Nuclear Level Densities in the Static-Path Approximation

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(Received 1 August 1988)

We propose a unified theory of nuclear level densities, encompassing both spherical and deformed nuclei, using the static-path approximation. The theory appears numerically tractable for a pairing-plus-quadrupole Hamiltonian.

PACS numbers: 21.10.Ma, 05.30.−d

Important problems remain in the theory of nuclear level densities after more than 50 years of study. On a practical level, low-energy nuclear reactions depend crucially on the level densities. In situations where the levels cannot be measured directly, for example in *r*-process nucleosynthesis, one relies on extrapolated level densities to calculate the cross sections.[1]

The theory of level densities is usually based on the Fermi-gas model, which ignores important degrees of freedom. For example, the role of deformation degrees of freedom has never been satisfactorily incorporated in the theory of level densities. There may be orders-of-magnitude difference in level densities between spherical and deformed nuclei, which was noted by Bjørnholm, Bohr, and Mottelson,[2] and included in a numerical study by Døssing and Jensen.[3] Small-amplitude shape fluctuations also have an important effect. Here there are two quite different approaches to the level density. In the Landau theory of Fermi liquids there is a parameter, the effective mass of the nucleon at the Fermi surface, which becomes modified by coupling to vibrations. The effective mass increases because of the coupling, which results in a higher level density.[4] One can also derive an effect from finite-temperature perturbation theory. This gives separate, nonfermionic contributions to the partition function, which, however, also cause the level density to increase.[5] The pairing degree of freedom, which significantly changes the low-lying spectrum, is usually treated in an *ad hoc* fashion by an energy shift in the Fermi-gas formula for the level density.[1]

The finite-temperature perturbation theory starts with the Hartree-Fock theory as the initial approximation. This theory has well known shortcomings in that it does not treat fluctuations adequately. Fluctuations are especially important in the transition between spherical and deformed nuclei, and we expect that they are important in any nucleus at a high excitation energy. The Hartree-Fock theory predicts a sharp transition from deformed to spherical nuclei as the temperature is increased at angular momentum zero; in reality, the mean square deformation may not significantly change when fluctuations are included.[6,7] This missing fluctuation physics is not well described by the small-amplitude effects which perturbation theory deals with. In this work, we investigate a quite different way to go beyond the finite-temperature Hartree theory, which we hope will treat fluctuations better. This is the static-path approximation to the path-integral representation of the partition function, defined in Refs. 8 and 9. We believe that the method will be computationally tractable, and it might enable one to formulate expectation values at a finite temperature when the quantities depend on deformation.

The level density is obtained as the Laplace transform of the nuclear partition function.[10] The density may be obtained with respect to any additive quantum number. For a specified energy E, particle number N, and a component M of the angular momentum vector, the level density is obtained from the grand partition function

$$Z(T,\lambda,\omega)=\mathrm{Tr}\{\exp[-(E-\lambda N-\omega M)/T]\}\,, \qquad (1)$$

where the trace is over all many-body states of the system. To evaluate the partition function, we write it in a path-integral formulation, using the Hubbard-Stratonovich transformation,[11,12] and employ the static-path approximation.[8,9] In this description both single-particle and collective degrees of freedom are taken into account in a unified manner, since the formulation encompasses deformed potential fields and fluctuations of the fields around their self-consistent values.

The Hubbard-Stratonovich transformation applies to interactions that are separable and attractive. The simplest such Hamiltonian that contains the essential physics is the pairing-plus-quadrupole model.[13] The Hamiltonian is written

$$H=H_0-\tfrac{1}{2}\chi\sum_\mu(-)^\mu Q_\mu Q_{-\mu}-GP^\dagger P,\quad \chi>0,\ G>0\,, \qquad (2)$$

where $Q_\mu=f(r)Y_{2\mu}$ is the quadrupole operator and $P^\dagger$ is the pair-creation operator. The single-particle Hamiltonian H_0 is assumed to be rotationally invariant and may include the spin-orbit interaction. The two-body interaction in (2) can be expressed as a negative definite quadratic form in the Hermitian operators Q_0, $(Q_1+Q_1^\dagger)$, $i(Q_1-Q_1^\dagger)$, $(Q_2+Q_2^\dagger)$, $i(Q_2-Q_2^\dagger)$, $(P^\dagger+P)$, and $i(P^\dagger-P)$. In the path-integral formulation, the partition function is written as an integral over seven auxiliary fields, σ_μ, ζ, and ζ^*. In the static-path approx-

imation to Z, the fields become simple integration variables,

$$Z=\left(\frac{\chi}{2\pi T}\right)^{5/2}\frac{1}{\pi GT}\int\prod_{\mu}d\sigma_{\mu}\,d\zeta\,d\zeta^{*}\exp\left(-\frac{\chi}{2T}\sum_{\mu}|\sigma_{\mu}|^{2}-\frac{\zeta\zeta^{*}}{GT}\right)\mathrm{Tr}\left\{\exp\left(-\frac{H'}{T}\right)\right\}, \tag{3}$$

$$H'=H_0-\chi\sum_{\mu}(-)^{\mu}\sigma_{\mu}Q_{-\mu}-GP_0-\zeta^{*}P-\zeta P^{\dagger}-\lambda N-\omega M\,. \tag{4}$$

The five independent fields σ_μ form the components of a spherical tensor and play the role of quadrupole deformation parameters while ζ and ζ^* are the pairing fields. The operator P_0 is related to the number operator N by $P_0=\frac{1}{2}(N-\Omega)$, where Ω is half the number of states in the single-particle space. It arises from the commutation of the pair-creation and the pair-destruction operators.

