Exact Removal of the Center-of-Mass Spurious States from Level Densities

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We give recursive formulae for the exact removal of the contribution of the center-of-mass spurious states from the fixed-spin and parity nuclear level density found in shell-model calculations, provided the total level density for restricted configurations is known. The method is valid for a large class of problems using a harmonic oscillator basis. Using our earlier methods based on statistical spectroscopy that utilize the centroids and widths for a restricted class of fixed-spin configurations, such as $N\hbar\omega$ excitations, one can calculate very accurately level densities free of spurious states. The approach is applicable to other fermion and boson systems trapped by an oscillator potential.

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Cross sections of nuclear reactions at energies of astrophysical interest are usually calculated with the Hauser-Feshbach method. This requires exact knowledge of level densities for certain spin and parity in the Gamow window of energies around the particle threshold [1]. Level densities are important in many applications. At not very high excitation energy, the growth of the level density reflects the interplay of interactions inside the system; the energy variation of the level density may indicate the phase transformations smoothed out in finite systems: pairing quenching in nuclei [2] and small metallic particles [3], or magnetic effects in small quantum dots [4]. The correct reproduction of the level density helps in recognizing the regular or chaotic nature of spectral statistics in nuclei [5] and quantum dots [6]. Similar questions arise in other mesoscopic systems, such as atoms in traps [7] and condensed matter microstructures [8].

Recently, we developed a strategy [9,10] of calculating the spin- and parity-dependent shell-model level density. The main ingredients are (i) extension of methods of statistical spectroscopy [11–13] by calculating the first and second moments for different configurations at fixed spin (the use of conventional approaches with the spin-cutoff factors is also possible [13]), (ii) exact decomposition of many-body configurational space into classes corresponding to different parities and numbers of harmonic oscillator excitations, (iii) development of new effective interactions for model spaces of interest starting with the G-matrix [14] and fixing or fitting monopole terms or/and linear combinations of two-body matrix elements to experimental data, and (iv) an accurate estimate of ground state energy using the exponential convergence method (ECM) [15,16]. Other methods of choice [17–20] calculate the *density of states* and later use approximations to extract the *level density*, with its spin and parity dependence.

One of the problems on the way to the reliable level density, as well as in shell-model calculations in general, is that of spurious (excited) center-of-mass (c.m.) states. Calculations of nuclear density and momentum distribution also require accounting for admixtures of c.m. motion [21,22]. Many applications of magnetic traps or optical lattices are based on the coupling of c.m. motion with intrinsic many-body excitations. Modern experiments on cooling of atoms, molecular association, study of many-body effects, phase transitions, scalability for quantum control and information, and decoherence rely on the relation between c.m. and intrinsic dynamics, see for example [23–25].

As a rule, the classification of states in terms of the harmonic oscillator $N\hbar\omega$ excitations is applied. The restriction to particular classes of configurations is necessary to eliminate the contribution of spurious c.m. states. In Ref. [10], we showed how one can use this approach to approximately exclude the spurious states for low excitation energies. Here, we describe a more general method of exact removal of the c.m. spurious states from the level density for a certain class of $N\hbar\omega$ excitations (or combinations of them). This method uses the recursive techniques similar to that of Ref. [26], where, however, all spins were mixed together.

As a prerequisite, one needs to find the level density for all the states (including the spurious one) for several classes of $N\hbar\omega$ excitations and their combinations. Although the shell model cannot give an exact solution of the many-body problem, its modern versions with good effective interactions are reliable for nuclei in the $sd - pf$ model space, and the area of applicability is constantly growing, both due to the computational progress and to new physical approaches. It is expected that $(0 + 2)\hbar\omega$ and $(1 + 3)\hbar\omega$ will be soon feasible for the $sd - pf$ region of high interest in nuclear structure and astrophysics. For certain parity, one needs to know the *nonspurious* level density ρ° at a given excitation energy E, spin J, and a combination of $N, (N + 2), \ldots, (N + 2M)$ harmonic oscillator excitations,

$$\rho^{\circ}[E, J; (N) + (N + 2) + \cdots + (N + 2M)] \equiv \rho^{\circ}[E, J]_N^M \quad (1)$$

(in practice, $N = 0$ for natural parity states and $N = 1$ for unnatural parity states). It is well known [27,28] that, for a *complete* set of $N\hbar\omega$ oscillator excitations taken as a configurational basis, the eigenfunctions of the many-body Hamiltonian (including only relative kinetic energy [29]) can be exactly factorized into the product $\Phi_{\rm CM}\Phi_{\rm int}$ of the c.m. and intrinsic functions,

$$H\Phi_{\rm CM}\Phi_{\rm int} = \Phi_{\rm CM}H\Phi_{\rm int} = E\Phi_{\rm CM}\Phi_{\rm int}. \quad (2)$$

