Nuclear Level Densities and Partition Functions with Interactions

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A general theory, based on central limit theorems and unitary-group decompositions of the microscopic H, is given for the nuclear level density. The density appears in terms of convolutions of noninteracting-particle densities with easily calculable interaction functions given explicitly in terms of the Hamiltonian matrix elements.

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The nuclear level density, and its decomposition by conserved symmetries and by configurations (partitionings of the active particles among orbits), are important on practical grounds—they are sometimes measurable, and they enter into the calculation of reaction cross sections—and, formally, because, when given as functions of the Hamiltonian parameters, they determine the smoothed partition function and hence much of the statistical behavior of the nucleus. The purpose of this paper is to outline a general theory for interacting nucleons which derives, directly and without free parameters, from the microscopic Hamiltonian. Among other things it will explain why the conventional noninteracting-particle (NIP) level-density theories[1,2] are often successful, and will give forms and measures for the various kinds of orbital admixings generated by the interaction which the NIP theories do not deal with. From the formal standpoint it should lead to a more fundamental statistical theory of nuclear reactions and should make contributions also to the theory of the effective interaction.

The basis of the theory is an elementary unitary-group decomposition of the interaction Hamiltonian, coupled with the use of spectral- and ensemble-averaging methods. It has been argued before,[3] and to a considerable extent demonstrated,[3,4] that spectral averaging should lead to a proper level-density theory. A problem of form, however, arises, with spectral averaging, from the initial restriction of the single-particle (sp) spectrum to a finite set of sp states. This leads to the level density as a superposition of configuration densities valid only for a restricted part of the spectrum. The consequence is that one loses contact with the essentially combinatorial NIP form. Moreover, as we extend the sp spectrum in order to proceed to higher energies we encounter a problem of substance, namely that the variances of all the configuration distributions increase indefinitely; this, on the face of it, generates ever larger orbital admixings and spreadings, destroying the shell-model stability. We shall dispose of both of these problems.

Let the single-particle model space be partitioned as usual according to major shells, and further via spherical (j) orbits. Then the m-particle states are described via configurations which we may catalog by s, the major-shell excitation; for example, if the $1s$ and $1p$ shells are regarded as filled, $(1d, 2s)^m$ with $0 < m \leq 24$ has $s = 0$ while $(1d, 2s)^{m-2}(1f)^2$ has $s = 2$. Writing $G(k)$ for a k-body operator we have $H = H(0) + h(1) + V(2)$ where $h = \sum \epsilon_i(1) n_i$ is determined by the single-particle energies (spe), and the interaction V by the matrix elements V_{ijkl}. V also has a major-shell decomposition, $V = \sum V_t$ with $t = 0, 2, \ldots$, where V_t generates $\pm t\hbar\omega$ excitations. When $V = 0$ we have the NIP density, $I_0(E)$ say, which consists of a number of degenerate sets ("spikes") labeled by configurations (c) with energies $\mathcal{E}_c$ and degeneracies d_c. The smoothed form of $I_0(E)$, which is essentially $\exp(bE)^{1/2}$, can be calculated by either conventional or spectral methods. For brevity, we do not deal with that here, nor with the (J, T) decomposition which, even with interactions, can be carried out spectrally; the parity decomposition comes automatically with the configurations.

Unitary transformations come into play because of the antisymmetry of the fermion states. With that in mind we first extract from V that part ($V^{[0]}$ with $[0] = [0, 0, \ldots]$) which is invariant with respect to the group of simultaneous unitary transformations in every orbit α. Thus $V = V^{[0]} + V^{[\Lambda]}$ where $[\Lambda]$ then stands for all the nonscalar irreps. Since it is necessarily a quadratic polynomial in the orbital number operators $n_\alpha = \sum_{i \in \alpha} a_i^\dagger a_i$, $V^{[0]}$ preserves the configuration degeneracies, has no matrix elements connecting configurations, and receives contributions only

from V_0. It does, however, shift the centroids, $\mathcal{E}_c \to \mathcal{E}_c + \Delta\mathcal{E}_c$. Moreover, because of its J-scalar two-body nature, $V^{[\Lambda]}$ cannot transform as a nontrivial ($\neq 1$) scalar in *any* orbit since any n_α operator appearing in V must be multiplied by some $n_\beta - \delta_{\alpha\beta}$ and must therefore belong to $V^{[0]}$. Thus all the centroids are fixed by $V^{[0]}$. Our first problem now is to investigate the centroid shifts $\Delta\mathcal{E}_c$, asking in particular whether they are compatible with a renormalization of the spe.

