مجلة كلية التربية – جامعة سرت
المجلد (2) العدد(3) يناير 2023

Spectral Distribution Method Calculations Of Nuclear Level Densities

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Abstract

The spectral distribution method offers an attractive framework in the study of nuclear level density with inclusion of the two-body force. We present a global parametrization of nuclear level densities taking into consideration the shell-model structures and residual interactions. The noninteracting and interacting particles parts of the Hamiltonian can be studied separately and then the results convoluted to calculate the total level density. The distribution for such a Hamiltonian shows that Gaussian distribution is a good approximation for the level density formalism.

Keyword: Spectral distribution method, Hamiltonian, Nilsson Model, Residual interaction, Gaussian.

الملخص:

تستخدم طريقة التوزيع الطيفي في دراسة كثافة المستوى النووي مع تضمين القوة المتبادلة. بين جسيمين بالأظافة لأستخدام نموذج الأغلفة النووية و نمودج التفاعلات المتبقية في حساب كثافة المستويات النووية، تم الأستعانة بنمودج نيلسون لطاقات الجسيمات الفردية وتفاعلات دلتا من أجل التفاعل الفعال بين الجسيمات.باستخدام هذه النظرية, تم الحصول علي كثافة المستويات النووية بناء علي معاملات الهاميلتونيان(الفردي+الثنائي) والتي يتم حسابها باستخدام طريقة التوزيع الطيفي. عن طريق دراسة الجزء الخاص بالجسيمات غير المتفاعلة والجزء الخاص بالتفاعل بشكل منفصل ثم الجمع بين النتائج النهائية تم حساب الكثافة الكلية للجسيمات النووية المتفاعلة. عند دراسة االهاملتونيان الكلي – مع الأخد بعين الاعتبار ان هناك تفاعل بين الجسيمات النووية– وجد أن التوزيع الجاوسي هو تقريب جيد لشكل كثافة المستويات النووية.

Introduction

One of the characteristic properties of a nucleus is the nuclear level density (NLD) as a function of excitation energy (Sano&Wakai, 1972; Ignatyuk, 1998; Majumdar *et al.*, 1996). Nuclear level density is basic quantity of the nucleus and plays an important role in both pure and applied physics. This importance comes from the wide needs for understanding the creation of consistent theoretical description of excited nucleus and the nuclear reaction cross-section calculations for many branches.

Because of the inherent computational and theoretical limitations in defining the effective interactions, most of researches on nuclear level density (Okuducu *et al.*, 2012; Mengoni& Nakajima, 1994; Hilaire& Goriely, 2006; Dilg *et al.*, 1973; Iljinov *et al.*,1992) based on the Fermi gas model with modification to include the nuclear interaction. The non-interacting Fermi gas model of particles moving in orbits independently of each other has led to various expressions for the density. The basic assumption is essentially based on treating the nucleons as non-interacting particles that move in an average one body field generated by all other particles. Under this assumption, the derived level density as function of excitation energy was originally introduced by Bethe in the form (Bethe, 1937) of:

$$\rho(E) = \rho_0 \exp(2\sqrt{aE}) \tag{1}$$

where *a* is the Bethe parameter and □□ is the density at ground state energy taken at 0 MeV.

Bethe formula modified later on taking into account additional interaction effects such as the shell effects and the pairing energy. This leads to the addition of other parameters such as the spin dependent parameter and the nuclear temperature. As an example for this modification, the back- shifted Fermi-gas model (BSFGM) for finite nuclei (Gilbert& Cameron, 1925; Newton, 1956). The excitation energy is moved -using the pairing energy- by amount of energy called pairing energy parameter (□). The parameter (□) is given by □ = U -E where *U* is the excitation energy.

The BSFG standard form for the observable level density corresponding to excitation energy and angular momentum can be presented as:

$$\rho(E,J) = \frac{\sqrt{\pi}\exp\left(2\sqrt{aE}\right)(2j+1)\exp\left(\frac{-\left(j+\frac{1}{2}\right)^2}{2\sigma^2}\right)}{12a^{\frac{1}{4}}E^{\frac{5}{4}}2\sqrt{2\pi}\sigma^3} \tag{2}$$

□ is the spin cut off factor defined using Bethe parameter for a given excitation energy E:

$$\sigma = (0.0888\sqrt{aE}A^{\frac{2}{3}})^{\frac{1}{2}} \tag{3}$$

where *A* is the nucleus mass number.

