beta\left[\frac{p^2}{2m}-\tfrac{1}{2}V(0)+\int V(x-x')\sum_{i=1}^{A}u_i(x',\eta)u_i(x',-\eta)dx'\right]\right\}u_k(x,\eta)=\lambda_k u_k(x,\eta)\ , \tag{5.5}$$

with the boundary conditions of (5.3c). They describe the tunneling as propagation in imaginary time, which is reflected by the absence of imaginary i in the time derivative and the presence of the combination $u_i(\eta)u_i(-\eta)$ in the expression of the mean field. As usual, the self-consistency involves A single-particle wave functions. As discussed in Ref. 15 the limit $\beta\rightarrow\infty$ leads to the behavior of $u_i(x,\eta)$ such that they start and end at the corresponding single-particle wave functions composing the Slater determinant of the ground state of the fissioning nucleus.

The relation of the sets (5.5) and (5.3) is very similar to the relation between the static zero-temperature mean-field equations for the ground state and the finite-temperature static mean-field equations with occupations discussed in Sec. II. In both (5.5) and (5.3) the η dependence of the mean-field $\widetilde{\sigma}_0$ enters through the combination $u_k(\eta)u_k(-\eta)$ and there is no i multiplying the time derivative. As was established in Ref. 15, this is the correct way to account for the quantum-mechanical tunneling in the dynamical mean-field description. The statistical averaging enters through the occupations $\widetilde{f}_k$ in (5.3d), which are determined by the eigenvalues λ_k. Owing to the boundary conditions of (5.3c) the mean-field potential $\int V(x-x')\times\widetilde{\sigma}_0(x',\eta)dx'$ is periodic and the eigenvalues λ_k are dimensionless quasienergies such as Bloch quasimomenta in space-periodic potentials. In the spontaneous fission Eq. (5.5) these quasienergies are similar to the single-particle energies in the static zero-temperature mean-field equations for the ground state. The mean-field potential in (5.5) does not depend explicitly on λ_k and is defined self-consistently by the A lowest single-particle wave functions $u_k(x,\eta)$. For finite excitation energies the potential $\int V(x-x')\widetilde{\sigma}_0(x',\eta)dx'$ becomes dependent on all $u_k(x,\eta)$ with occupations $\widetilde{f}_k$ determined by the quasienergies λ_k, again in close analogy with the static case.

The spontaneous fission limit (5.5) is obtained from (5.3) when the energy E tends to the ground state energy. Then the mean temperature $\widetilde{\beta}_0{}^{-1}$ tends to zero with α_0/β_0 remaining fixed by the value of A. In this limit the eigenvalues of λ_k become very large, the occupations f_k tend to a step function over the lowest single-particle states $u_k(x,\eta)$, and the interval over which the imaginary time variable $\tau=\beta\eta$ varies increases to infinity. As a result the wave functions $u_k(x,\eta)$ start and end at the corresponding ground-state functions and the conserved excitation energy in Eq. (5.4a) decreases to the mean-field energy of the ground state. Since we do not include the Gaussian correction in our discussion this is the Hartree energy without the RPA correlations.

We now examine the expression for the action $\mathscr{S}[\alpha,\beta,\sigma]$ in (5.1) when calculated at the saddle point $\alpha=\widetilde{\alpha}_0$, $\beta=\widetilde{\beta}_0$, $\sigma=\widetilde{\sigma}_0$ defined by Eqs. (5.3) and (5.4). Using these equations we transform (5.2) into

$$\mathscr{S}(E,A)=\widetilde{S}(E,A)-W(E,A)\ , \tag{5.6a}$$

$$\widetilde{S}(E,A)=-\left\{\sum_{i=1}^{\infty}[\widetilde{f}_i\ln\widetilde{f}_i+(1-\widetilde{f}_i)\ln(1-\widetilde{f}_i)]\right\}+\{\ \infty\ \}\ , \tag{5.6b}$$

$$W(E,A)=\sum_{i=1}^{\infty}\widetilde{f}_i\left\langle\frac{\partial}{\partial\eta}\right\rangle_i\ . \tag{5.6c}$$

The occupations $\widetilde{f}_i$ are defined in (5.3e) and we used the notation of (5.4c).

The effective action is thus composed of two parts. The first part, defined by (5.6b), has a form of the entropy corresponding to the statistical population of the single-particle states $u_i(x,\eta)$ which describe the nucleons as the nucleus penetrates the fission barrier. The quasienergies λ_i determining $\widetilde{f}_i$ depend functionally on the whole range of mean-field configurations through which the system passes on its way to scission. Accordingly, the entropy $\widetilde{S}(E,A)$, which is expressed through $\widetilde{f}_i$, can be interpreted as representing an effective counting of the dynamically averaged many-nucleon states available to the system during the fission process. We will discuss the nature of this averaging in more detail after expression (5.10) for the fission width.