Anticipating that the abnormally large orbital admixings will be eliminated, we see that at energy E there will be some finite subset of active orbits, containing, say, $N = N(E)$ sp states. We can now decompose that part of $V^{[0]}$ which involves the active orbits into U(N) tensors, $V^{[0]} = \sum V^{\nu,[0]}$ where V^ν, with "unitary rank" $\nu = 0, 1, 2$, belongs to the Young columnar shape $[N-\nu, \nu]$ and contains $\binom{n-\nu}{\nu}$ as a factor[3,5]; here $n = \sum n_\alpha$, summed over the active orbits. For fixed particle number m, V^0 behaves as a constant, V^1 as a one-body operator, and V^2 as a "true" two-body operator.

Now we "turn on" V as follows:

(1) $V^{0,[0]}$ which locally shifts the NIP spectrum. This adds to $H(0)$ and may for present purposes be ignored.

(2) $V^{1,[0]}$ which contains $(n-1)$ as a factor and therefore gives only a number-dependent renormalization of the spe. Thus $I_0(E) \to I_1(E)$ where $I_1(E)$ is locally of NIP form.

(3) $V^{2,[0]}$ which preserves the NIP degeneracies but moves the $\mathcal{E}_c$ in a way *not* given by changes in the spe. We shall see that $V^{2,[0]}$ is negligible.

(4) $V_0^{[\Lambda]}$, the part of the residual H which generates excitations only within a major shell, preserving the oscillator symmetry. This term produces the $0\hbar\omega$ admixings and spreadings (variances $\hat{\sigma}_c^2$) of the configurations. In conjunction with $I_1(E)$ it gives rise to the level density $I_2(E)$ which is valid for $E \lesssim \hbar\omega$.

(5) $V_{t>0}^{[\Lambda]} = V_{t>0}$. If treated like $V_0^{[\Lambda]}$ this term would generate the anomalously large orbital admixings. But by connecting configurations which are too far apart to be strongly interacting, it generates multimodal distributions which require a special treatment.

$V^{[0]}$ is obviously defined by the quantities $V_{\alpha\beta}$, the average interaction between two particles, one in orbit α and one in β (which may coincide). With N_α the orbital degeneracy, the dimensionality of the corresponding two-particle space is $N_{\alpha\beta} = N_\alpha(N_\beta - \delta_{\alpha\beta})(1 - \frac{1}{2}\delta_{\alpha\beta})$. Recognizing that $n_{\alpha\beta}$, defined similarly, is the projection operator for these states, we have, with $i<j$ when $\alpha = \beta$,

$$V^{[0]} = \sum_{\alpha\le\beta} V_{\alpha\beta} n_{\alpha\beta};$$
$$V_{\alpha\beta} = N_{\alpha\beta}^{-1} \sum_{i\in\alpha} \sum_{j\in\beta} V_{ij\,ij}. \tag{1}$$

To carry out the local decomposition referred to above we restrict the orbits to those active in the region of interest; then $N = \sum N_\alpha$. By simple intuitive arguments, or more formally,[3] we find

$$V^{0,[0]} = \bar{V}\binom{n}{2};\quad \bar{V} = \binom{N}{2}^{-1} \sum_{\alpha\le\beta} N_{\alpha\beta} V_{\alpha\beta},$$
$$V^{1,[0]} = (n-1)\sum \epsilon_\alpha(2) n_\alpha, \tag{2}$$
$$\epsilon_\alpha(2) = (N-2)^{-1} \sum (N_\gamma - \delta_{\alpha\gamma})(V_{\alpha\gamma} - \bar{V}).$$

$V^{0,[0]}$ is of no interest to us. The form of $V^{1,[0]}$ displays explicitly the renormalization of the sp Hamiltonian, $h \to \hat{h} = h + V^{1,[0]}$, while

$$\epsilon_\alpha(1) \to \epsilon_\alpha = \epsilon_\alpha(1) + (m-1)\epsilon_\alpha(2).$$

The unitary decomposition of $\hat{h}$ is

$$\hat{h} = \hat{h}^0 + \hat{h}^1 = \bar{\epsilon} n + \sum (\epsilon_\alpha - \bar{\epsilon}) n_\alpha$$

with $\bar{\epsilon} = N^{-1}\sum N_\alpha \epsilon_\alpha$; similarly for h with $\epsilon_\alpha(1)$ instead of ϵ_α. The results that $\binom{n}{2} = \sum_{\alpha\le\beta} n_{\alpha\beta}$ and $(n-1)n_\alpha = \sum_{\alpha\le\beta}(1+\delta_{\alpha\beta}) n_{\alpha\beta}$, while $V^{2,[0]} = V^{[0]} - V^{0,[0]} - V^{1,[0]}$, enables us to write "two-body" forms $\sum V_{\alpha\beta}{}^\nu n_{\alpha\beta}$ for each V^ν.

