Exact Level Densities for the Harmonic Oscillator

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The number of levels of a many-fermion system confined by a harmonic-oscillator potential is computed as a function of excitation energy. Because of its exact nature, the formalism accounts for effects of shell structure on the level density. The method is easily extended to a variety of situations as is illustrated with the inclusion of isospin and deformation effects as well as a calculation of the number of spurious states.

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A simple but commonly used estimate of the level density of a nucleus is known since the work of Bethe [1]. It assumes a gas of noninteracting fermions and, through a statistical analysis, arrives at the following expression for the level density (see also Chap. 2 of [2]):

$$\rho(A, E) = \frac{1}{\sqrt{48}E} \exp\sqrt{2\pi^2 g(\epsilon_{\mathrm{F}})E/3}, \qquad (1)$$

where A is the particle number and E is the excitation energy. The A dependence in this formula arises through the density $g(\epsilon_{\mathrm{F}})$ of single-particle levels at the Fermi-surface energy ϵ_{F}. The Fermi-gas estimate (1) cannot be reliably applied at low excitation energy E where a low level density precludes a statistical analysis. At high excitation energy E, its derivation relies on the neglect of higher-order derivatives of the single-particle level density $g(\epsilon)$ and might be incorrect if this condition is not fulfilled [2]. Its most important limitation, however, is that it assumes independent particles.

After Bethe's work, it was soon realized that his approach is an approximation to exact state-counting formulas [3]. With the advent of the nuclear shell model, effects of shell structure on nuclear densities were investigated in this way [4], and combinatorial counting techniques were used to evaluate the level density of Fermi systems consisting of equally spaced single-particle levels [5]. This approach continues to inspire research in this field (see, e.g., [6,7]). Nevertheless, formulas based on the statistical estimate (1) (and its extensions) continue to be widely used [8] in applications where nuclear level densities are needed, e.g., in astrophysical studies [9]. A calculation of level densities that goes beyond the Fermi-gas model and takes account of the residual interactions between particles is much more involved. Because of the rapidly increasing size of the model space with mass, a direct diagonalization of the Hamiltonian matrix quickly becomes impossible. One way to get at the level density is via spectral averaging methods which have been applied to the spherical [10] and deformed [11] shell model. Alternatively, the Monte Carlo shell model (which also avoids diagonalization) has been proposed recently [12] to obtain nuclear level density distributions. Applications to nuclei in the $50 \leq A \leq 70$ mass region were considered for a pf [13] or $pf + g_{9/2}$ [14] single-particle space with a multipole interaction.

The approach presented in this Letter can be viewed as a counting method. A recurrence relation is established which allows the calculation of the exact number of harmonic-oscillator configurations with a given energy. The algorithm for computing such numbers can be established by relating them to those of a harmonic oscillator in a lower dimension [15].

Consider A identical fermions with spin s in an isotropic three-dimensional harmonic oscillator (HO). A single-particle state is labeled by three quantum numbers n_1, n_2, and n_3 which denote the numbers of oscillator quanta in the 1-, 2-, and 3-directions. Since the particles carry spin s, an additional quantum number σ is needed which labels the spin degeneracy. A many-body Slater determinant is specified by the occupation numbers $k^{\sigma}_{n_1 n_2 n_3}$ with indices that run over all possible values (i.e., $n_i = 0, 1, \ldots$ and $2s + 1$ distinct values for σ). For fermions, a single-particle level can be either occupied ($k^{\sigma}_{n_1 n_2 n_3} = 1$) or empty ($k^{\sigma}_{n_1 n_2 n_3} = 0$). The occupation numbers $k^{\sigma}_{n_1 n_2 n_3}$ of an A-particle state with total energy E_{t} must satisfy the following equations:

$$\begin{aligned} \sum_{n_1 n_2 n_3=0}^{\infty} \sum_{\sigma} k^{\sigma}_{n_1 n_2 n_3} &= A, \\ \sum_{n_1 n_2 n_3=0}^{\infty} \sum_{\sigma} (n_1 + n_2 + n_3) k^{\sigma}_{n_1 n_2 n_3} &= \mathcal{N}, \end{aligned} \qquad (2)$$

where $\mathcal{N}$ is the total number of oscillator quanta $\hbar\omega$ of the state, related with the total energy E_{t} through $E_{\mathrm{t}} = (\mathcal{N} + \frac{3}{2})\hbar\omega$. The enumeration of all solutions $k^{\sigma}_{n_1 n_2 n_3}$ determines the number of distinct A-particle states which shall be denoted as $c_3(A, \mathcal{N})$ with the index 3 referring to the dimensionality of the HO.

