Lowest eigenvalue of the nuclear shell model Hamiltonian

J. J. Shen,[1,2] Y. M. Zhao,[1,3,4,*] and A. Arima[1,5]

[1]*Institute of Nuclear, Particle, Astronomy and Cosmology, Department of Physics, Shanghai Jiao Tong University, Shanghai 200240, China*

[2]*Nishina Center, RIKEN, the Institute of Physical and Chemical Research, Hirosawa 2-1, Wako-shi, Saitama 351-0198, Japan*

[3]*Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou 730000, China*

[4]*China of Advanced Science and Technology (CCAST), World Laboratory, Post Office Box 8730, Beijing 100080, China*

[5]*Chancellor, Musashi Gakuen, 1-26-1 Toyotamakami Nerima-ku, Tokyo 176-8533 Japan*

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In this paper, we investigate regular patterns of matrix elements of the nuclear shell model Hamiltonian H, by sorting the diagonal matrix elements from the smaller to the larger values. By using simple plots of nonzero matrix elements and lowest eigenvalues of artificially constructed submatrices h of H, we propose a new and simple formula, which predicts the lowest eigenvalue with remarkable precision.

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The diagonalization of matrices is a fundamental practice in nuclear structure physics as well as in many other fields. However, diagonalization becomes difficult if the dimension of the matrix is very large. Statistical approaches are very suggestive and have been developed (e.g., in Refs. [1–7]), where the lowest eigenvalue is presented in terms of the energy centroid and spectral moments.

Recently, we showed, in Ref. [8], that sorting diagonal matrix elements of a given nuclear shell model Hamiltonian from the smaller to the larger values provides us with a new approach to evaluate the eigenvalues. By sorting the diagonal matrix elements, we are able to evaluate all eigenvalues based on a very strong linear correlation between the diagonal matrix elements and the exact eigenvalues. This method was found to work very well for medium eigenvalues but deviates for the lowest ones. However, in nuclear structure physics as well as in many other fields of sciences, we are interested in the low-lying states. Therefore, it is very desirable to refine the approach toward more and more accurate evaluation of the low-lying eigenvalues, by sorting the diagonal matrix elements.

In this paper, we propose a new approach to predict the lowest eigenvalue of the nuclear shell model Hamiltonian. To exemplify our method, we will use a few realistic examples of nuclear shell model calculations. All results in this paper are based on the shell model code by the Kyushu group [9–11]. The shell model basis states of this code are constructed by using the coefficients of fractional parentage discussed in Ref. [11]. In this paper, we take the universal sd-shell (USD) effective interactions of Ref. [12]. Other interactions such as the Yukawa-type interactions of Refs. [10,13] give similar results.

Let us denote the matrix of spin I states of the nuclear shell model Hamiltonian H by $H^{(I)}$, and the matrix elements of $H^{(I)}$ by $H^{(I)}_{ij}$, where i and j represent indices of basis states. In Fig. 1, we present two typical examples of distributions of the magnitude of $H^{(I)}_{ij}$, based on the $J^\pi = 0^+$ and $J^\pi = 2^+$ states of the ^{24}Mg nucleus. The color from blue to red corresponds to values from zero to large magnitudes. From panels (a) and (b) of Fig. 1, one sees that the values of $H^{(I)}_{ij}$ look random. However, if one sorts the diagonal matrix elements from the smaller to larger values, as in Ref. [8], the values of $H^{(I)}_{ij}$ decrease rapidly and become zero if they are far enough from the diagonal line, as shown in panels (a′) and (b′) of Fig. 1.

Let us investigate this behavior in another form. We study the probability for $H^{(I)}_{ij}$ to be nonzero (after sorting the diagonal matrix elements of $H^{(I)}_{ij}$), while moving away from the diagonal line, versus d, denoted by $\rho(d) = \frac{\sum |\mathrm{sgn}(H^{(I)}_{i,i+d})|}{D-d}$, $d = 1, 2, 3, \ldots, D$. Here, d is the distance of $H^{(I)}_{ij}$ from the diagonal line, and D is the dimension of matrix $H^{(I)}_{ij}$ for spin I states. As shown in Figs. 2(a) and 2(b) for the $I^\pi = 0^+$ and 2^+ states of the ^{24}Mg nucleus, $\rho(d)$ becomes zero at a critical value $d = d_0$; the value of $\ln d_0$ equals 6.75 and 8.22, respectively.

