Approximation for shell-model level densities: Ergodicity

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Received: 28 June 1994/Revised version: 9 May 1995

Abstract. Using the supersymmetry method, we show that the maximum entropy approach for the calculation of nuclear shell-model partial and total level densities, developed in a previous paper, is ergodic.

PACS: 21.60.Cs; 21.10.Ma

1. Introduction

The calculation of nuclear level densities is a long-standing problem in nuclear structure physics. The spectroscopic interest in the total densities is self-evident. As shown recently, the partial level densities defined by projection onto suitably chosen subspaces play a fundamental role in the theory of precompound reactions [1, 2]. A method for calculating such partial densities is therefore also much needed. However, in spite of much work done in this field, a quantitatively reliable approach for calculating the densities for a wide range of mass numbers and excitation energies which accounts for the residual interaction is still missing.

In a previous paper, we have added a novel procedure to the existing armory [3]. Starting point was the nuclear shell model with residual interactions. We constructed a particular Gaussian ensemble of random matrices using the maximum entropy hypothesis [4] and the following conditions. Given a division of the shell-model Hilbert space into subspaces, the first and second subspace moments of the ensemble should be equal to the corresponding traces of the underlying shell-model Hamiltonian. The ensemble-averaged total and partial level densities obtained from this construction compared favorably with the results derived by an exact diagonalization of the underlying Hamiltonian. The method which was used to calculate the ensemble-averaged level densities employs a representation of the Green's function of a random Hamiltonian in terms of a Grassmann integral, and a saddle-point approximation. In a more complex but also more realistic framework, this approach has meanwhile been used for practical calculations [5, 6]. In principle, the approach can be used for estimating the level densities of general Hamiltonians which act in a finite-dimensional Hilbert space.

The saddle-point approximation can be viewed as the contribution of lowest order in an asymptotic (saddle-point) expansion. This expansion proceeds in inverse powers of the dimensions $N_j$ of the subspaces mentioned above. The implicit assumption that the asymptotic series, for values of $N_j$ which are of physical interest, are accurately approximated by their lowest order terms, was analyzed in a more recent paper [7]. In this paper, the validity of the saddle-point approximation has been examined by explicitly constructing all terms of first and second order in inverse powers of $N_j$ in what in fact would be called a loop expansion in field theory. In doing so, we found that except for the tails of the level distributions, where the saddle-point expansion itself becomes unrealistic, these corrections behave smoothly, and, as numerical simulations show, tend to correct the leading approximation towards the true ensemble-averaged density. We have found that even for subspace dimensions $N_j$ as small as ten or so, the saddle-point approximation is quite reliable, the first order corrections are small, and the second order corrections are negligible.

To complete the theoretical framework of the proposed method, it remains to demonstrate the ergodicity of the procedure, i.e. the implicitly assumed generic equality of the spectral-averaged level densities (partial, total) referring to one member of the ensemble and of the corresponding ensemble-averaged level densities. The proof of this assumption is the subject of the present paper. In Sect. 2, we introduce the notation and give brief summary of basic equations of the method. The ergodicity is demonstrated in Sect. 3.

2. The ensemble and the ensemble-averaged level densities

We follow closely the terminology and notation of [3]. We consider a given real and symmetric shell-model
Hamiltonian $H_{sm}$ acting in an $N$-dimensional shell-model Hilbert space $\mathcal{S}$ of states of given quantum numbers (spin, parity), and the partial densities referring to a given $s$-fold partitioning of $\mathcal{S}$ into a direct sum $\mathcal{S} = \bigoplus_{j=1}^{s} \mathcal{S}_j$ of orthogonal subspaces $\mathcal{S}_j$, $j = 1, \ldots, s$. The dimensions and projectors of $\mathcal{S}_j$ are denoted by $N_j$ and $\mathcal{P}_j$ respectively, with $\sum_j N_j = N$ and $\sum_j \mathcal{P}_j = 1$, and their orthonormal basic states by $|jm\rangle$, $m = 1, \ldots, N_j$. In this notation, the defining equations for the normalized shell-model total and partial level densities $\rho_{sm}(E)$ and $\rho_{sm,j}(E)$ are

$$\rho_{sm}(E) = \frac{1}{N} \text{tr}[\delta(E - H_{sm})],$$

$$\rho_{sm,j}(E) = \frac{1}{N_j} \text{tr}[\mathcal{P}_j \delta(E - H_{sm})].$$

with $N \rho_{sm}(E) = \sum_j N_j \rho_{sm,j}(E)$. Following [3], simple estimates of (spectral-averaged) $\rho_{sm}(E)$ and $\rho_{sm,j}(E)$ are given by the average densities (we denote the ensemble averaging by overbars)

$$\bar{\rho}(E) = \frac{1}{N} \text{tr}[\delta(E - H)], \quad \bar{\rho}_j(E) = \frac{1}{N_j} \text{tr}[\mathcal{P}_j \delta(E - H)]$$

of the ensemble of random Hamiltonians $H$, which is linked to $H_{sm}$ by the moment constraints

$$\text{tr}(\mathcal{P}_j H) = \text{tr}(\mathcal{P}_j H_{sm}), \quad \text{tr}(\mathcal{P}_j H \mathcal{P}_j H) = \text{tr}(\mathcal{P}_j H_{sm} \mathcal{P}_j H_{sm}),$$

and has maximum entropy compatible with these restrictions. Solving the arising variational problem for the ensemble distribution function shows that the ensemble is a generalized Gaussian orthogonal ensemble (generalized GOE), in which the matrix elements $H_{nm}^{ij} = \langle jm|H|jn\rangle$ of the individual random Hamiltonians $H$ are distributed according to the weight functions

$$W(H_{nm}^{ij}) = (2\pi B_{nm})^{-1/2} \exp \{-2(B_{nm})^{-1} (H_{nm}^{ij} - M_{nm}^{ij})^2\}.$$