The derivation of the algorithm to calculate $c_3(A, \mathcal{N})$ requires elementary algebraic manipulations only and is as follows. Equation (2) can be rewritten as

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$$\sum_{n_1 n_2=0}^{\infty}\sum_{n_3=1}^{\infty}\sum_{\sigma} k^{\sigma}_{n_1 n_2 n_3} = A - A',$$
$$\sum_{n_1 n_2=0}^{\infty}\sum_{n_3=1}^{\infty}\sum_{\sigma}(n_1+n_2+n_3)k^{\sigma}_{n_1 n_2 n_3} = \mathcal{N} - \mathcal{N}', \tag{3}$$

where A' and $\mathcal{N}'$ are defined through

$$\sum_{n_1 n_2=0}^{\infty}\sum_{\sigma} k^{\sigma}_{n_1 n_2 0} = A',$$
$$\sum_{n_1 n_2=0}^{\infty}\sum_{\sigma}(n_1+n_2)k^{\sigma}_{n_1 n_2 0} = \mathcal{N}'. \tag{4}$$

A new set of unknowns $k'^{\sigma}_{n_1 n_2 n_3} \equiv k^{\sigma}_{n_1 n_2 n_3+1}$ is now introduced. The sums in (3) have again n_3 running from 0 to ∞ in terms of the new unknowns, and by subtraction of the first from the second equation, one finds

$$\sum_{n_1 n_2 n_3=0}^{\infty}\sum_{\sigma} k'^{\sigma}_{n_1 n_2 n_3} = A - A',$$
$$\sum_{n_1 n_2 n_3=0}^{\infty}\sum_{\sigma}(n_1+n_2+n_3)k'^{\sigma}_{n_1 n_2 n_3} = \mathcal{N} - \mathcal{N}' - A + A'. \tag{5}$$

Equation (5) has a structure identical to the original one but with smaller numbers of particles and quanta; Eq. (4) is also of a similar type but for a two-dimensional HO. In fact, the entire derivation can be carried out for a d-dimensional HO and yields the following recurrence relation:

$$c_d(A, \mathcal{N}) = \sum_{A'\mathcal{N}'} c_{d-1}(A', \mathcal{N}') \times c_d(A - A', \mathcal{N} - \mathcal{N}' - A + A'). \tag{6}$$

One needs, in addition, some boundary values for $c_d(A, \mathcal{N})$. They are

$$c_d(A = 0, \mathcal{N}) = \delta_{\mathcal{N}0},$$
$$c_d(A, \mathcal{N}) = 0, \quad \text{if } \mathcal{N} < \mathcal{M}^A_d, \tag{7}$$

where $\mathcal{M}^A_d$ denotes the minimum number of quanta for A particles in a d-dimensional HO. Note that the dependence on the spin degeneracy is introduced in the boundary values only, in particular, via the minimum number of quanta $\mathcal{M}^A_d$. An analysis of the one-dimensional case shows that (6) remains valid, provided one takes

$$c_0(A, \mathcal{N}) = \frac{(2s+1)!}{A!(2s+1-A)!}\,\delta_{\mathcal{N}0}. \tag{8}$$

The algorithm (6) is easily implemented numerically through a recursive procedure. An illustration of it is given in Fig. 1 which shows the level density $\rho(A, E)$ for 70 particles (a closed-shell number for the three-dimensional HO with spin $s = \frac{1}{2}$) up to an excitation energy of $30\hbar\omega$. The dots are calculated from $\rho(A, E) \equiv c_3(A, \mathcal{N} = \mathcal{M}^A_3 + E/\hbar\omega)/\hbar\omega$ for discrete values $E = 0, \hbar\omega, 2\hbar\omega, \ldots$ and with $\mathcal{M}^{70}_3 = 210$, the minimum number of oscillator quanta for 70 $s = \frac{1}{2}$ particles. The curve