An argument for the regular patterns described in Figs. 1, 2(a), and 2(b) is as follows. With the diagonal matrix elements sorted from the smaller to the larger values, one classifies configurations from the lowest to the largest in energy, roughly by particle-hole excitations. Configurations that come first are the lowest, and the states that come last are n-particle-n-hole excitations out of those low configurations. Because the shell model Hamiltonian consists of one-body and two-body operators, one cannot connect those configurations that are distant (e.g., the configurations with the lowest energy and n-particle-n-hole configurations with $n > 2$). This explains the reason why all values of $H^{(I)}_{ij}$ become zero for $d \geqslant d_0$. Soon, we will find that the value of d_0 is very important in predicting the lowest eigenvalue of the matrix $H^{(I)}$.

In Refs. [3,6,7] the lowest eigenvalue is presented in terms of $\ln D$, where D is the dimension of the matrix $H^{(I)}$. Although the formulas of the lowest eigenvalues presented in Refs. [3,6,7] are applicable to the random ensemble average (not to *individual* sets of interactions parameters), one naturally asks whether or not certain plots of the lowest eigenvalue versus the dimension could be useful in evaluating the lowest eigenvalue of realistic systems studied in this paper. Let us sort the diagonal matrix elements from the smaller to the larger, as in Refs. [8]. Then, we artificially truncate the matrix $H^{(I)}$

*ymzhao@sjtu.edu.cn

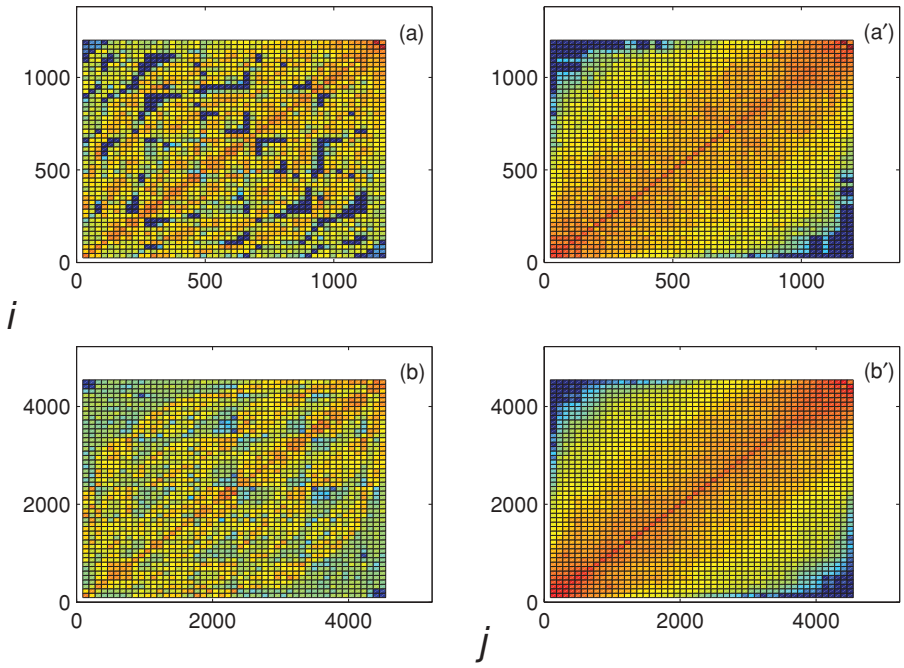

FIG. 1. (Color online) Magnitude of the matrix elements without [panels (a) and (b)] and with [panels (a′) and (b′)], which sort the diagonal matrix elements from the smaller to the larger. The color from blue to red corresponds to values from zero to large magnitudes. The results are based on $I^\pi = 0^+$ [panels (a) and (a′)] and $I^\pi = 2^+$ [panels (b) and (b′)] states of the ^{24}Mg nucleus, obtained by using the USD interactions. The magnitude of $H^{(I)}_{ij}$ without sorting the diagonal matrix elements (left-hand side) are close to random, and those with sorting the diagonal matrix elements (right-hand side) decrease rapidly as going farther from the diagonal line.

and obtain a submatrix h with dimension d ($d < D$), and $h_{ij} = H^{(I)}_{ij}$ ($i, j = 1, 2, \ldots, d$). We diagonalize h and obtain the lowest eigenvalue ϵ_d of the matrix h, and plot ϵ_d versus $\ln d$. In Figs. 2(a′) and 2(b′) we present the ϵ_d-$\ln d$ plots for the $I^\pi = 0^+$ and 2^+ states of the ^{24}Mg nucleus. One sees that ϵ_d decreases linearly with $\ln d$ when d is smaller than a critical dimension $d = D_0$, and decrease again linearly with $\ln d$ but with a smaller slope. Apparently, the value of D_0 and the slopes for both $d < D_0$ and $d > D_0$ suffice for the evaluation of the lowest eigenvalue of $H^{(I)}_{ij}$.

