Correlation between eigenvalues and sorted diagonal elements of a large dimensional matrix

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We show the functional dependence of eigenvalues in terms of sorted diagonal elements of a Hamiltonian matrix in the nuclear shell model (NSM), a matrix with uniform distribution and that with normal distribution. For a realistic two-body interaction, its relation is approximately expressed by a linear function, especially for the most elements in the intermediate region. We also derive their functional dependences for the uniform distribution and the normal distribution analytically. As a special case, the functional relation for the normal distribution turns out to be approximated by a hyperbolic-tangent function.

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Introduction. In many-body theories most problems are reduced to such problems how to solve eigenenergies of a large dimensional Hamiltonian matrix. However, eigenvalues of a large matrix are difficult to obtain. There are various ways to obtain eigenvalues either exactly or approximately. One is the exact diagonalization of a matrix. Usually, the Lanczos method is efficient and practical to obtain a few lowest eigenvalues in the nuclear shell model, but the dimension of the matrix is limited up to 10^9 even using big computers [1]. The Monte Carlo shell model method is one of the promising methods and attracts considerable attention, although it takes a lot of computational time [2,3].

Another method to tackle the problem is to make the original hamiltonian simpler without spoiling the important feature of the Hamiltonian. In this respect the random matrix theory [4] is useful to study the Hamiltonian with strong chaotic properties. Especially, the Gaussian orthogonal ensemble (GOE) deals with systems of the time-reversal symmetry. There have been also many efforts to obtain eigenvalues by using the energy centroid and spectral moments, and typical works along this line can be found in, e.g., Refs. [5–10].

Recently, Shen *et al*. showed that eigenvalues have a strong linear relation with diagonal matrix elements for individual runs of the two-body random ensemble or Gaussian orthogonal random matrices, if both eigenvalues and diagonal matrix elements are sorted from smaller values to larger ones [11]. They exemplified these correlations for various cases starting from the realistic shell model interactions to random matrices.

In this Brief Report we give a mathematical background for the correlation between sorted eigenvalues and sorted diagonal elements, which was exemplified in various cases in our previous paper [11]. We first show that eigenvalues have a strong linear dependence on the sorted diagonal elements for a realistic nuclear shell model Hamiltonian. Next we investigate their functional dependences in the case of the random Hamiltonians with the uniform and normal distributions. We will give their functional relations between the sorted diagonal elements of a matrix and its sorted eigenenergies for realistic shell model Hamiltonian, the GOE distribution and the uniform distributions.

Functional relations between eigenvalues and diagonal matrix elements. Let us consider a real symmetric matrix H with dimension d. First we sort the matrix elements h_{ij} such that the diagonal elements are sorted from smaller values to larger ones $h_{ii}(h_{11} \leqslant h_{22} \leqslant \cdots \leqslant h_{dd})$ by changing the order of the basis states. The eigenvalues E_i $(i = 1, \ldots, d)$ of the original matrix are not changed by this operation. We assume a functional dependence of the sorted eigenvalues $E_i(E_1 \leqslant E_2 \leqslant \cdots \leqslant E_d)$ in terms of sorted diagonal elements h_{ii}, namely, we assume that $E_i = f(h_{ii})$. Since the number of states for a given energy interval is the same for both eigenvalues and diagonal elements, we have the relation

$$\mathrm{P}(E_i)\, dE_i = \rho(h_{ii})\, dh_{ii}, \tag{1}$$

where $\mathrm{P}(E_i)$ and $\rho(h_{ii})$ are the density of states for E_i and h_{ii}, respectively. Then we have the differential equation

$$\mathrm{P}(E_i) f'(h_{ii}) = \rho(h_{ii}), \tag{2}$$

where $f'(h_{ii}) = \frac{dE_i}{dh_{ii}}$. Once $\mathrm{P}(E_i)$ and $\rho(h_{ii})$ are given, Eq. (2) can be solved to give the functional relation $E_i = f(h_{ii})$.

Realistic two-body interactions. The eigenenergies for a realistic two-body shell model interaction follow the Gaussian distribution [12–14]. As seen in Ref. [11], each distribution is well described by a Gaussian curve although Gaussian approximation is not so good as compared with the case for eigenenergies.

Let us obtain the functional dependence of the eigenvalues of a GOE matrix in terms of the sorted diagonal elements. Through numerical studies it is natural to assume that we approximately have for the distribution of eigenenergies E_i

$$\mathrm{P}(E) = \frac{d}{\sqrt{2\pi}\,\Sigma} \exp\left[-\frac{(E-\bar{E})^2}{2\Sigma^2}\right] \tag{3}$$

and for the distribution of diagonal matrix elements h_{ii}

$$\rho(h) = \frac{d}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{(h-\bar{h})^2}{2\sigma^2}\right]. \tag{4}$$

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TABLE I. Correlation factors R^2 and matrix dimensions for various spin states in ^{24}Mg and ^{28}Si nuclei.