To understand the action of $V^{[0]}$ in the m-particle space of the active orbits we need, for the traceless operators h^1, $V^{1,[0]}$, and $V^{2,[0]}$, their relative magnitudes and their correlation coefficients. These are defined (for traceless operators F) in terms of the unitary norm $|F|^m$ whose square is $\langle F^\dagger F\rangle^m \equiv \binom{N}{m}^{-1} \mathrm{Tr}(F^\dagger F)$, the average eigenvalue of the Hermitian square, which is easily evaluated.[3] Three general results are that operators of different unitary rank are uncorrelated, that the correlation coefficient for operators of the same ν are independent of m, and that the norm of $F^\nu(k)$ grows asymptotically with m as $m^{k-\nu/2}$ so that $|h^1|^m \sim m^{1/2}$, $|V^{1,[0]}|^m \sim m^{3/2}$, and $|V^{2,[0]}|^m \sim m$. With typical interactions[6] we find that, in the two-particle space, $V^{1,[0]}$ and $V^{2,[0]}$ are of comparable magnitude, but very much smaller than h^1; moreover h^1 and $V^{1,[0]}$ have a strong positive correlation [$\gtrsim 0.9$ in (ds), 0.99 in the space generated by the first fifteen orbits, the primary one-body H in the latter case being taken as that of a harmonic oscillator]. Then, because the primary and induced one-body Hamiltonians add coherently, and because the latter grows more rapidly than $V^{2,[0]}$, the $V^{2,[0]}$ effects are negligible, giving a norm correction

~2% in (ds) and ~0.2% in the larger case. Taking for granted that this result extends to larger nuclei, and leaving for the future on explanation of its origin in terms of the spatial and spin properties of V, we conclude that the entire centroid-generating Hamiltonian $V^{[0]}$ is well represented by an effective one-body operator so that, under its inclusion, the NIP level-density form is still maintained.

As we have said, the $t=0$ part of the remaining interaction $V^{[\Lambda]}=V^{2,[\Lambda]}$ generates the $0\hbar\omega$ admixings and configuration spreadings. Though there will be fluctuations in the shapes of individual configuration distributions it is adequate for us to take them as Gaussian,[7] defined therefore by $(d_c, \mathcal{E}_c, \hat{\sigma}_c{}^2)$ with d_c the dimensionality, and $\hat{\sigma}_c{}^2=\sigma_c{}^2(t=0)$. It has been observed in many numerical calculations that m-particle configuration variances, calculated for realistic interactions, fluctuate very little about the average which, properly weighted, is

$$\sigma_A{}^2=d^{-1}\sum d_c\sigma_c{}^2=\langle(V^{[\Lambda]})^2\rangle^m, \tag{3}$$

where $\langle\cdots\rangle^m$, essentially a trace, is defined above. To calculate the variance of the $\sigma_c{}^2$ (similarly for $\hat{\sigma}_c{}^2$) we first construct a variance-generating operator K (analogous to the centroid generator above, and also expressed in terms of the n_α operators) and then evaluate *its* variance in the m-particle space. We find, as a compact operator version of an earlier result,[3] that

$$K=\sum_{\alpha\le\beta,\,\gamma\le\delta}\{\langle n_{\alpha\beta}n_{\gamma\delta}{}^{\times}\rangle^2\}^{-1}K_{\alpha\beta\gamma\delta}n_{\alpha\beta}n_{\gamma\delta}{}^{\times}. \tag{4}$$

Here $N_{\alpha\beta}K_{\alpha\beta\gamma\delta}$ is the sum of squares of the matrix elements of $V^{[\Lambda]}$ connecting the two-particle configurations $(1_\alpha, 1_\beta)$ and $(1_\gamma, 1_\delta)$, so that $K_{\alpha\beta\gamma\delta}$ is a partial $(1_\alpha, 1_\beta)$ variance, while $F^{\times}$ is the hole-particle adjoint of F, $n_\alpha{}^{\times}$ then being $N_\alpha-n_\alpha$, and of course $\langle K\rangle^m=\sigma_A{}^2$. The fractional rms deviation of the σ_c is then $\delta(m)=(|K|^m)^2/2\sigma_A{}^4(m)$; schematically $\sigma_c(m)=\sigma_A(m)[1\pm\delta(m)]$. The evaluation of the quadratic and quartic traces, in terms of the V_{ijkl}, follows easily[3] from their values for two, three, and four particles.

For ds-shell interactions ($N=24$) we find $\sigma_c(m)$ ~$8(1\pm0.03)$ MeV. Spaces whose sp spectra span several major shells are immense, and then simple averaging may be misleading. The appropriate averages, also easily calculable, are over the subspaces with fixed $s\hbar\omega$ excitation, which so far are noninteracting since $t=0$. For example, a ten-orbit interaction ($N=80$) with $m=24$ has $s_{\max}=44$ and gives $\hat{\sigma}_c=30\pm1.5$ MeV on the gross average. But for $s=0$, 2, and 4 we find $\hat{\sigma}_c=7.5(1\pm0.03)$, $11.9(1\pm0.11)$, and $15.2(1\pm0.10)$ MeV. We note incidentally a secular increase of the spreading widths with energy, $\hat{\sigma}_A{}^2(m)\to\hat{\sigma}_A{}^2(m,s)$.