In Fig. 2, one sees that the values of d_0 where $\rho(d_0) = 0$ in Figs. 2(a) and 2(b) coincide with D_0 in Figs. 2(a′) and 2(b′), respectively. Panels (a) and (b) are based on the same matrices as (a′) and (b′), respectively. For convenience, we use the same scale in panels (a) and (a′) and (b) and (b′), and plot two dotted lines to guide the eyes to see such coincidence. From Fig. 2, one also sees that the slope for $d > d_0$ (denoted by k') is smaller than that for $d < d_0$ (denoted by k).

An intuitive understanding of the facts that $d_0 \simeq D_0$ and $k' < k$ is given as follows. Because $H^{(I)}_{ij}$ are zero when $d > d_0$

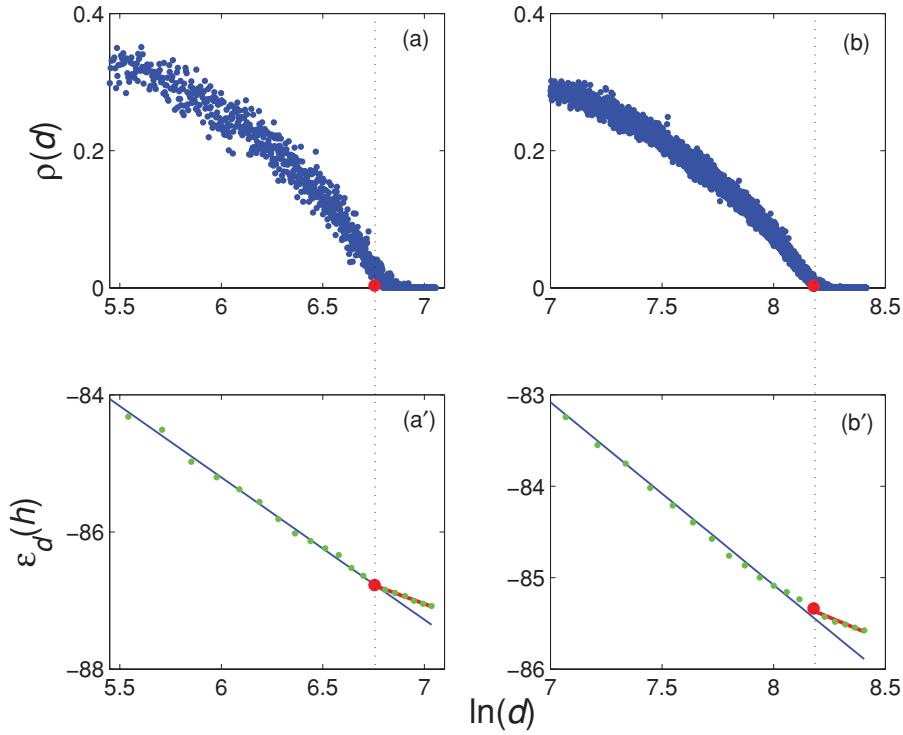

FIG. 2. (Color online) Distribution for $H^{(I)}_{ij}$ to be nonzero, denoted by $\rho(d)$, and the lowest eigenvalues of h, denoted by $\epsilon_d(h)$. The results of (a), (a′) and (b), (b′) are obtained for the $J^\pi = 0^+$ and $J^\pi = 2^+$ states of ^{24}Mg, respectively. One sees that the values of d where $\rho(d_0) = 0$ and where the $\epsilon_d(h)$-$\ln d$ plots change the slope (D_0) coincide (i.e., $d_0 = D_0$). We use the same scale in (a), (a′) or (b), (b′). The dotted lines are used to guide the eye.