The distribution parameters $B_{nm}^{ij}$, $M_{nm}^{ij}$ are uniquely specified by the subspace moments of $H_{sm}$,

$$M_{nm}^{ij} = \delta_{ij} \delta_{nm} M_j, \quad M_j = h_j N_j^{-1},$$

$$B_{nm}^{ij} = B_{jj}(1 + \delta_{ij} \delta_{nm}),$$

$$B_{jj} = (h_{jj} - \delta_{jj} h_j^2 N_j^{-1}) [N_j (N_j + \delta_{jj})]^{-1},$$

where $h_j$ and $h_{jj}$ denote the first and the second of the traces of $H_{sm}$ appearing in (3), respectively. We assume that the shell-model Hamiltonian $H_{sm}$ couples all $s$ subspaces.

An explicit expression for $\bar{\rho}_j(E)$, derived in [3], reads

$$\bar{\rho}_j(E) = -\frac{1}{2^{3/2} \pi} \sum_{fj'} \text{tr}[\delta\sigma_j \text{tr}((E - M_j - \lambda_j \sigma_j)^{-1} I)] \exp \left\{ -\frac{1}{4} \sum_{lfj} \text{tr}[A_{jj'} \sigma_f \sigma_{j'}] \right\},$$

Here, the integration is over $s$ graded $4 \times 4$ matrices $\sigma_j$, $j = 1, \ldots, s$, defined in [3]. $\mathcal{S}$ stands for imaginary part, $I$ for the diagonal matrix $I = \text{diag}(1, 1, -1, -1)$, and $\lambda_j$ and $A_{jj'}$ denote the width parameters and the elements of the coupling matrix defined by

$$\lambda_j = [N_j(B^{-1})_{jj}]^{1/2}, \quad A_{jj'} = (B^{-1})_{jj'} \lambda_j \lambda_{j'}. \quad (7)$$

The desired density estimates follow by taking the Grassmann integral (6) in the saddle-point approximation. For the $j$th partial density, the explicit result is (to simplify the notation, we write $k_j$ and $x_j$ without denoting their dependence on $E$, and use the same symbol for the exact density and for its saddle-point approximation)

$$\bar{\rho}_j(E) = -\frac{1}{\pi x_j} 2\kappa_j, \quad \kappa_j = \lambda_j(E - M_j - \lambda_j x_j)^{-1},$$

where $x_j$ denotes the solution of the ‘scalar saddle-point equation’

$$\sum_{j'} A_{jj'} x_j = N_j \lambda_j (E - M_j - \lambda_j x_j)^{-1},$$

uniquely specified by demanding all $x_j$ have negative imaginary parts.

3. The ergodicity of the procedure

We start by examining the ergodicity of the partial densities. For the spectral averaging interval $\Delta E$, the spectral average of the $j$th partial level density referring to the ensemble member $H$ is given by the integral (we denote the spectral averaging by angular brackets)

$$\langle \rho_j(E) \rangle = \frac{1}{\Delta E} \int_{E - \Delta E/2}^{E + \Delta E/2} dE' \rho_j(E')$$

$$= \frac{1}{\Delta E} \int_{E - \Delta E/2}^{E + \Delta E/2} dE' \frac{1}{N_j} \text{tr}[\mathcal{P}_j \delta(E' - H)].$$

According to Pandey’s discussion of ergodic behaviour in ensembles of random matrices [8], for $\rho_j(E)$ to be ergodic, $\langle \rho_j(E) \rangle \rightarrow \bar{\rho}(E)$, a limit must exist where the ensemble variance $\text{var}(\rho_j(E))$ of $\langle \rho_j(E) \rangle$ vanishes, and the ensemble average of $\langle \rho_j(E) \rangle$ becomes equal to $\bar{\rho}_j(E)$,

$$\text{var}(\rho_j(E)) = (\langle \rho_j(E) \rangle - (\rho_j(E)))^2 \rightarrow 0,$$

$$\langle \rho_j(E) \rangle \rightarrow \bar{\rho}_j(E).$$

As we shall show, like in the case of GOE [8], the ergodic limit is essentially the limit of large $N_j$, small $\Delta E$, and large $\Delta N = \Delta E N \bar{\rho}(E)$. From the technical point of view, the proof of the ergodicity of $\rho_j(E)$ practically reduces to the calculation of the variance $\text{var}(\rho_j(E))$, or better, of the (jth) density correlation function

$$C_j(E_1, E_2) = \langle \rho_j(E_1) \rho_j(E_2) \rangle_{\text{comm}}$$

(12)