Summing over all spins yields the total level density in the form of:

$$\rho(E) = \sum \rho_J(E,J) = \frac{\sqrt{\pi}\exp\left(2\sqrt{aE}\right)}{12a^{\frac{1}{4}}E^{\frac{5}{4}}\sqrt{2\pi}\sigma} \qquad (4)$$

Also, the Constant Temperature (CT) model (Gilbert& Cameron, 1965) includes the back shift energy and determines the level density as a function of the temperature. The corresponding expression of level density is obtained by taking the derivative of the cumulative number of levels with respect to the excitation energy*:*

$$\rho(E) = \frac{1}{T} exp\frac{(E-E_0)}{T} \qquad (5)$$

where the two free parameters T and E_0 are to be adjusted to the experimental discrete levels.

Further, Gilbert and Cameron in their papers have shown that, Bethe formula and CT model give a good fit provided that the CT model is used at lower energies while Bethe formula is used at higher ones.

In this work we present the spectral distribution methods (French *et al.*, 2006; French& Kota, 1983; Chang *et al.*, 1971; Hag& Wong, 1980, Wong, 1986) of French for the calculation of level density. The basis of this method is to determine the level density not from the nuclear spectrum itself but from the level distribution defined in terms of the moments of the Hamiltonian. The one-body (mean field) and two-body (effective interaction) parts can be treated separately and the results convoluted to calculate the total level density.

1-Nuclear Level Density Calculation

The nucleus is a complex system containing a fixed number of positively charged protons and electrically neutral neutrons bound together by the nuclear force. As a first approximation, each nucleon may be regarded as moving independently in a mean field resulting from the interactions with other nucleons. Further, the effects of the residual nuclear interaction can be taken into account by an effective two-body interaction.

Theoretically, the calculation of level density starts by defining the Hamiltonian of the system and calculating the eigenvalues and eigenfunctions. In a finite space of the basis states (ϕ_i, i = 1,…, n), the essential problem is to solve the eigenvalue equation:

$$H\Psi = E\Psi \tag{6}$$

where H is the Hamiltonian of the system with energy E and described by the wavefunction Ψ.

In term of given nuclear interaction (V), the Hamiltonian can be written as the sum of the one-body operator- which describes the independent motion of the nucleons- plus the residual interaction.

$$H = h + V \tag{7}$$

The one body Hamiltonian (h) is composed of the single particle energies□ε_i:

$$h\phi_i = \varepsilon_i \phi_i \tag{8}$$

The corresponding wave function Ψ in term of individual basis states can be determined as:

$$\Psi = \sum_{i=1}^{n} c_i \phi_i \tag{9}$$

The focus in spectral distribution method is not to determine the individual states (energies) exactly but to obtain the frequency function in terms of the various moments of the distribution. It turns out that for the two-body nuclear interaction, the distribution of the eigenvalues converges to a simple characteristic distribution (Gaussian with a few high moment correction). These moments are related to various traces of the Hamiltonian and the first few moments can be determined rather than easily.

If we represent the Hamiltonian as a matrix H, all moments can be written in terms of the matrix traces of powers of H.

The zeroth moment is the dimension of the space d(m).

The first moment or the centroid is:

$$E_c(m) = \langle H\rangle \frac{1}{\mathrm{d(m)}} \sum \langle \Psi_{\mathrm{i}} | \mathrm{H} | \Psi_{\mathrm{i}} \rangle \tag{10}$$

The other moments are computed relative to the central moment:

$$\mu_p = \langle (H - E_c(m))^p \rangle \tag{11}$$

1.1-Non-Interacting Particle (NIP) Level Density

Spectral Distribution Method Calculations Of Nuclear Level Densities

The calculation of nuclear level density assuming that the nucleons do not interact with one another but move independently in a mean field created by a single particle Hamiltonian h. We first define the Hamiltonian in terms of the single particle energies and then calculate the moments of h in this given spectroscopic space. The non-interacting particle (NIP) level density is then constructed in terms of these low-order moments.

1.1.1 Moments of the Hamiltonian

The one-body Hamiltonian h in terms of the single particle energies of the various orbits is given by:

$$h = \sum_{i=1}^{n} n_i \, \varepsilon_i \tag{12}$$

Where n_i and $\square_i$ (i = 1, 2 3,.. n) represent the orbital number operator

$n_i = a_i^\dagger a_i$ and the single particle energy for orbit i respectively.