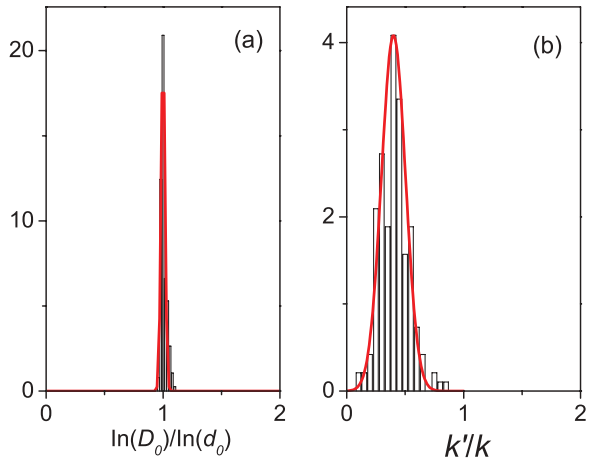

FIG. 3. (Color online) Distribution for $\ln(D_0)/\ln(d_0)$ and k'/k for 200 $H^{(I)}$ matrices for a number of nuclei in the sd shell, the dimension D of which goes from 500 to 10 000, by taking the USD interactions. One sees that $\ln(D_0)/\ln(d_0) \simeq 1$, and that $k' \sim \frac{2}{5}k$ with considerable fluctuations. In this paper, we assume that $\ln(D_0)/\ln(d_0) = 1$ and $k' = \frac{2}{5}k$ when we predict the lowest eigenvalue of $H^{(I)}$, for simplicity.

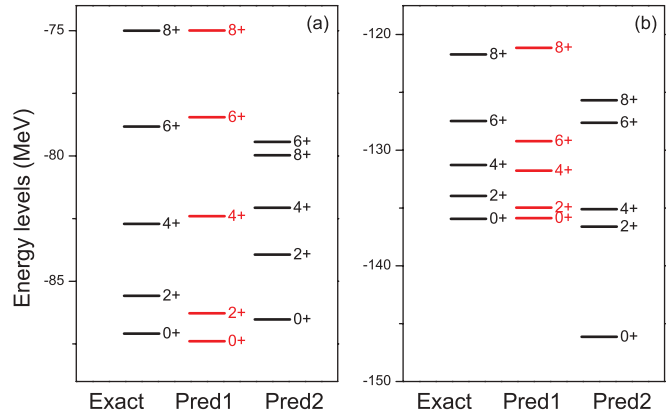

FIG. 4. (Color online) Comparison of low-lying levels obtained by exact diagonalization (denoted by exact) and those predicted by using Eq. (1) (denoted by pred1) and the linear correlation formula suggested in Ref. [8] (denoted by pred2) for the ^{24}Mg nucleus in panel (a), and the ^{28}Si nucleus in panel (b). The results are obtained by using the Yukawa-type interaction of Refs. [10,13]. One sees substantial improvement of predictions for the lowest eigenvalues for each spin I by using Eq. (1) of this paper.

[i.e., $\rho(d_0) = 0$ for $i, j > d_0$], there is no contribution to the lowest eigenvalue from these matrix elements. On the other hand, some of matrix elements $H_{ij}^{(I)}$ and $H_{ji}^{(I)}$, with $0 < i < D - d_0$ and $j > D - d_0$, are nonzero [see Figs. 1(a′) and 1(b′)], which lower down the smallest eigenvalue of the h matrix. The slope of the ϵ_d-ln d plot, therefore, changes at $d = d_0$ and becomes smaller for $d > d_0$ than that of h for $d < d_0$.

In Fig. 3, we present our results of $\ln(D_0)/\ln(d_0)$ and k'/k, based on 200 examples of $H^{(I)}$ for a number of sd shell nuclei by using the USD interactions.One sees that $\ln(D_0)/\ln(d_0)$ are very close to 1.0 and that $k' \simeq \frac{2}{5}k$ with fluctuations. For simplicity, we assume that $\ln(D_0)/\ln(d_0) = 1$ and $k' = \frac{2}{5}k$ for *all cases* throughout this paper.

By making use of these regularities, we obtain a new and simple formula to evaluate the lowest eigenvalue of the matrix $H^{(I)}$,

$$E_{\min}^{(I)} = \frac{2k}{5}\ln D + \left(k \ln d_0 + b - \frac{2k}{5}\ln d_0\right) = \frac{2k}{5}\ln(D) + \frac{3k}{5}\ln(d_0) + b, \quad (1)$$

where k and b are the slope and the intercept of the ϵ_d-ln d plot for $d < d_0$; d_0 is determined by $\rho(d_0) = 0$, and D is the number of spin I states. Because the ϵ_d-ln d plot shows a nice linearity [see Figs. 2(a′) and 2(b′)], we extract the values of k and b based on submatrices h of $H^{(I)}$ with $d \leqslant D/10$ for all cases.