Whereas the first part $\widetilde{S}(E,A)$ in the effective action (5.6a) represents the statistical effects, the second part $W(E,A)$ is a quantum penetrability factor. In order to clarify this interpretation let us recall the expression for such a factor in the limiting case of spontaneous fission, which was derived in Ref. 15:

$$W(E_g,A)=\sum_{i=1}^{A}\left\langle\frac{\partial}{\partial\eta}\right\rangle_i\equiv\sum_{i=1}^{A}\int_{-1/2}^{1/2}d\eta\int dx\,u_i(x,-\eta)\frac{\partial}{\partial\eta}u_i(x,\eta)\ . \tag{5.7}$$

Here, u_i are solutions of Eqs. (5.5) and (5.3c). As explained in Ref. 15 the functions $u_i(x,\eta)$ and $u_i(x,-\eta)$ play the role of canonically conjugate variables and Eq. (5.7) is a mean-field analog of the tunneling action $\int p\dot{q}\,d\tau$ in the one-dimensional WKB treatment.

Comparing (5.7) with (5.6c) we see that $W(E,A)$ in the induced fission case is a statistically averaged penetrability in which every single particle wave function is weighted according to its occupation. The action $\mathscr{S}$ of (5.6) thus consists of a statistical contribution with dynamical averaging and a dynamical contribution with statistical averaging. Clearly, when the mean temperature $\beta_0{}^{-1}$ is decreased to zero, the entropy $\widetilde{S}(E,A)$ vanishes and the penetrability $W(E,A)$ coincides with the spontaneous fission expression (5.7).

The contribution of the fission solution (5.3d) to the microcanonical partition function is

$$\rho_f(E,A)=\rho_f^{(0)}e^{\mathscr{S}(E,A)}\,, \tag{5.8}$$

where $\mathscr{S}(E,A)$ is given by (5.6) while the factor $\rho_f^{(0)}$ arises from the Gaussian integral around the saddle point of the expression (5.1) at $\sigma=\widetilde{\sigma}_0$, $\alpha=\widetilde{\alpha}_0$, $\beta=\widetilde{\beta}_0$. One should also consider mean-field solutions with multiple reflections. These are important in the vicinity of the fission barrier energy and we comment on them later on.

With all the saddle points included, the mean-field approximation for the microcanonical partition function of the fissioning nuclear system is given by the sum

$$\rho(E,A)=\rho_{\rm CN}(E,A)+\rho_f(E,A)+\cdots\,. \tag{5.9}$$

Here $\rho_{\rm CN}$ is the density of compound states (where CN represents the compound nucleus) corresponding to the static mean field discussed in the previous sections. The term $\rho_f(E,A)$ is the fission contribution (5.8). The rest of the sum represents contributions from mean-field configurations of various fission fragments, their motion, etc., as was indicated in the beginning of this section.

Given the sum (5.9), it is reasonable to employ the usual phase space considerations and to argue that the relative fission probability is determined by the ratio of the contributions from fission $\rho_f(E,A)$ and the initial compound nucleus $\rho_{\rm CN}(E,A)$. Following our discussion of the action $\mathscr{S}$, we identify the exponential in (5.8) as an effective penetrability factor which combines both statistical effects and quantum mechanical tunneling. On this basis we suggest the following expression for the averaged fission width:

$$\Gamma(E,A)=\frac{D(E,A)}{2\pi}e^{\widetilde{S}(E,A)-W(E,A)}\,, \tag{5.10}$$

where the compound level spacing $D(E,A)=\rho_{\rm CN}{}^{-1}(E,A)$ and $\widetilde{S}(E,A)$, $W(E,A)$ given by Eqs. (5.6).

The quantities D, $\widetilde{S}$, and W in (5.10) are determined by the microscopic mean-field equations. At the same time our derivation of the expression for the fission width is only heuristic and follows considerations similar to the usual phenomenological discussions[31] of the compound nucleus fission. In this respect it is different from the mean-field theory[15] of spontaneous fission, where it was possible to determine the fission width more rigorously using the complex poles of the many-nucleon Green's function. At the moment it is not clear to us how to generalize this approach to finite excitation energies with the proper statistical averaging of the fission width. More work in this direction is required together with a detailed treatment of the Gaussian correction factor $\rho_f^{(0)}$ in (5.8).