Scalar Averaging

Denoting the degeneracy of the i-th spherical orbit of angular momentum j_i as $N_i = 2j_i + 1$, the total number of 1-particle states N is:

$$N = \sum_{i=1}^{n} N_i \tag{13}$$

Then for m particles distributed in these N single particle states, the total dimensionality d(m) is given by:

$$d(m) = \binom{N}{m} = \frac{N!}{m!\,(N-m)!} \tag{14}$$

This dimensionality *d(m)* also referred to as the scalar dimensionality may be regarded as the zeroth order moment of the Hamiltonian. In this scalar averaging, the centroid of the distribution is the average of h over all m-particle states. The spectral distribution methods propagate information from simple to complicated spectroscopic spaces and allow one to write the m- particle centroid in terms of the one-particle centroid. The one-particle scalar centroid is the first moment of the Hamiltonian which can be defined as:

$$E_c(1) = \langle \mathrm{h} \rangle^1 \frac{1}{N} \sum_{i=1}^{n} N_i \, \varepsilon_i \tag{15}$$

The m-particle centroid is:

$$E_c(m) = m \, E_c(1) \tag{16}$$

The propagation of information extends to powers of the Hamiltonian and for the second central moment we first write the one-particle variance as:

$$\sigma^2(1) \equiv \langle (h - \langle h \rangle^1)^2 \rangle = \frac{1}{N} \sum_{i=1}^{n} N_i \left(\varepsilon_i - E_c(1)\right)^2 \tag{17}$$

Then the m-particle variance may be written as:

$$\sigma^2(m) = m \frac{(N-m)}{(N-1)} \sigma^2(1) \tag{18}$$

In terms of the dimensionality, centroid and variance of the distribution, the density can be approximately described as a Gaussian function may be written as:

$$\rho(m, E) = \frac{d(m)}{\sqrt{2\pi\sigma^2(m)}} \exp\left(-\frac{(E - E_c))^2}{2\sigma^2(m)}\right) \tag{19}$$

Calculating the density using scalar moments is relatively simple and straight forward. However, for a large number of particles and several orbits, the dimensionality of the space becomes huge and a single Gaussian density leads to inaccuracies. Since we are interested in the density up to a few MeV excitation energy, this region necessarily falls in the tail of the distribution. A finer partition of the space in terms of configurations is necessary.

Configuration Averaging

We start by distributing m particles over a set of n single particle orbits each with degeneracy Ni to generate the m-particle configurations. Each configuration is labeled by $\mathbf{m} \equiv \{m_1, m_2, \dots m_n\}$

The dimensionality of the configuration is given by the product of the different number of ways to arrange m_i particles in single particles states N_i:

$$d(\boldsymbol{m}) = \prod_{i=1}^{n} \binom{N_i}{m_i} \tag{20}$$

Because of the non-interacting nature of the particles, the total energy for a configuration is additive and given by:

$$E(\boldsymbol{m}) = \sum_{i=1}^{n} m_i \varepsilon_i \tag{21}$$

Further, the configuration centroids and variances are related to the scalar ones as:

$$E_c(m) = \frac{1}{d(m)} \sum_{m} d(\boldsymbol{m}) E(\boldsymbol{m}) \tag{22}$$

$$\sigma^2(m) = \frac{1}{d(m)} \sum_{m} d(\boldsymbol{m}) E(\boldsymbol{m}) - E_c(m))^2 \tag{23}$$

2.1-Interacting Particle (IP) Level Density

In order to obtain the influence of the nuclear interaction on the non-interacting particle density, the full nuclear Hamiltonian may be determined as a sum of three parts*:*

$$H = C(0) + h(1) + V(2) \tag{24}$$

The first part, $C(0)$, represents the zero-body part and defines the inactive core. The second part, $h(1)$, specifies the one-body Hamiltonian and its defined by the external single particle energies of the spherical orbits. The third part, $V(2)$**,** is the residual two-body interaction and defines how the nucleons interact with each other.

If $V(2) = 0$, we have the NIP density which involves a number of degenerate sets (spikes) marked by configurations, energies and degeneracies. With the inclusion of V, these spikes will spread and admix resulting in the IP density.

In order to examine what the effect of the interaction various parts will have on the density, we make a unitary decomposition of h and V following [12]. First, we consider the decomposition of the one-body interaction $h(1)$ with respect to spherical configuration group, into two parts:

$$h(1) = h^{0[0]} + h^{1[0]} \tag{25}$$

$$h^{0[0]} = \sum_{\boldsymbol{r}} \epsilon_{\boldsymbol{r}} n_{\boldsymbol{r}} \quad ; \quad \epsilon_{\boldsymbol{r}} = N_{\boldsymbol{r}}^{-1} \sum_{n \in \boldsymbol{r}} \epsilon_r N_r \tag{26}$$

$$h^{0[1]} = \sum_{\boldsymbol{r}} \epsilon_r{}^{[1]} n_r \quad ; \quad \epsilon_r{}^{[1]} = \epsilon_r - \epsilon_{\boldsymbol{r}} \tag{27}$$

The unitary rank zero part $h^{0[0]}$ is added to the zero-body part C(0) of the Hamiltonian. The remaining unitary rank one part is defined in terms of the single particle energies.