Nucleus	Spin$^{\text{Parity}}$	Dimension	R^2
^{24}Mg	0^+	1161	0.9985
	2^+	4518	0.9995
	3^+	4968	0.9996
	4^+	4734	0.9995
	5^+	3843	0.9992
	6^+	2799	0.9992
^{28}Si	0^+	3372	0.9985
	2^+	13562	0.9992
	3^+	15385	0.9994
	4^+	15089	0.9994
	5^+	12876	0.9995
	6^+	9900	0.9995

Then Eq. (2) is easily solved to give a linear function,

$$E_i = a h_{ii} + b, \tag{5}$$

where $a = \Sigma/\sigma$, $b = -\Sigma\bar{h}/\sigma + \bar{E}$. We can estimate the coefficients a and b in Eq. (5) without knowing the width Σ and mean $\bar{E}$ for E_i, the width σ and mean $\bar{h}$ for h_{ii}. Using relations, $\sum_{i=1}^{d} E_i = \mathrm{Tr}(H) = \sum_{i=1}^{d} h_{ii}$ and $\sum_{i=1}^{d}(E_i)^2 = \mathrm{Tr}(H^2)$, we have $b = \bar{h}(1-a)$ and $a = \sqrt{(\overline{H^2} - \bar{h}^2)/(\overline{h^2} - \bar{h}^2)}$ where $\bar{h} = \mathrm{Tr}(H)/d$, $\overline{h^2} = \sum_{i=1}^{d}(h_{ii})^2/d$ and $\overline{H^2} = \mathrm{Tr}(H^2)/d$. In order to obtain the coefficients a and b, we need to calculate $\mathrm{Tr}(H^2)$, $\mathrm{Tr}(H)$, and $\overline{h^2}$. However, it is much easier than diagonalizing the original Hamiltonian.

We define the correlation factor R between two d-dimensional vectors $\vec{A}$ and $\vec{B}$ as the cosine of the angle between two vectors: $R \equiv \cos\theta = \frac{\vec{A}\cdot\vec{B}}{|\vec{A}||\vec{B}|}$. If both vectors are parallel, $R = 1$, while $R = -1$ if both are antiparallel. In our case we define the components of vectors $\vec{A}$ and $\vec{B}$ as $A_i = h_{ii} - \bar{h}$ and $B_i = E_i - \bar{h}$.

The values of the factor R^2 for various spin states in ^{24}Mg and ^{28}Si nuclei are listed in Table I. All factors are found to be nearly equal to one, showing the linearity relation between eigenvalues and diagonal elements.

Uniform distribution. In the uniform distribution the distribution of diagonal matrix elements is given as

$$\rho(h) = d, \tag{6}$$

for $-0.5 < h < 0.5$ and $\rho(h) = 0$ for otherwise. The distributions of eigenvalues are shown in Fig. 1(a) and (b) for the dimension $d = 3,000$ and $d = 5,000$, respectively. As seen in the figure each distribution of eigenvalues is well approximated as a semicircle

$$\mathrm{P}(E) = B\sqrt{A^2 - E^2}, \tag{7}$$

where numerically we know $A = \sqrt{d/3}$ for a large d. The lowest eigenvalue is thus given by $E_1 = -A = -\sqrt{d/3}$. The constant B is determined later.

Assuming the functional dependence $E_i = f(h_{ii})$, Eq. (2) now becomes

$$d = B\sqrt{A^2 - [f(h)]^2}\, f'(h). \tag{8}$$

By integrating, we have

$$d\int_{-1/2}^{h_0} dh = B\int_{-A}^{f_0} \sqrt{A^2 - f^2}\, df, \tag{9}$$

where h_0 and f_0 are the upper limits for the variables h and f, respectively. This integration can be carried out exactly to give

$$(h_0 + 1/2)d = \frac{A^2 B}{2}\left\{\left[\arcsin\left(\frac{f_0}{A}\right) + \frac{\pi}{2}\right] + \frac{f_0}{A}\sqrt{1 - \left(\frac{f_0}{A}\right)^2}\right\}. \tag{10}$$