Equation (3) is exact in the high-temperature limit, $T\rightarrow\infty$, cf. Ref. 9. When σ_μ and ζ are given by their self-consistent values $\sigma_\mu=\langle Q_\mu\rangle$ and $\zeta=G\langle P\rangle$, the single-particle Hamiltonian (4) is equivalent to the usual cranked Hartree-Bogolyubov Hamiltonian. Note, however, that the cranking axis is specified relative to a fixed axis in the laboratory system, which we take to be the z axis. The trace in Eq. (3) is over an exponential of a one-body operator and may be evaluated as a determinant,

$$\mathrm{Tr}\left\{\exp\left(-\frac{H'}{T}\right)\right\}=e^{-U/T}\prod_{i}[1+\exp(-E_i/T)]\,, \tag{5}$$

where U is the zero-point energy and E_i is the quasiparticle energies of H'.

The partition function simplifies somewhat when the Hamiltonian is transformed to the intrinsic system of the principal axis of the quadrupole potential

$$\sigma_{\mu}=\frac{1}{\chi}M\omega_0^2\sum_{\nu}a_{\nu}D^{2}_{\mu\nu}(\phi,\theta,\psi)\,,$$

$$a_{-1}=a_1=0,\quad a_0=\beta\cos\gamma,\quad a_{-2}=a_2=\frac{1}{\sqrt{2}}\beta\sin\gamma\,. \tag{6}$$

Here $D^2(\phi,\theta,\psi)$ is Wigner's rotation matrix. The normalization in (6) is chosen so that for a harmonic-oscillator potential of frequency ω_0 the self-consistent values of the deformation parameters β and γ agree with the parameters used in the Bohr Hamiltonian.[14] Here, however, β and γ give the deformation of the potential and not of the wave functions. The pairing fields can be brought to a simpler form by our writing

$$\zeta=\Delta e^{i\alpha}\,, \tag{7}$$

and noting that the spectrum of the Hamiltonian (4) does not depend on the gauge angle α. With these transformations, the partition function becomes

$$Z=\frac{4\pi}{GT}\left(\frac{a}{2\pi}\right)^{5/2}\int_0^{\infty}d\Delta\Delta\int_0^{\pi}d\psi\int_0^{\pi}d\theta\sin\theta\int_0^{\infty}d\beta\beta^4\int_0^{\pi/3}d\gamma\,|\sin(3\gamma)|$$

$$\times\exp\left(-\frac{1}{2}a\beta^2-\frac{\Delta^2}{GT}\right)\mathrm{Tr}\left\{\exp\left(-\frac{H'}{T}\right)\right\},\quad a=\frac{M^2\omega_0^4}{\chi T}\,, \tag{8}$$

and the quasiparticle Hamiltonian is

$$H'=H_0-M\omega_0^2f(r)\beta\left(\cos\gamma\,Y_{20}+\sin\gamma\frac{1}{\sqrt{2}}(Y_{22}+Y_{2,-2})\right)-GP_0-\Delta(P^{\dagger}+P)$$

$$-\lambda N-\omega(\cos\theta I_3-\sin\theta\cos\psi I_1+\sin\theta\sin\psi I_2)\,. \tag{9}$$

The intrinsic coordinate system is labeled (1,2,3) and the spherical harmonics and the angular momentum operator are given with respect to this system.

The integrand of (8) has the appearance of a thermodynamic probability $e^{-F(\tau)/T}$, with a free energy F given in terms of the field variables τ. One would certainly like to define a free energy to calculate the expectation values of quantities that depend on deformation.[15] At first sight, Eq. (8) appears to satisfy this goal. However, the variables τ measure the deformation of the potential and not that of the density and, consequently, expectation values of quantities depending on density cannot be directly calculated.