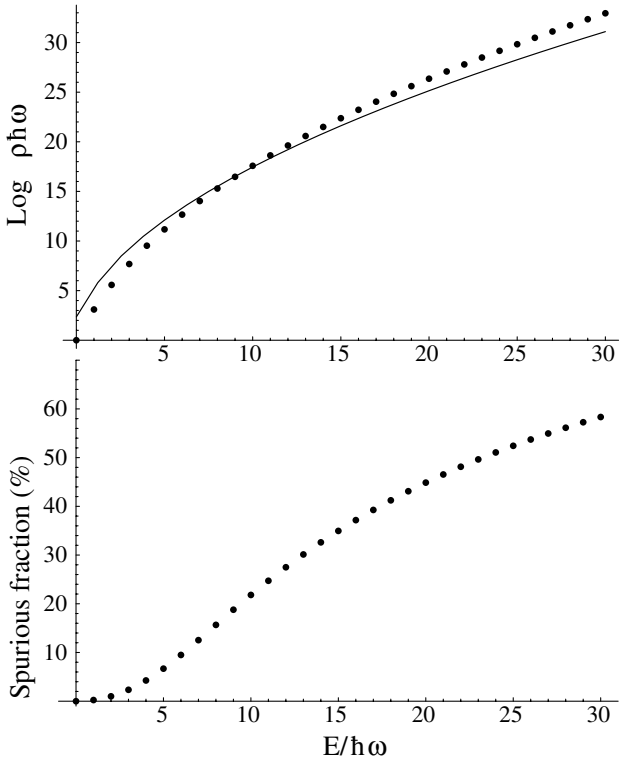

FIG. 1. Top: The level density $\rho(A, E)$ for $A = 70$ $s = \frac{1}{2}$ particles. The full curve is the level density computed from Bethe's one-component Fermi-gas formula, and the dots represent $c_3(A, \mathcal{N})$. Bottom: The number of spurious states as a fraction of the total number of states.

shows the Fermi-gas result (1) with the HO single-particle level density [in units $(\hbar\omega)^{-1}$] $g(\epsilon) = \frac{1}{2}(2s+1)(N+1)\times(N+2)$, with $\epsilon = N\hbar\omega$ and N the major-shell quantum number. For $A = 70$ particles, the Fermi energy corresponds to $N = 4$, $g(\epsilon_F) = 15(2s+1)$. Deviations from the statistical treatment occur at low energy but also at high energy because the dependence of $g(\epsilon)$ on ϵ is quadratic. Note that the number of configurations is huge but is nevertheless given *exactly* by (6).

The recurrence relation (6) defines the problem in the simplest possible situation but can be easily adapted to a variety of cases as will be illustrated with some examples.

A first application concerns the enumeration of spurious states. To estimate nuclear level densities, one is interested only in states that are in the ground configuration with respect to the center-of-mass excitation, while the solutions of (2) include nonphysical ones which represent a collective translation of the nucleus as a whole. Let us denote the number of *physical* solutions of (2) as $\tilde{c}_3(A, \mathcal{N}_e)$ where $\mathcal{N}_e \equiv \mathcal{N} - \mathcal{M}^A_3$ is the number of HO quanta above the minimum required for A particles. The number $\tilde{c}_3(A, \mathcal{N}_e)$ is found by subtracting from the total number those that can be constructed by acting (possibly several times) with the step-up operator for the center-of-mass motion, $B^{\dagger}_{\mu} \equiv \sum_i b^{\dagger}_{\mu}(i)/\sqrt{A}$, on any physical state (see Chap. 4 of [16]). Hence,

$$\tilde{c}_3(A, \mathcal{N}_e) = c_3(A, \mathcal{N}) - \sum_{\mathcal{N}'_e=1}^{\mathcal{N}_e} \frac{1}{2}(\mathcal{N}'_e + 1)(\mathcal{N}'_e + 2) \times \tilde{c}_3(A, \mathcal{N}_e - \mathcal{N}'_e). \quad (9)$$

This recurrence relation allows an easy determination of the fraction of spurious states, $1 - \tilde{c}_3/c_3$, and is illustrated in Fig. 1 for $A = 70$.

An important generalization concerns systems consisting of two different types of fermions, e.g., nuclei with neutrons and protons. The occupation numbers in this case are $k^{\sigma\tau}_{n_1 n_2 n_3}$, where τ is the intrinsic label of the fermion, say, $\tau = +$ for a neutron and $\tau = -$ for a proton. The number of possible configurations for N neutrons, Z protons, and $\mathcal{N}$ quanta, $c_3(N, Z, \mathcal{N})$, can again be obtained with recursive techniques. Alternatively, it follows from

$$c_3(N, Z, \mathcal{N}) = \sum_{\mathcal{N}'} c_3(N, \mathcal{N} - \mathcal{N}')c_3(Z, \mathcal{N}). \quad (10)$$

The quantities $c_3(N, Z, \mathcal{N})$ can be evaluated for closed as well as for open shells and this provides a simple way for estimating the effect of shell structure on nuclear level densities. This is illustrated in Fig. 2 which shows the exact HO results for systems corresponding to the nuclei ^{16}O and ^{28}Si and compares them to the two-component Fermi-gas estimate [see Eq. (2B-42) of [2] together with the single-particle density (6.519) of [17]]. This procedure clearly underestimates the level density of an open-shell nucleus. The figure also illustrates that the Bethe formula with *fitted* single-particle level density a and back shift Δ (i.e., replace E by $E + \Delta$) is able to reproduce the exact HO level density very well.