With $h_0 = \frac{1}{2}$ and $f_0 = A$, we have $d = \frac{A^2 B}{2}\pi$, which determines the constant $B(B = 6/\pi)$. Replacing h_0 and f_0 by h_{ii} and E_i, we finally get the relation between eigenenergies and

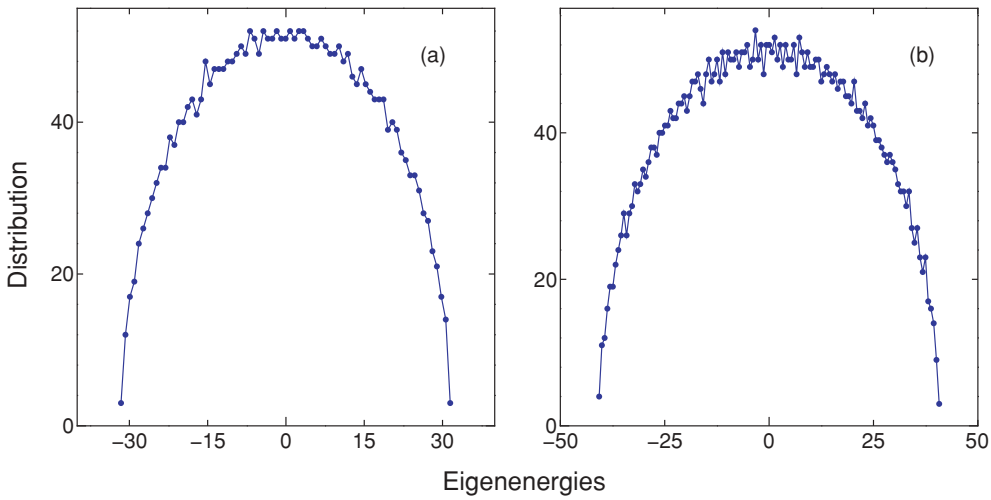

FIG. 1. (Color online) Distribution of eigenvalues for the matrix with the uniform distribution: (a) $d = 3,000$, (b) $d = 5,000$.

diagonal elements as

$$h_{ii} = \frac{1}{\pi}\left[\arcsin\left(\frac{E_i}{A}\right) + \frac{E_i}{A}\sqrt{1-\left(\frac{E_i}{A}\right)^2}\right]. \quad (11)$$

This gives the exact functional relation between the diagonal elements h_{ii} and the eigenvalues E_i for a uniform distribution. Around the origin $h_{ii} \sim E_i \sim 0$, we have the linear expression $E_i = \frac{\pi A}{2} h_{ii} = \frac{\pi}{2}\sqrt{\frac{d}{3}} h_{ii}$, where we have used $A = \sqrt{d/3}$. This relation indicates that the linearity holds around the origin. Although the functional relation in Eq. (11) is not further simplified analytically, it is approximately expressed as

$$E_i = \sqrt{\frac{d}{3}} \tan\left(\frac{\pi}{2} h_{ii}\right), \quad (12)$$

for a whole range of h_{ii}.

Figure 2 shows eigenvalues as a function of diagonal elements for $d = 3000$ and $d = 5000$ for the uniform distribution. The functional relation given by Eq. (11) is also shown in the figure.

Gaussian distribution. The distribution of diagonal matrix elements h of dimension d for the normal distribution with width σ centered at origin is given as

$$\rho(h) = \frac{d}{\sqrt{2\pi}\sigma} \exp\left(-\frac{h^2}{2\sigma^2}\right). \quad (13)$$

The distribution of eigenvalues E for a large dimension d is known to be a semicircle

$$\mathrm{P}(E) = B\sqrt{A^2 - E^2}, \quad (14)$$

where $A = \sqrt{2d}$ for a large d. The lowest eigenvalue is given by $E_1 = -A = -\sqrt{2d}$. The constant B is determined later by considering normalization.

Assuming the functional dependence $E_i = f(h_{ii})$ with width $\sigma = 1$, Eq. (2) now becomes

$$\frac{d}{\sqrt{2\pi}} \exp\left(-\frac{h^2}{2}\right) = B\sqrt{A^2 - [f(h)]^2} f'(h). \quad (15)$$

By integrating, we have

$$\frac{d}{\sqrt{2\pi}} \int_{-\infty}^{h_0} \exp\left(-\frac{h^2}{2}\right) dh = \frac{A^2 B}{2}\left\{\left[\arcsin\left(\frac{f_0}{A}\right) + \frac{\pi}{2}\right] + \frac{f_0}{A}\sqrt{1-\left(\frac{f_0}{A}\right)^2}\right\}, \quad (16)$$

where h_0 and f_0 are the upper limits for the variables h and f, respectively. The normalization condition $d = \frac{A^2 B}{2}\pi$ is obtained by considering the case when $h_0 = +\infty$ and $f_0 = A$.