The interaction may be regarded as consisting of two parts, the part which generates the centroids of the configurations $V^{[0]}$ and the rest of $V^{\wedge}$ represents the residual interaction. The centroid generator can be decomposed into three parts with unitary ranks 0, 1, and 2.

$$V^{[0]} = \sum_{v=0}^{2} V^{v[0]} \tag{28}$$

$$V^{[0]} = \sum_{r \geq s} V_{rs} \frac{n_r(n_s - \delta_{rs})}{(1 + \delta_{rs})} \tag{29}$$

where n_r is the orbital number operator, and V_{rs} is the average interaction between two particles one in r orbit and one in s orbit.

$$n_r = \sum_{r \in \boldsymbol{r}} a_r^{\dagger} a_r \tag{30}$$

$$V_{rs} = \left\{\frac{1}{N_r(N_r - \delta_{rs})}\right\} \left\{\sum_J (2J+1) V_{rsrs} \, (1 + \delta_{rs})\right\} \tag{31}$$

$$V^{0[0]} = \sum_{\boldsymbol{r} > \boldsymbol{s}} [V_{\boldsymbol{rs}}] \frac{n_r(n_s - \delta_{\boldsymbol{rs}})}{(1 + \delta_{\boldsymbol{rs}})} \tag{32}$$

$$V_{\boldsymbol{rs}} = [N_{\boldsymbol{rs}}]^{-1} \left[\sum_{r \in \boldsymbol{r}, s \in \boldsymbol{s}} N_{rs} V_{rs} \right] \tag{33}$$

$$V^{1[0]} = \sum_r \{\sum_s (m_s - \delta_{rs})[\epsilon^{[1];s}]\} n_r \tag{34}$$

$$\epsilon^{[1];s} = (N_s - 2\delta_{rs})^{-1} \times \{[\sum_{s\in s} (N_s - \delta_{rs})V_{rs}] - (N_s - \delta_{rs} V_{rs}\} \tag{35}$$

$$V_{t=0} = \sum_v V^{v[0]} + V^{\Lambda} \tag{36}$$

The term $v = 0$ shifts the entire NIP spectrum and is added to $C(0)$ part. The $v= 1$ part renormalizes the single particles energies thereby changing the spectrum without moving the centroids. The remaining part $v = 2$ is small and is therefore neglected [12, 13].

Finally, the three parts of the Hamiltonian can be expressed as:

$$C = C(0) + h^{0[0]} + V^{0[0]} \tag{37}$$

$$h = h^{1[0]} + V^{1[0]} \tag{38}$$

$$V = V^{\Lambda} \tag{39}$$

The zero body Hamiltonian *C* is absorbed in the one body Hamiltonian *h* without loss of generality. Thus, we rewrite the total Hamiltonian as:

$$H = h + V \tag{40}$$

In terms of the interacting particle Hamiltonian, the total density can be written as a convolution of the non-interacting particle (NIP) density with a zero centered spreading Gaussian function. Mathematically,

$$\rho^{H} = \rho^{h} \otimes \rho^{V} \tag{41}$$

Where □ ^{h} is the density due to the effective one-body Hamiltonian *h* constructed by calculating a few lower order moments. Meanwhile, □ ^{V} is a zero-centered Gaussian due to the irreducible two body part V of the interaction [13]. Here, we convolute through the addition of moments and thereby calculate the total density□□ ^{H}.

1.2.1-Moments of the Hamiltonian

We first describe the low-order scalar moments of the Hamiltonian *H*.