The main drawback of the Fermi-gas estimates is that these are based on an independent-particle assumption. Interactions between the particles are ignored and collective effects have to be introduced in a semiempirical way. Likewise, the formalism developed so far assumes independent particles in a HO and thus suffers from the same problem. However, a simple generalization to an *anisotropic* HO leads to a formulation that accounts for an important collective effect, namely, deformation. Although the problem can be formulated for a HO with complete anisotropy, assume by way of example that the quanta in two directions, say, 1 and 2, have the same energy which is different from the 3-quantum energy, $\hbar\omega_1 = \hbar\omega_2 \equiv \hbar\omega_{12} \neq \hbar\omega_3$. This is appropriate for a deformed nucleus with axial symmetry; a prolate nucleus corresponds to $\omega_{12} > \omega_3$ while an oblate one has $\omega_{12} < \omega_3$. A Slater determinant is specified by the occupation numbers $k^{\sigma\tau}_{n_1 n_2 n_3}$ and its energy is

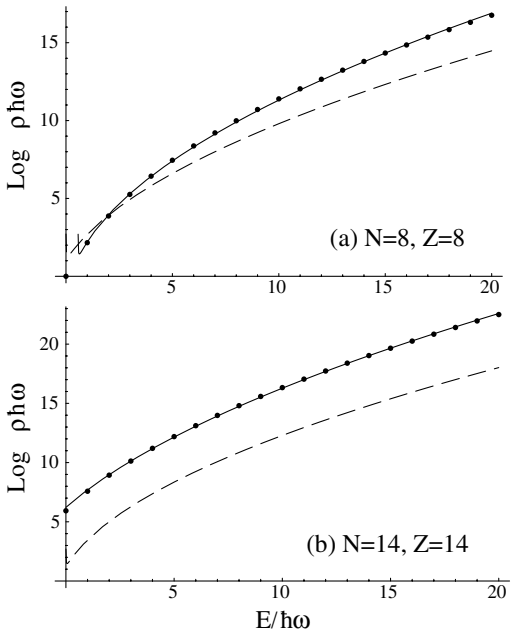

FIG. 2. The level density $\rho(N, Z, E)$ for (a) $N = Z = 8$ and (b) $N = Z = 14$. The dashed curves are the level densities computed from Bethe's two-component Fermi-gas formula and the dots represent $c_3(N, Z, \mathcal{N})$. The full curves result from a fit to the dots with the *back-shifted* Bethe formula.

$$E_t = (\mathcal{N}_{12} + 1)\hbar\omega_{12} + (\mathcal{N}_3 + \tfrac{1}{2})\hbar\omega_3, \quad (11)$$

where $\mathcal{N}_{12}$ is the number of quanta in the 1- and 2-directions, and $\mathcal{N}_3$ that of quanta in the 3-direction. The number of distinct states for $A^+ = N$ neutrons and $A^- = Z$ protons with $\mathcal{N}_{12}$ and $\mathcal{N}_3$ quanta is determined by the solutions of

$$\sum_{n_1 n_2 n_3=0}^{\infty} \sum_{\sigma} k^{\sigma\tau}_{n_1 n_2 n_3} = A^\tau, \qquad \tau = \pm,$$
$$\sum_{n_1 n_2 n_3=0}^{\infty} \sum_{\sigma\tau} (n_1 + n_2) k^{\sigma\tau}_{n_1 n_2 n_3} = \mathcal{N}_{12}, \quad (12)$$
$$\sum_{n_1 n_2 n_3=0}^{\infty} \sum_{\sigma\tau} n_3 k^{\sigma\tau}_{n_1 n_2 n_3} = \mathcal{N}_3,$$

and shall be denoted as $c_3(N, Z, \mathcal{N}_{12}, \mathcal{N}_3)$. The relevant recurrence relation in this case is

$$c_3(N, Z, \mathcal{N}_{12}, \mathcal{N}_3) = \sum_{N' Z' \mathcal{N}'_{12}} c_2(N', Z', \mathcal{N}'_{12}) \times c_3(N - N', Z - Z', \mathcal{N}_{12} - \mathcal{N}'_{12}, \mathcal{N}_3 - N + N' - Z + Z'), \quad (13)$$