The description of the compound nucleus fission given by the set of Eqs. (5.3), (5.4), and (5.10) is adequate for the energies between the ground state and the fission barrier. As was already indicated earlier, the entropy $\widetilde{S}$ is dynamically averaged over many-nucleon states available during the fission process. These states correspond to a range of deformations encountered in the collective motion of the mean field. The relative *weight* of a particular deformation depends on how rapidly the mean field is changing in the vicinity of this deformation. It can be seen from Eqs. (5.3)–(5.5) that when the excitation energy is small (and accordingly the inverse mean temperature $\widetilde{\beta}_0$ is large) the system is heavily weighted near the compound nucleus shape with a smaller weight on the fast transition to the scission configuration. In this situation the quasienergies λ_i are nearly equal to the dimensionless static energies $\widetilde{\beta}_0\epsilon_i$. Thus the dynamical entropy $\widetilde{S}$ of Eq. (5.6b), which is determined by λ_i via the occupations $\widetilde{f}_i$, is also nearly equal to the entropy $\widetilde{S}_p$, Eq. (4.6), of the compound nucleus. Since $D\sim e^{-\widetilde{S}_p}$, this simply means that expression (5.10) for the fission width is mainly determined by the quantum penetrability $W(E,A)$ as expected for the energies near the ground state.

When the excitation energy increases, the mean field starts farther from the compound nucleus shape and the contributions in the entropy $\widetilde{S}$ of the deformations close to the scission configuration become more significant. When the fission barrier is approached, the barrier deformation becomes dominant.

In the region close to the barrier the dynamics of the mean field is expected to concentrate in one mode. This is the unstable mode of harmonic vibrations around the static mean-field which represents the barrier saddle point configuration. In this energy region, multiple reflections of the tunneling solution become important, which leads to the replacement[31] of the penetrability factor $\exp(-W)$ in Eq. (5.10) by the more appropriate expression $(1+\exp W)^{-1}$. For energies above the barrier the quantum effects should gradually disappear and only the statistical phase space contributions should remain. These can be calculated on the basis of the static mean-field solution representing the barrier saddle point shape in the same way the compound nucleus level density was calculated in the preceding chapters. The foregoing discussion of the energy region close to the fission barrier is based on arguments which seem to be physically plausible. It is not clear to us at the present time how to make these arguments more rigorous or precise.

Finally, we comment on the practical solution of the induced fission Eqs. (5.3). They represent a set of coupled nonlinear equations and, of course, we cannot supply a general proof of the existence of solutions. Numerically, however, they are very similar to the static mean-field equations with temperature discussed in Sec. II. The standard iteration procedure can be used, the added complication being one more dimension, the imaginary time variable η. In Ref. 15 the limiting case of spontaneous fission was discussed in the framework of a model many-fermion system and the tunneling solutions were demonstrated. Work is now in progress to extend these calculations to energies above the ground state. Preliminary results show the existence of solutions for these energies. A full account of the calculations will be reported in a separate publication.

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APPENDIX A: TEMPERATURE DEPENDENT RPA EQUATIONS

Equation (3.13) represents a natural generalization of the ordinary RPA to finite temperature.[19] It is easy to show that if ξ_{ik}^{ν} is a solution of (3.13) with an eigenvalue ω_ν, then $\zeta_{ik}^{(\nu)} \equiv \xi_{ki}^{(\nu)*}$ is also a solution with an eigenvalue $(-\omega_\nu)$. This fact and the Euler formula

$$\frac{\sinh z}{z} = \prod_{N=1}^{\infty} \left[1+\frac{z^2}{N^2\pi^2}\right] \tag{A1}$$

are used in evaluating the ratio of products in (3.14). Consider first the terms with $N \neq 0$:

$$\prod_{N\neq 0} \frac{\prod_\nu \left[1+\dfrac{i\beta\omega_\nu}{2\pi N}\right]}{\prod_{j,k}\left[1+\dfrac{i\beta\Delta\epsilon_{jk}}{2\pi N}\right]} = \frac{\prod_\nu \prod_{N>0}\left[1+\dfrac{\beta^2\omega_\nu{}^2}{4\pi^2N^2}\right]}{\prod_{j,k}\prod_{N>0}\left[1+\dfrac{\beta^2\Delta\epsilon_{jk}{}^2}{4\pi^2N^2}\right]} = \frac{\prod_\nu \dfrac{\sinh(\beta\omega_\nu/2)}{\beta\omega_\nu/2}}{\prod_{j,k}\dfrac{\sinh(\beta\Delta\epsilon_{jk}/2)}{\beta\Delta\epsilon_{jk}/2}} . \tag{A2}$$

Together with the terms with $N=0$ this gives for (3.14)

$$\det(1+\beta VD) = \frac{\prod_\nu \sinh(\beta\omega_\nu/2)}{\prod_{j,k}\sinh(\beta\Delta\epsilon_{jk}/2)} . \tag{A3}$$

Using the symmetry property of the eigenvalues ω_ν discussed in the beginning of this appendix and Eq. (3.11), one obtains the final result (3.15).