For removing the c.m. spurious components of the low-lying states, the Lawson method [30] is frequently used that adds to the actual Hamiltonian a shifted c.m. Hamiltonian multiplied by a positive constant β,

$$H' = H + \beta\mathcal{H}_{\rm CM} \equiv H + \beta\left[\left(H_{\rm CM} - \frac{3}{2}\hbar\omega\right)\frac{A}{\hbar\omega}\right]. \quad (3)$$

Here, the energies are expressed in units of $\hbar\omega$, and $\mathcal{H}_{\rm CM}\Phi_{\rm CM} = AN\Phi_{\rm CM}$, where $\Phi_{\rm CM}$ is the wave function describing the $N\hbar\omega$ c.m. excitations. Reasonably large values of β can be used to filter out the spurious wave functions [31,32]. However, this method is not very useful for calculating the nonspurious density of states with the aid of statistical spectroscopy because $\beta\mathcal{H}_{\mathcal{CM}}$ would distort the higher moments of the Hamiltonian.

Considering the complete set of $N\hbar\omega$ excitations, one can show that the dimensions $D^\circ(J, N)$ of the nonspurious subspaces for given total spin J can be calculated using the recursive formula

$$D^\circ(J,N) = D(J,N) - \sum_{K=1}^{N}\sum_{J_K=J_{K\min}}^{K,\text{step}\,2}\sum_{J'=|J-J_K|}^{J+J_K} D^\circ(J', N-K). \quad (4)$$

This is a logical identity similar to that used in Ref. [26], but with account of possible spins of the set of excitations. One can check the validity of Eq. (4) by inspecting the factorized classes of eigenstates in a particular case, say $N = 2$,

$$\Psi(J, N=2)\text{: } \Phi_{\rm CM}(J=0, N=0)\Phi_{\rm int}(J, 2), \quad [\Phi_{\rm CM}(1,1)\Phi_{\rm int}(J', 1)]_J, \quad [\Phi_{\rm CM}(2,2)\Phi_{\rm int}(J', 0)]_J, \quad \Phi_{\rm CM}(0,2)\Phi_{\rm int}(J, 0). \quad (5)$$

Since the c.m. wave function is symmetric with respect to particle permutations, the intrinsic wave functions are assumed to be constructed according to appropriate statistics; therefore, the method should work for bosons as well. Note that the $N - K = 0$ subspaces are always nonspurious, i.e., $\rho^\circ(E, J, 0) = \rho(E, J, 0)$. Consequently, the nonspurious level density for given J and N is defined by a similar formula [33]:

$$\rho^\circ(E,J,N) = \rho(E,J,N) - \sum_{K=1}^{N}\sum_{J_K=J_{K\min}}^{K,\text{step}\,2}\sum_{J'=|J-J_K|}^{J+J_K} \rho^\circ(E, J', N-K), \quad (6)$$

where E is the total energy. As an example, we consider the case $J = 2$ and $N = 1$ that gives

$$\rho^\circ(E,2,1) = \rho(E,2,1) - \sum_{J'=1}^{3}\rho(E,J',0). \quad (7)$$

Figure 1 shows the components of Eq. (7) for 20 particles (^{20}Ne) in the $s - p - sd - pf$ model space (the WBT interaction [34] was used). The exact level density can be obtained by diagonalization of Hamiltonian (1) with $\beta = 5$ shifting the spurious contribution to higher energies (around +10 MeV in Fig. 1). For comparison, Fig. 2 shows the effect of subtracting the second term in the r.h.s. of Eq. (7) from the first term. The result is the l.h.s. of Eq. (7) that exactly reproduces the nonspurious level density calculated with the Lawson procedure.