and has the following boundary values:

$$c_3(N = 0, Z = 0, \mathcal{N}_{12}, \mathcal{N}_3) = \delta_{\mathcal{N}_{12}0}\delta_{\mathcal{N}_3 0}, \qquad c_3(N, Z, \mathcal{N}_{12}, \mathcal{N}_3) = 0, \quad \text{if } \mathcal{N}_{12} + \mathcal{N}_3 < \mathcal{M}_3^{N,Z}, \quad (14)$$

where $\mathcal{M}_3^{N,Z} \equiv \mathcal{M}_3^N + \mathcal{M}_3^Z$ denotes the minimum number of quanta for N neutrons and Z protons.

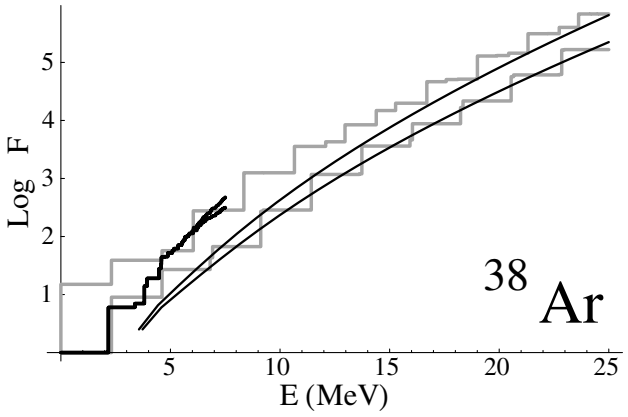

FIG. 3. The number of levels $F(E)$ in ^{38}Ar. The black jagged lines are lower and upper limits obtained from counting levels [18]. The smooth curves are the lower and upper limits for $F(E)$ obtained by fitting Bethe's two-component Fermi-gas formula (with back shift) to the experimental densities from [19]. The grey lines are calculated following the procedure explained in the text for two different deformations $\beta_2 = -0.2$ (lower) and $\beta_2 = 0.2$ (upper).

Possible applications of this formalism can be illustrated with a simple example. Figure 3 shows for ^{38}Ar the cumulative number of levels $F(E)$ up to a certain energy E, $F(E) = \int_0^E \rho(E')dE'$. The calculation of the theoretical level density requires the determination of the oscillator frequencies which can be taken from (see Chap. 5 of [17]) $\omega_{12} = \omega(1 + \frac{1}{3}\delta)$ and $\omega_3 = \omega(1 - \frac{2}{3}\delta)$ where $\hbar\omega = 41A^{-1/3}$ MeV sets the energy scale and $\delta = \sqrt{45/16\pi}\beta_2$, with β_2 the quadrupole deformation. For a given β_2, one then looks for the values of $\mathcal{N}_{12}$ and $\mathcal{N}_3$ that minimize the energy (11) and for which the corresponding number of configurations $c_3(N, Z, \mathcal{N}_{12}, \mathcal{N}_3)$ is nonzero. This defines the ground-state configurations. The number of configurations at nonzero excitation energy is obtained by increasing the number of quanta or by transforming 3-quanta into 12-quanta if $\omega_{12} > \omega_3$ or *vice versa* if $\omega_{12} < \omega_3$. The results of such a calculation at two different deformations, $\beta_2 = -0.2$ and 0.2, are shown in Fig. 3 in grey. Given the simplicity of the approach, the agreement can be called satisfactory. A possible source of uncertainty is the choice of the deformation parameter. It should be noted that the agreement is not always as gratifying as it is in ^{38}Ar: If one repeats a similar exercise for nuclei such as Fe or Ni, the calculation overestimates the observed densities because of the propinquity of the $N, Z = 28$ shell closure which is absent from the HO.

The applications of the recursive formalism discussed in this Letter have centered around the harmonic oscillator mainly because of the intrinsic interest of such a system and also because it can readily accommodate deformation. It is, however, easy to generalize the present recursive method to a system of fermions distributed over a set of single-particle levels with arbitrary energies ϵ_i and degeneracies Ω_i. It leads to recurrence relations [20] that are similar but not identical to the ones derived from partitions functions [21]. In fact, the applications reported in [21] and, in particular, the method to exclude continuum levels [22], can also be carried out with the current formalism. The use of realistic single-particle energies in combination with deformation effects and a reliable estimate of the number of spurious states should lead to fruitful applications of the present formalism in the domain of nuclear level densities.

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