The terms with $j=k$ are not included in the product of (3.15) since there is a corresponding number of zero eigenvalues ω_ν in Eq. (3.13). This is due to the presence of the matrix F in (3.13) which decouples the nondiagonal components $\xi_{ik}^{(\nu)}$ from the diagonal ones. The latter have all eigenvalues $\omega_\nu = 0$.

In the zero temperature limit the matrix F,

$$\begin{aligned} F_{pn,rs} &\equiv \delta_{ps}\delta_{rn}(f_n - f_p) \\ &\equiv \delta_{ps}\delta_{rn}[f_n(1-f_p) - f_p(1-f_n)] , \end{aligned} \tag{A4}$$

becomes a projector on the particle-hole subspace.

The corresponding components of $\xi_{ik}^{(\nu)}$ in (3.13) become decoupled from the particle-particle and hole-hole components. The former satisfy the ordinary zero temperature RPA equations while the latter have eigenvalues ω_ν equal to the differences of particles or holes energies, respectively. These cancel against the corresponding terms in the numerator of (3.15) and only particle-hole differences are left in the zero-temperature expression (3.19). Further discussion of the finite temperature RPA can be found in Ref. 19.

APPENDIX B: SINGLE-PARTICLE CONTINUUM STATES IN THE NUCLEAR FREE ENERGY

In the saddle-point approximation (2.14) the free energy of a particular mean-field configuration is represented as a sum of two terms: $\Omega_p[\alpha,\beta,\sigma_0] + \Omega_c[\alpha,\beta,\sigma_0]$. In this Appendix we discuss the volume dependence of this expression arising from the single-particle continuum states in the self-consistent potential, which are populated at finite temperatures.

Consider first the single-particle term $\Omega_p[\alpha,\beta,\sigma_0]$ given by the expression (2.11). The sums over continuum states present in this expression should be replaced by integrals

$$\sum_i \to \int d\epsilon\, g(\epsilon) , \tag{B1}$$

where $g(\epsilon)$ is the single-particle density of states $g(\epsilon)$ in the mean-field potential generated by σ_0.

In the continuum the density $g(\epsilon)$ is a sum

$$g(\epsilon) = g_0(\epsilon) + \Delta g(\epsilon) , \tag{B2}$$

where $g_0(\epsilon)$ corresponds to a state density of free nucleons and $\Delta g(\epsilon)$ reflects the effect of the scattering from the mean-field potential. For instance, in the spherically symmetric potential the continuum wave functions at large distances $r^{-1}\sin(kr - \pi l/2 + \delta_l)$ with the quantization $kR - \pi l/2 + \delta_l = \pi n$, at large radius R, imply for (B1) in the k space

$$\sum_i \to \sum_{l=0}^{\infty} (2l+1) \int_0^\infty dk \left[\frac{R}{\pi} + \frac{1}{\pi}\frac{d\delta_e}{dk} \right] . \tag{B3}$$

The terms containing R in (B3) are associated with g_0 in (B2) while the rest depend on the scattering phase shifts and represent Δg in (B2).

The free part g_0 is proportional to the volume of the system, whereas the scattering part Δg is independent of the volume. Obviously, in the corresponding free energy $\Omega_p[\alpha,\beta,\sigma_\infty]$ of the exterior nucleon gas with the constant density σ_∞, the integrals over the single-particle states contain only the free density of states g_0. Thus the subtraction of $\Omega_p[\alpha,\beta,\sigma_\infty]$ removes the volume dependence of $\Omega_p[\alpha,\beta,\sigma_0]$ in such a way that the remaining, volume-independent part accounts for the continuum states only as far as they are modified by the self-consistent potential well, as seems appropriate for the definition of the compound nucleus.

We now turn to the discussion of the volume dependence of the RPA correlation term $\Omega_c[\alpha,\beta,\sigma_0]$, which is given by the first term in expression (4.3). The double sum over single-particle states appearing in this term is converted into an integral using the level density

$$G_0(\epsilon,\epsilon') = g(\epsilon)g(\epsilon') , \tag{B4}$$

with $g(\epsilon)$ of (B2). This obviously has a leading quadratic dependence of the volume when both ϵ and ϵ' belong to the continuum.