Assuming that one knows the spurious level densities for different J' and different combinations of N, $(N + 2)$, ..., $(N + 2M)$ excitations, and the nonspurious level densities for N, $(N + 2)$, ..., $(N + 2M - K)$ excitations ($K > 0$), we come to the total nonspurious level density in the form

$$\rho^\circ[E,J]_N^M = \rho[E,J]_N^M - \sum_{K=1}^{N+2M}\sum_{J_K=J_{K\min}}^{K,\text{step}\,2}\sum_{J'=|J-J_K|}^{J+J_K} \rho^\circ[E,J']_{N-K}^M, \quad (8)$$

with the condition that, if $(N - K) < 0$, then

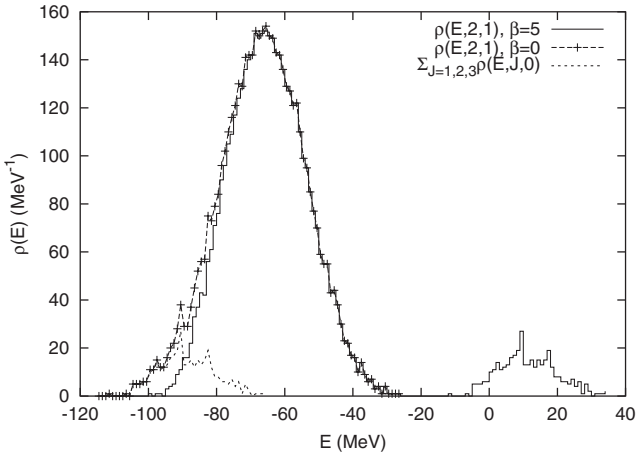

FIG. 1. Different contributions to the level density for 20 particles in the $s - p - sd - pf$ model space, as described by Eq. (7) (see text for details).

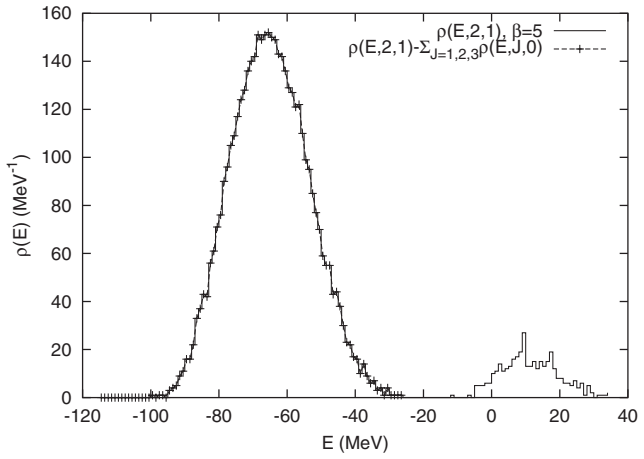

FIG. 2. The $\sum_{J=1,2,3}\rho(E,J,0)$ subtracted from the $\beta = 0$ level density of Fig. 1 exactly reproduces the nonspurious part of the level density (the lower part of the $\beta = 5$ spectrum).

$\rho^{\circ}[E,J']^{M}_{N-K} = \rho^{\circ}[E,J']^{M}_{N+2-K}$. In Eq. (8), we use for the total level density ρ the same abbreviation as in Eq. (1) for ρ°.

As an example, we take the particular case $J = 2$, $N = 0$, and $M = 1$, when the recursion is relatively short,

$$\rho^{\circ}[E,2]^{1}_{0} = \rho[E,2]^{1}_{0} - \sum_{J'=1}^{3}\rho^{\circ}(E,J',1) - \sum_{J_K=0}^{2,\mathrm{step}2}\sum_{J'=|2-J_K|}^{2+J_K}\rho(E,J',0). \quad (9)$$

Figure 3 shows separately (up to the signs) the three terms on the r.h.s of Eq. (9) for 10 particles (^{10}B) in the $s-p-sd-pf$ model space, with the same WBT interaction. The exact level density can be obtained by the direct diagonalization of the Hamiltonian (1) with $\beta = 10$ that shifts the spurious contribution due to the second term on the r.h.s. of Eq. (9), $\rho^{\circ}(E,*,1)$, to higher energies (around +120 MeV in Fig. 3), and the third term on the r.h.s. of Eq. (9), $\rho^{\circ}(E,*,0)$, to around +190 MeV in Fig. 3. Here, "*" stands for any necessary value J' in Eq. (9). We see the significant difference at low energies between the nonspurious density ($\beta = 10$, continuous line) and the density that mixes spurious and nonspurious states (labeled by dashes and pluses in Fig. 3). Figure 4 shows the effect of subtracting the second and third terms in the r.h.s. of Eq. (9) from the first term. The result is the l.h.s. of Eq. (9) that exactly reproduces the nonspurious level density calculated with the Lawson procedure.