The scalar centroid can be written as a sum of two parts:

$$E_c(m) = \langle H \rangle^{(m)} = mE_c(1) + \frac{m(m-1)}{2}\bar{V} \qquad (42)$$

where $\overline{\mathrm{V}}$ is given by:

$$\bar{V} = \frac{2}{N(N-1)} \sum_{rsJT} (2J+1)(2T+1) V_{rsrs}^{JT} \qquad (43)$$

The variance is given by:

$$\sigma^2(m) = \langle (H - \langle H \rangle^m)^2 \rangle^{(m)} = \langle H^2(1,0) + H^2(2,0) \rangle^{(m)} \qquad (44)$$

For details regarding the second moment propagation we refer to Ref [14-16]. The complete expression for the variance can be obtained as:

$$\sigma^2(m) = \binom{N}{m}^{-1} \left[\binom{N-2}{m-1} \sum_{rs} [r] \varepsilon_{rs}\, \varepsilon_{rs} \delta_{rs}^{a.m} \binom{N-4}{m-2} \sum_{\substack{r \le s \\ t \le u \\ \Gamma}} [\Gamma] \{\mathcal{W}_{rstu}^{\Gamma}\}^2 \right] \qquad (45)$$

$$\mathcal{E}_{rs} = \tilde{\epsilon} \delta_{rs} + \epsilon_{rs} + (\hat{n} - 1) \bar{V}_{rs} \qquad (46)$$

Where $\mathcal{W}_{\mathrm{rstu}}^{\Gamma}$ denotes the two -body matrix element of the unitary rank-two part of the Hamiltonian H.

For accuracy in large spectroscopic spaces, we use the configuration moments rather than the scalar ones to construct the density.

The dimensionality of a configuration is:

$$d(\mathbf{m}) = \prod_r \binom{N_r}{m_r} \qquad (47)$$

The configuration centriod is given by:

$$E_c(\mathbf{m}) = \langle H \rangle^{\mathbf{m}} = \sum_r m_r \varepsilon_r + \sum_{r \le s} \bar{V}_{rs} \frac{m_r(m_s - \delta_{rs})}{1 + \delta_{rs}} \qquad (48)$$

where r, s label the spherical orbits, represents the two body operator of the interaction part **V** and □$_{\mathrm{rs}}$ is kronecker delta needed for the two body operator.

$$\bar{V}_{rs} = \frac{1+\delta_{rs}}{N_r(N_s-\delta_{rs})}\sum_{JT}(2J+1)(2T+1)V^{JT}_{rsrs} \qquad (49)$$

Where $V^{JT}_{rsrs} = \langle rsJT|V|rsJT\rangle$ defines the matrix elements of the interaction part V of a pair of nucleons in the same orbit.

The configuration variance is such as a sum of square of one and two parts of the Hamiltonian

$$\sigma^2(\mathbf{m}) = \langle (H - \langle H\rangle^{\mathbf{m}})^2\rangle^{(\mathbf{m})} = \langle H^2(1,0) + H^2(2,0)\rangle^{(\mathbf{m})}$$
$$= \frac{1}{4}\sum_{rstu}\frac{(N_r-m_r)(N_s-m_s-\delta_{rs})m_t(m_u-\delta_{tu})}{(N_r-\delta_{rt}-\delta_{ru})-(N_s-\delta_{st}-\delta_{su}-\delta_{rs})N_t(N_u-\delta_{tu})}$$
$$\times\sum_{JT}(2J+1)(2T+1)(\mathcal{W}^{\mathrm{JT}}_{rstu})^2(1+\delta_{rs})(1+\delta_{tu}) \qquad (50)$$

Where $\mathcal{W}^{\mathrm{JT}}_{\mathrm{rstu}}$ is the coupled, antisymmetrized the two-body matrix elements.

For r=t, s=u, $\mathcal{W}^{\mathrm{JT}}_{\mathrm{rstu}}$ can be written as:

$$\mathcal{W}^{\mathrm{JT}}_{\mathrm{rstu}} = V^{\mathrm{JT}}_{\mathrm{rstu}} - \bar{V}_{rs} \qquad (51)$$

Similarly, the expression used for the level density of the whole Hamiltonian with a given excitation energy can be also approximated as a Gaussian function as follow:

$$\rho(\mathbf{m},E) = \frac{d(\mathbf{m})}{\sqrt{2\pi\sigma^2(\mathbf{m})}}\exp\left(-\frac{(E-E_c(\mathbf{m}))^2}{2\sigma^2(\mathbf{m})}\right) \qquad (52)$$

Summary

In summary, the spectral distribution methods developed for studying quantities of general interest in nuclear structure enable us to go beyond and calculate nuclear level density.. The method is based on using the Nilsson Hamiltonian for the single particle energies and the surface delta interaction for the two-body effective interaction. The density is constructed in terms of the moments of the Hamiltonian which are calculated using spectral distribution methods. By including the effects of both the noninteracting and interacting parts of the full Hamiltonian, the level density and related parameters could be calculated. We convoluted through the addition of moments, in particular, the dimensionality, centroid and variance of the distribution, and then expressed the total density in the form of Gaussian function.

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