The corresponding level density in the sum over the eigenfrequencies ω_ν in Eq. (4.3b) is of the form

$$G(\epsilon,\epsilon') = G_0(\epsilon,\epsilon') + \Delta G(\epsilon,\epsilon') , \tag{B5}$$

with $\omega = \epsilon - \epsilon'$. This follows from Eq. (3.13) determining ω_ν, which shows that G reduces to G_0 when the interaction term VF is turned off. A useful interpretation of ΔG in (B5) is therefore similar to ΔG in (B2). For ϵ and ϵ' in the continuum the generalized RPA Eq. (3.13) written in coordinate space can be regarded as a scattering of a particle and an "antiparticle," i.e., a hole in the presence of the potential well generated by σ_0.

The corresponding part of the first term in expression (4.3d) can be written as

$$\int_0^\infty d\epsilon' \int_0^\infty d\epsilon [G(\epsilon,\epsilon') - G_0(\epsilon,\epsilon')] \ln\sinh[\beta(\epsilon-\epsilon')/2] \tag{B6}$$

so that the volume dependence of $\Omega_c[\alpha,\beta,\sigma_0]$ is determined by $\Delta G(\epsilon,\epsilon')$. It should be obvious from the interpretation of $\Delta G(\epsilon,\epsilon')$ given above that it has only one power of the volume. This can be easily understood if one recognizes that the scattering via the interaction VF in Eq. (3.13), which determines $\Delta G(\epsilon,\epsilon')$, can occur anywhere in space including regions far outside the potential well.

Again in this case the subtraction of the term $\Omega_c[\alpha,\beta,\sigma_\infty]$, corresponding to a constant density σ_∞ of the exterior nucleon gas, removes the remaining linear volume dependence from $\Omega_c[\alpha,\beta,\sigma_0]$ so that the difference $\Omega_c[\alpha,\beta,\sigma_0]-\Omega_c[\alpha,\beta,\sigma_\infty]$ is independent of the volume of the system and is appropriate for use in the definition of the compound nucleus level density.

APPENDIX C: DYNAMICAL σ FIELD

Slater determinants built of solutions of (5.3) represent eigenfunctions of the operator U_σ in (5.2) for a given $\sigma(x,\eta)$. The eigenvalues are

$$\exp \sum_{i=1}^{\infty} (-n_i\lambda_i)\,, \tag{C1}$$

with $n_i=0$ or 1 and $\sum_{i=1}^{\infty} n_i = A$. Similar to Eq. (2.9) we can write the last term of (5.2) in the form

$$\mathrm{Tr} e^{\alpha\hat{A}} U_\sigma(\beta) = \sum_{A=0}^{\infty} \sum_{\{n_i\}} \exp \sum_{i=1}^{\infty} n_i(\alpha-\lambda_i)\,. \tag{C2}$$

In this expression for a general η-dependent σ, λ_i plays the same role as the single particle energy $\beta\epsilon_i$ for a static σ.

As in Sec. II we transform the σ dependent terms of (5.2) and obtain

$$\mathscr{S} = -\alpha A + \beta E + \beta/2(\sigma,V\sigma) + \sum_{i=1}^{\infty} \ln(1+e^{\alpha-\lambda_i})\,. \tag{C3}$$

In order to apply the saddle-point condition $\delta\mathscr{S}/\delta\sigma=0$ we need to evaluate $\delta\lambda_i/\delta\sigma$, i.e., to determine how the eigenvalues λ_i of Eq. (5.3) change with σ. As will be seen shortly the self-consistent σ obeys $\sigma(\eta)=\sigma(-\eta)$. Under this condition it is easy to verify[15] that the operator $\partial/\partial\eta+\beta h_\sigma$ is Hermitian in the space of (5.3c) provided the inner product is defined as

$$(v,u) = \int_{-1/2}^{1/2} d\eta \int dx\, v(x,-\eta)\, u(x,\eta)\,. \tag{C4}$$

Using this information we apply perturbation theory to Eq. (5.3) and find

$$\frac{\delta\lambda_i}{\delta\sigma(x,\eta)} = \beta \int dx' V(x-x') u_i(x',-\eta)\, u_i(x',\eta)\,. \tag{C5}$$

Differentiating (C3) we obtain from the condition $\delta\mathscr{S}/\delta\sigma=0$ the expression (5.3d) for the η-dependent mean field. The conditions $\partial\mathscr{S}/\partial\beta=0$ and $\partial\mathscr{S}/\partial\alpha=0$ are evaluated in a similar way and lead to Eqs. (5.4).

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