By replacing h_0 and f_0 by h_{ii} and E_i, and using the normalization condition, we have

$$\mathrm{Err}(h_{ii}) = \frac{1}{\pi}\left[\arcsin\left(\frac{E_i}{A}\right) + \frac{E_i}{A}\sqrt{1-\left(\frac{E_i}{A}\right)^2}\right], \quad (17)$$

where the error function is defined as $\mathrm{Err}(x) = \frac{1}{\sqrt{2\pi}} \int_0^x \exp(-\frac{t^2}{2}) dt$. Around the origin $h_{ii} \sim E_i \sim 0$, we have

$$E_i = \frac{\pi A}{2\sqrt{2\pi}} h_{ii} = \frac{\sqrt{d\pi}}{2} h_{ii}, \quad (18)$$

where we have used $A = \sqrt{2d}$. As suggested in Ref. [11], the functional relation is well approximated by a hyperbolic tangent function,

$$E_i = \sqrt{2d} \tanh\left(\frac{c}{2} h_{ii}\right). \quad (19)$$

By comparing Eq. (19) with Eq. (18) around $h_{ii} \sim E_i \sim 0$, we have $c = \sqrt{\frac{\pi}{2}} \sim 1.25$.

Figure 3 shows eigenvalues as a function of diagonal elements for $d = 3000$ and $d = 5000$ for the normal distribution. The functional relations given by Eqs. (17) and (19) are also shown in the figure. If one uses Eq. (19), one observes small deviations around $E_{\min} = -\sqrt{2d}$ and $E_{\max} = \sqrt{2d}$.

Summary and conclusions. In this Brief Report we showed the functional dependences of eigenvalues as functions of sorted diagonal elements for realistic nuclear shell model

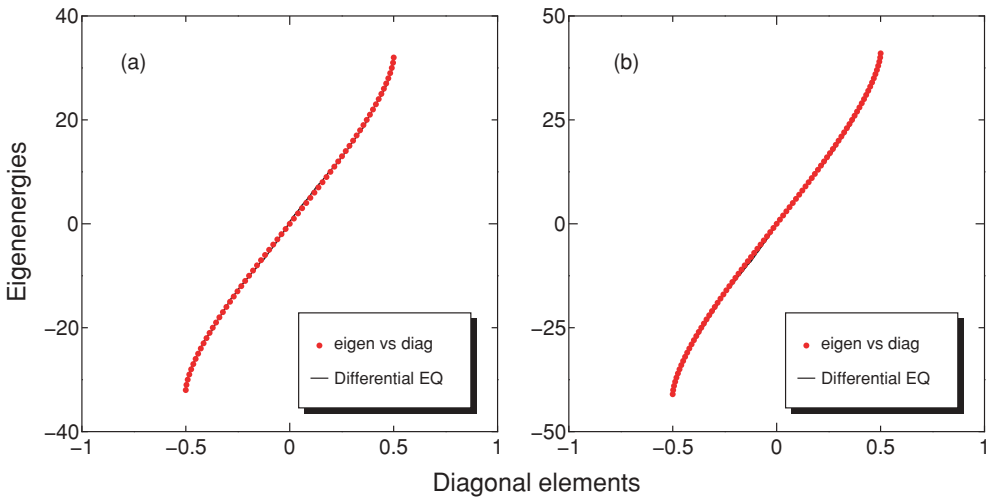

FIG. 2. (Color online) Functional dependence between eigenvalues and diagonal matrix elements (eigen vs diag) for the uniform distribution. The functional relation given by Eq. (11) is denoted by the solid line (Differential EQ): (a) $d = 3,000$, (b) $d = 5,000$.