In the shown examples, we used the exact shell-model level density for all necessary combinations of $(N + 2M)\hbar\omega$ excitations. It was demonstrated that one can use our methods [9,10] to obtain the same level density with high accuracy. An important ingredient in these calculations is the accurate knowledge of energy for the ground and yrast states in order to identify the excitation energy of the system and thresholds in the spectrum for all spins J' of interest. These energies are calculated either by the direct diagonalization in the corresponding shell-model space, or by using the ECM [15,16] that provides these energies with an error of about 100 keV after appropriate truncation up to less than 1% of total dimension. As was shown in [15], the exponential extrapolation based on generic properties of complicated ("chaotic") states correctly accumulates the pressure of excluded highly excited configurations on more regular ground and yrast states. The yrast energies are used in the expansion in terms of finite range Gaussians [9] to enforce the correct threshold behavior of the level density.

Since the number of partitions grows fast, in practice the calculation of fixed-J centroids and widths is not an easy

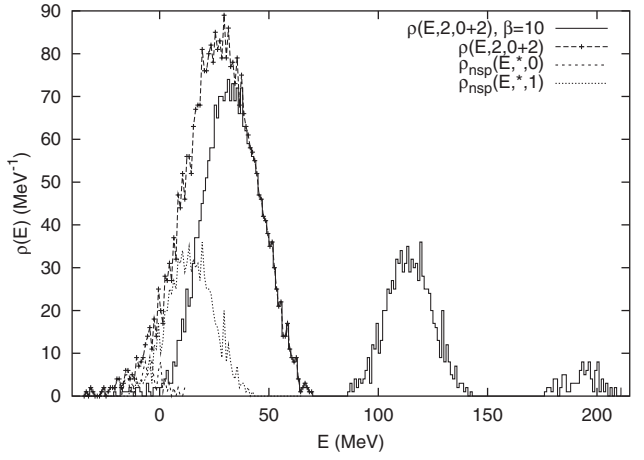

FIG. 3. Different contributions to the level density for 10 particles (^{10}B) in the $s-p-sd-pf$ model space ($\rho_{\mathrm{nsp}} \equiv \rho^{\circ}$), as described by Eq. (9) (see text for details).

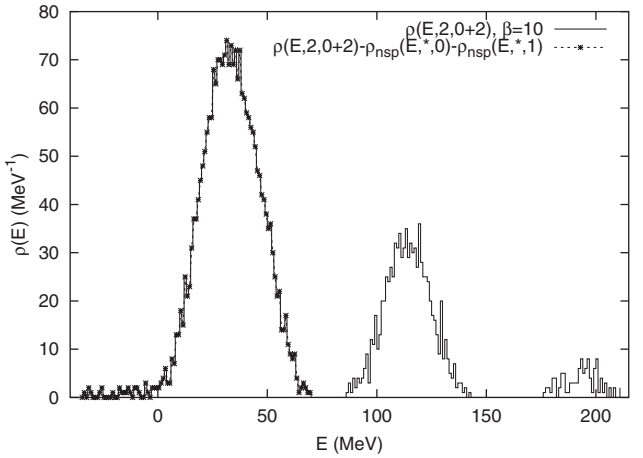

FIG. 4. The nonspurious $\rho(E,*,1)$, and $\rho(E,*,0)$ level densities subtracted from the total level density $\rho(E,2,0+2)$ of Fig. 3 calculated with $\beta = 0$; the nonspurious part of the level density (lower part of the $\beta = 10$ spectrum) is exactly reproduced.

task, and the required computational effort is comparable with that in the shell model for yrast energies. However, these calculations can be parallelized as shown by recent progress; further efforts are underway. As shown in [10], the use of the energy-dependent spin-cutoff factor is also a possibility, even if less accurate. The computational errors can accumulate in the process of using the recurrent relations. Although it is hard to estimate this uncertainty, our experience shows that an error in individual level densities does not exceed 10% and is even less for $N_{\max} \leq 3$.

In conclusion, we presented a new way for calculating the spin- and parity-dependent level densities in finite quantum many-body systems by proposing an exact method of removing the spurious c.m. contribution. This method requires knowledge of the level densities with fixed spin and parity for different combinations of $N\,\hbar\omega$ excitations. We worked out two examples with ten and 20 particles in the first few major harmonic oscillator shells and demonstrated that the method works practically exactly. The conventional Lawson method can compete with this procedure only if it allows to filter out the spurious contributions with a relatively small value of β. This is more plausible for low-lying states but not for the level density. Although our primary purpose was in applications to nuclear reactions of astrophysical interest and nuclear structure, the same approach could be applied to other many-fermion and many-boson systems trapped by a harmonic oscillator potential, provided that the trap is harmonic and one can use the same oscillator frequency for the basis expansion and for the trapping potential.

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