In Fig. 4, we present a comparison of the lowest states of spin I predicted by Eq. (1), and those obtained by the linear correlation (i.e., Eq. (3) of Ref. [8]), with those calculated by diagonalizing $H^{(I)}$ $(I = 0, 2, 4, 6, 8)$ for two nuclei, ^{24}Mg and ^{28}Si.One sees the remarkable agreement between the exact eigenvalues (the column exact) and our predicted ones (pred1), and substantial improvements achieved by Eq. (1) in comparison with Eq. (3) of Ref. [8] (pred2 in Fig. 4). Without going into detail, we mention that the overall root-mean-squared deviation $\mathcal{E}$ for the 200 cases we checked in Fig. 3 [defined by $\mathcal{E} = \sum_i^N \sqrt{(E_i^{\text{exact}} - E^{\text{pred}})^2/N}$, where N is the number of examples that we checked and, here, $N = 200$] is 0.38 MeV, by assuming that $d_0 = D_0$, $k' = \frac{2}{5}k$ for all examples.

Here, we give a brief discussion of formulas in Refs. [3,4,6–8] and the formula proposed in this paper. Reference [4] reported a correlation between the lowest eigenvalue and the spectral width σ of the spin I states. Reference [3] suggested a simple formula $E_{\min}^{(I)} = \bar{E}_I - \sqrt{\ln D/\ln 2}\sigma$, where $\bar{E}_I$ is the average energy of spin I states. Reference [6] suggested a formula $E_{\min}^{(I)} = \bar{E}_I - \sqrt{a \ln D + b}\sigma$ (similar to Ref. [3]), with $a \simeq 1.00$ and $b \simeq 0.40$. Reference [8] refined the results of Ref. [6] by including the third moment analytically, with an additional factor $[1 - \frac{\sqrt{\pi}}{6\sqrt{2}}(\frac{\sigma_3}{\sigma})^3]$ multiplied in the second term of the formula in Ref. [6]. Here, σ_3 is the third moment of the eigenvalues. These formulas are applicable to the random Hamiltonians statistically (i.e., the ensemble average), not to the individual Hamiltonians such as for realistic systems. In Ref. [8], the formula by using the linear correlation between the eigenvalues and the diagonal matrix elements is applicable to individual sets of parameters and works well for medium eigenvalues, but it does not work very well for the lowest (or the largest) eigenvalues. The formula proposed in this paper is found to predict the lowest eigenvalues of the nuclear shell model Hamiltonian remarkably well, as shown in Fig. 4. We should also add that there are many other efforts toward overcoming the limitation of dimension in diagonalizing large matrices, see Refs. [14–17].

To summarize, in this paper, we first investigated the distribution of nonzero off-diagonal matrix elements of the nuclear shell model Hamiltonian. We demonstrated that the

nonzero off-diagonal matrix elements exhibit regular patterns, if one sorts the diagonal matrix elements from the smaller to the larger values; without sorting the diagonal matrix elements, the off-diagonal matrix elements look random. Almost all matrix elements become zero, if the matrix elements are distant enough from the diagonal line, after sorting the diagonal matrix elements.

A very simple formula of the lowest eigenvalue for the shell model Hamiltonian matrix $H^{(I)}$ is proposed, based on the regular patterns of the $\rho(d)$ and ϵ_d-ln d plots for submatrices h. There exists a critical dimension D_0 at which the slope of the ϵ_d-ln d plot changes. The slope for $d > D_0$ is empirically found to be equal to 2/5 of that for $d < D_0$ with fluctuations. The value of D_0 is found to be equal to d_0, which can be obtained easily by using $\rho(d_0) = 0$. Here, $\rho(d)$ represents the probability for H_{ij} to be nonzero while moving away from the diagonal line.

The overall root-mean-squared deviation for 200 shell model Hamiltonians of nuclei in the *sd* shell is 0.38 MeV (the relative deviation is about 0.003), which assumes that $d_0 = D_0$ and $k' = \frac{2}{5}k$, with k and b obtained from the submatrices h of $H^{(I)}$. The dimension of h is much smaller than D, and, here, we take $d \leqslant D/10$. This demonstrates that our predicted results of the lowest eigenvalue based on our new formula are in very good agreement with the exact values, even if one treats much smaller submatrices of $H^{(I)}$. Therefore, we expect that our new formula has significance for future theoretical studies of nuclear structure. It will also be interesting to investigate whether or not other low-lying states have similar features.

What has not yet been understood at a microscopic level is why the ϵ_d-ln d plot exhibits a remarkable linearity. Further consideration of these issues is warranted in future studies.

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