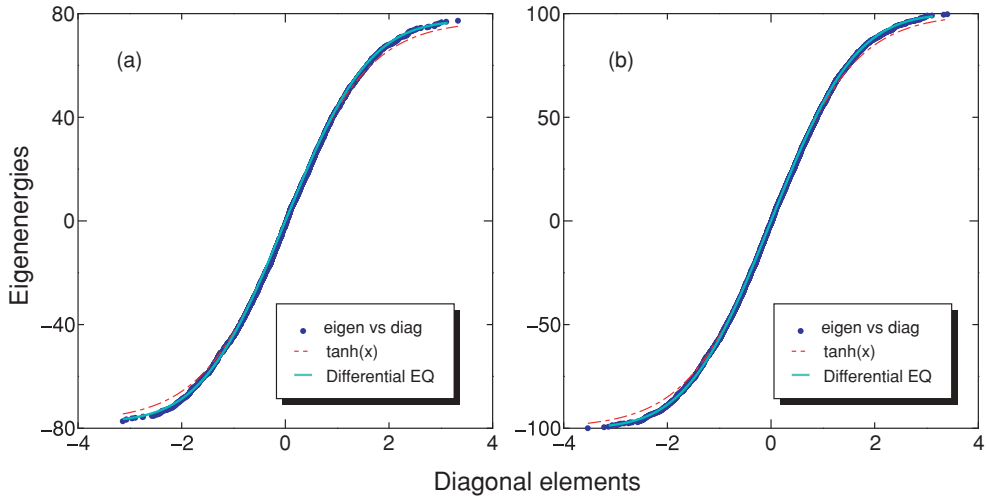

FIG. 3. (Color online) Functional dependence between eigenvalues and diagonal matrix elements (eigen vs diag) for the normal distribution. The functional relation (Differential EQ) given by Eq. (17) is denoted by the solid line in addition with its approximate solution [$\tanh(x)$] in Eq. (19): (a) $d = 3,000$, (b) $d = 5,000$.

(NSM) Hamiltonian matrix, the matrices for the uniform distribution and the normal distribution. In the NSM case, the dependence is approximately observed as a linear function since both eigenenergies and diagonal elements obey approximately gaussian distributions. For the cases of ^{24}Mg, ^{26}Mg, and ^{28}Si, using the USD interactions, we showed that those energies are actually predicted using linear functions whose curvatures and constants are determined by the first and the second moments of the original Hamiltonian [Tr(H) and Tr(H^2)] and the second moment of the diagonal elements $\overline{h^2}$. For the uniform and normal distributions we obtained their analytical functional dependences explicitly by solving differential equations. Their functional dependences are shown to be approximately expressed as tangential and hyperbolic-tangent functions.

In summary we discovered the functional dependences between eigenvalues and sorted diagonal elements for three classes of large real symmetric matrices. In many-body theories most problems are reduced to those problems how to solve eigenenergies of a large dimensional Hamiltonian matrix. Although eigenvalues obtained here are not exact, they are reasonable approximations to exact values. We therefore believe that the functional relations between exact eigenvalues and diagonal matrix elements is very useful in studying many-body problems, for which one needs approximate eigenvalues while other methods are not feasible.

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[1] S. A. Teukolsky and B. P. Flannery, *Numerical Recipes in C++* (William H. Press, Austin, TX, 1992); T. Pang, *An Introduction to Computational Physics* (Cambridge University Press, Cambridge, 1997).
[2] G. H. Lang, C. W. Johnson, S. E. Koonin, and W. E. Ormand, Phys. Rev. C **48**, 1518 (1993).
[3] M. Honma, T. Mizusaki, and T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995).
[4] M. L. Mehta, *Random Matrix Theory* (Academic Press, New York, 1991).
[5] K. F. Ratclif, Phys. Rev. C **3**, 117 (1971).
[6] F. J. Margetan, A. Klar, and J. P. Vary, Phys. Rev. C **27**, 852 (1983).
[7] V. Velazquez and A. P. Zuker, Phys. Rev. Lett. **88**, 072502 (2002).
[8] T. Papenbrock and H. A. Weidenmuller, Phys. Rev. Lett. **93**, 132503 (2004); Phys. Rev. C **73**, 014311 (2006).
[9] N. Yoshinaga, A. Arima, and Y. M. Zhao, Phys. Rev. C **73**, 017303 (2006).
[10] J. J. Shen, Y. M. Zhao, A. Arima, and N. Yoshinaga, Phys. Rev. C **77**, 054312 (2008).
[11] J. J. Shen, A. Arima, Y. M. Zhao, and N. Yoshinaga, Phys. Rev. C **78**, 044305 (2008).
[12] J. B. French and S. S. M. Wong, Phys. Lett. **B33**, 449 (1970); **B35**, 5 (1971); C. H. Chien *et al.*, *ibid.* **B35**, 261 (1971); O. Bohigas and J. Flores, *ibid.* **B35**, 383 (1971).
[13] T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. Wong, Rev. Mod. Phys. **53**, 385 (1981).
[14] V. Zelevinsky, B. A. Brown, N. Frazier, and M. Horoi, Phys. Rep. **276**, 85 (1996).
[15] B. H. Wildenthal, Prog. Part. Nucl. Phys. **11**, 5 (1984); B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Part. Sci. **38**, 29 (1988).