Ignoring the small variance fluctuations we see now that for $E\lesssim\hbar\omega$, for which only $s=0$ is relevant, the $t=0$ level density is a simple convolution[8] of the renormalized NIP density $I_1(E)$ with an "interaction Gaussian" of unit integral and variance $\hat{\sigma}_A{}^2(s=0)$, $I_2(E)=I_1\otimes\rho_G{}^{(s=0)}[E]$. For the general case we have a sum of convolutions,

$$I_3(E)=\sum I_3{}^{(s)}(E)=\sum I_1{}^{(s)}\otimes\rho_G{}^{(s)}[E], \tag{5}$$

which displays the simple connection between the interacting- and noninteracting-particle densities. The s decomposition of the NIP level density follows directly from the configuration decomposition[3] and is very simply done by spectral methods. It is noteworthy that, in their phenomenological introduction of interactions into an NIP theory, Haq and Wong[9] have *assumed* a somewhat similar convolution form, as well as an increase of the effective configuration variances with energy.

The $t\ge2$ excitations make such large contributions to all the configuration variances that the corresponding Gaussian distributions could not be reconciled with the low-energy shell structure; with $(ds)^8$ configurations in our ten-orbit case $\sigma_c{}^2(t)=\sum_{c'}\sigma_{cc'}{}^2(t)\simeq64$, 280, and 550 MeV^2 for $t=0$, 2, and 4, giving widths ~8, 19, and 30 MeV. But these variances are still small compared with $(t\hbar\omega)^2$ where $t\hbar\omega$ is the separation of spherical configurations connected by V_t. Hence V_t generates admixings too weak to produce a unimodal (Gaussian) distribution. Formally the admixing parameter, which must be $\gtrsim1$ for Gaussian, is $\tau(t)=\sigma^2(t)/(t\hbar\omega)^2=0.18$, 0.09, and 0.03 for $t=2$, 4, and 6 excitations of $s=0$ configurations in our example. When $\tau(t)\ll1$ the configuration distributions become multimodal,[10] each of the well separated modes having a dominant s value. The $t\ge2$ variances then mainly describe not configuration spreading but rather the transport of small configuration intensities over a wide energy range. This effect, of no present interest, is measured by the anomalous variances. But the interesting quantities are the modal variances.

For small τ we can ignore the t admixings or treat them perturbatively. A procedure valid for arbitrary τ represents the intershell interactions

by a random matrix. We illustrate this for $t=2$ excitations of an $s=0$ configuration (adequate for $E\lesssim 30$ MeV), ignoring the internal variance σ_{00}^2 to begin with, as well as the fine structure associated with the $t=2$ excitations, both being much smaller than Δ^2. We thus have two spikes separated by $\Delta\simeq 2\hbar\omega$ with a two-body interaction whose elements we draw from an off-diagonal Gaussian orthogonal ensemble defined in the two-particle space but acting in the $(m\gg 2)$-particle space. Solving this we find that the $s=0$ distribution, ρ_G in (5), is replaced by a bimodal form which vanishes in $0<W<\Delta$, where $W=E-\mathcal{E}_c$, and otherwise is

$$\rho(W;\, s=0)=\sigma_{02}^{-2}|W-\Delta|\exp\{-W(W-\Delta)/\sigma_{02}^2\}. \tag{6}$$

In the weak-interaction limit ($\tau\ll 1$) (6) gives the perturbation result, a Gaussian modal distribution with variance $\sigma_{00}^2+\tau\sigma_{02}^2$. At the other limit ($\tau\gg 1$) we get $(1-\pi/4)\sigma_{02}^2$ for the modal variance; the model in this limit is artificial because of the $t\leq 2$ restriction, without which the configuration distributions would of course be Gaussian with anomalous variances. For the physically relevant intermediate strengths we have a true bimodal distribution, the "lost" $s=0$ intensity being replaced by $s=2$ and the modal variance taking on part of the intershell variance. For $\tau=0.18$, found for $(ds)^8$ in the ten-orbit case, the modal variance is $0.08\sigma_{02}^2\simeq 20$ MeV^2 which will increase the effective $s=0$ configuration widths from 8 to 9 MeV rather than to 19 MeV as in the naive treatment. We thus have disposed of the problem of the anomalous variances. It is the procedures used here which should have special relevance to effective-interaction theory.

A more complete account, with an extended treatment of the multi-$\hbar\omega$ excitations, and applications to level densities and other statistical quantities, will be given later. We acknowledge useful conversations with J. P. Draayer and C. Jacquemin. This work has been supported in part by the U. S. Department of Energy.

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