The partition function (8) contains a prefactor that depends on the temperature. This has the unsavory consequence that at low excitation energy the heat capacity becomes negative and thus the solution is thermodynamically unstable. In order to investigate this and to check the overall approximation, we have numerically evaluated the partition function in the seniority model. The Hamiltonian contains only the pairing interaction, operating in 2Ω degenerate single-particle levels. The exact result for the partition function is given by the seniority model,[16] while the static-path approximation is

$$Z=\frac{2}{GT}\int_0^{\infty}d\Delta\Delta\exp\left[-\frac{1}{T}\left(\frac{\Delta^2}{G}-\Omega(\lambda+E)\right)\right]$$

$$\times[1+\exp(-E/T)]^{2\Omega}\,. \tag{10}$$

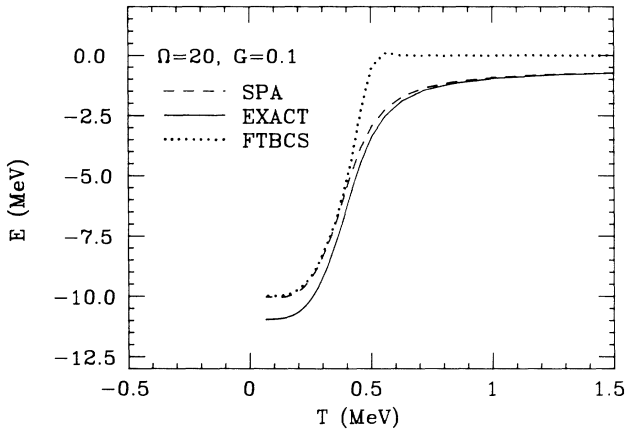

FIG. 1. Energy as a function of the temperature in the seniority model. The various curves show the results obtained in the exact calculation, in the static-path approximation (SPA), and in the finite-temperature BCS theory (FTBCS), as indicated in the figure.

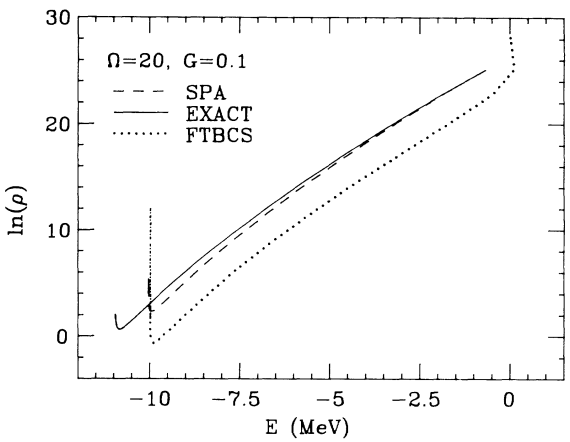

FIG. 2. Level density as a function of the energy in the seniority model. See caption to Fig. 1.

We specialize to a half-filled shell, $\lambda = -G/2$; $\langle N \rangle = \Omega$ and $E = \Delta$. In the low-temperature limit the energy becomes

$$E = -\frac{\partial \ln Z}{\partial (1/T)} + \lambda N \approx \tfrac{1}{4} G \Omega^2 - \tfrac{1}{2} T. \qquad (11)$$

Mathematically, the last term arises from the fact that the integrand in Eq. (3) is not peaked at a point in the space of ζ and ζ^*. Normally, each integration contributes a factor $T^{1/2}$, canceling a similar term in the prefactor of the partition function. However, when one of the variables is cyclic with the integrand peaking on a line, as in the seniority model, the powers of T are not canceled in the integration. A similar thing happens with the Euler angles in the pairing-plus-quadrupole model. Each of the Euler angles gives rise to an additional $-\frac{1}{2} T$ in the energy expansion at low temperature, provided that the ground state is well deformed. At high temperature, the exponential peaks at zero deformation and the energy approaches the exact result.

In Fig. 1 we show the energy as a function of temperature, and in Fig. 2 the level density $\ln(\rho)$ is given as a function of energy. In the static-path approximation, the level density is not a single-valued function of the energy but as seen from the figures this is only a problem at very low excitation energy. Also shown in the figures are the results obtained by replacement of the partition function by the maximum of the integrand. This is equivalent to the finite-temperature BCS theory in the Hartree approximation. It is seen that the static-path approximation is superior to the finite-temperature BCS result. In practical calculations the energy difference between the static-path approximation and the exact ground state may pose a problem, since calculated energies are usually fitted to the experimental ground-state energy.

The final topic we discuss is the numerical difficulty in the evaluation of the static-path partition function. It is no more complex than our summing over constrained Hartree partition functions; in fact, it is somewhat simpler in that no self-consistency requirement is ever imposed. However, compared to a single Hartree calculation it is considerably more complex. There are six integrations required to deal with both neutrons and protons in Eq. (8), if we assume an isoscalar quadrupole interaction. A minimal mesh in this many variables would require about 500 points. This is to be compared with the number of iterations required in a Hartree calculation, which is only of the order of 10.

We believe the model is sufficiently realistic to be interesting in a space of a major shell, which involves about $N \approx 50$ particles. Each integration point requires a diagonalization in this space, which according to Ref. 17 requires about $30N^2$ operations. Also, the partition function needs to be computed over a mesh in ω, λ, and T, in order to make the Laplace transform to get level density at fixed angular momentum and particle number.

Support for this work was provided by the National Science Foundation under Grant No. 87-14432 and by the Carlsberg Foundation.

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