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Eigenvalues of Large Matrices*

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Abstract: We recently performed a series of improvement on evaluation of eigenvalues without complicated iterations. In this work we first discuss evaluation of the lowest eigenvalue for given systems, by which one conveniently obtains the value of the lowest eigenvalue based on the dimension and width of given matrix. We also discuss a strong correlation between eigenvalues and diagonal matrix elements for large matrices, by which one is able to predict eigenvalues approximately without iterations.

Key words: eigenvalue; large matrix; correlation

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1 Introduction

Diagonalization of matrices is a very common practice in many fields. It is important to obtain eigenvalues of large matrices, not only in nuclear structure physics, but also in many other branches of sciences. For some cases the lowest few eigenvalues are of the most interest in physics. However, when the dimension becomes large, the diagonalization becomes prohibitively difficult.

It is therefore interesting and important to study whether we can obtain the lowest ones and also all eigenvalues if possible, without complicated diagonalizations. The purpose of this proceeding paper is to review our recent efforts along this line. We shall give a brief introduction to evaluation of the lowest eigenvalue and all eigenvalues for a given system.

This paper is organized as follows. In Sec. 2 we explain our recent work on evaluation of lowest eigenvalues by a statistical method. In Sec. 3 we present the correlation between eigenvalues and diagonal matrix elements. Summary and discussions are given in Sec. 4.

2 The Lowest Eigenvalues

I was told the following fact for some years. Usually one does not need a very big number of iterations to obtain exact the lowest eigenvalues by computer. The time of iteration in many cases is around or less than 50. Then there must be some clever quantities which play essential roles in the diagonalization process, although we do not know what they are.

There is a very naive idea. It is some-what hand-waving but it is almost precisely the way people working on this problem: first one studies the

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average energy of eigenvalues which is nothing but trace divided by dimension. Since it is well known that average energy is not much related to and far from the lowest eigenvalue, one next considers proper modifications on the average energy.

The paper by Ratcliff[1] and the paper by Margetan et al. were along this line[2]. They suggested that one might use various moments to evaluate the lowest eigenvalues. Suppose we have the width σ, then one easily has a hunch that we can subtract a quantity which is proportional to σ, from the average energy, in order to get the lowest eigenvalue. In Ref. [3] Zuker obtained that

$$E_I^{\text{lowest}} = \bar{E} - \sigma\sqrt{2\ln d_I} \ , \qquad (1)$$

where d_I is the dimension of matrix in consideration. He derived this formulas seven years ago. Unfortunately, this formula does not work well.

Another interesting work is by Papenbrock and Weidenmueller[4]. They noticed there exists an approximate correlation between sigma and the lowest eigenvalues for random interacting systems. Namely, $|E_I| \simeq \alpha\sigma$. The factor α is determined case by case empirically.

Yoshinaga et al. tried this problem by using the error function method[5]. He applied the asymptotic behavior of error function and obtained a similar result as Zuker's. Enlightened by this result, Yoshinaga, Arima and I suggested an empirical formula as follows

$$E_I^{\min} = \bar{E}_I - \Phi(d_I)\sigma_2 \, , \qquad (2)$$

where

$$\Phi(d_I) = \sqrt{a\ln d_I + b} \, ,$$

$$\sigma_2 = \sqrt{\frac{\sum_{i=1}^{d_I}(E_i - \bar{E})^2}{d_I}} = \int (E-\bar{E}_I)^2 \rho(E)\mathrm{d}E,$$

is the width of eigenvalues of all spin I states, d_I is the dimension of spin I states, and a and b were determined empirically to be 0.99 and 0.36, respectively. This empirical formula was found to be well applicable to many different systems which include fermions in a single-j shell and in many-j shells, systems of valence protons and neutrons, and sd-boson systems.

It is also interesting to improve Eq. (2) by considering the third central moment of eigenenergies, which partly compensates the deviation from Gaussian distribution of eigenvalues. The formula of Eq. (2) is based on the assumption that the eigenvalues follow a Gaussian distribution and thus odd central moments should be zero. However, distributions of eigenvalues deviate from Gaussian in many cases. Here in order to consider the skewness, we assume the distribution width of eigenvalues on the left (right) hand side with respect to $\bar{E}_I$ has a very small deviation δ from σ_2 ($\sigma_2^{\text{left}} = \sigma_2 - \delta$, $\sigma_2^{\text{right}} = \sigma_2 + \delta$), and that both the left hand side and the right hand side follow Gaussian distributions with slight different widths. Eq. (2) becomes

$$E_I^{\min} = \bar{E}_I - \Phi(d_I)\ (\sigma_2 - \delta) \ , \qquad (3)$$

let us define $\sigma_3^3 = \int (E-\bar{E}_I)^3 \rho(E)\mathrm{d}E$. We obtain

$$E_I^{\min} = \bar{E}_I - \Phi\left(1 - \frac{\sqrt{\pi}}{6\sqrt{2}}\left(\frac{\sigma_3}{\sigma_2}\right)^3\right)\sigma_2 . \qquad (4)$$

According to our numerical experiments, the deviation of predicted results of $E_I^{\min}$ by using Eq. (4) from exact results obtained by exact diagonalizations can be reduced $\sim 40\%$ on average, in comparison with those obtained by the formula of Eq. (2).

3 Correlation between Eigenvalues and Diagonal Matrix Elements

One would be surprised at any correlation between eigenvalues and diagonal matrix elements. Indeed, there can not be any correlation between eigenvalues and diagonal matrix elements when the dimension is very small, say, 2 or even for 10. Also one sees no correlation if all diagonal matrix elements are equal.

Such correlation arises when one goes to more complicated cases. Here we discuss a many-body hamiltonian interacting by two-body interactions. Let us begin with Hamiltonian matrices which conserve the angular momentum. In Fig. 1 we present the correlation between exact eigenvalues of spin $I=0$, 2, 3, 4, 5, 6 states of ^{24}Mg and corresponding diagonal matrix elements (sorted from the smaller to the larger values) by using the USD interaction[6]. One sees a remarkable linear correlation. Assuming such linearity, one obtains

$$E_i = AH_{ii} + B \ , \tag{5}$$

where

$$A = \sqrt{\frac{\overline{H^2} - \overline{H}^2}{\sum_i H_{ii}^2/D - \overline{H}^2}} \ ,$$
$$B = (1-A)\ \overline{H} \tag{6}$$

This means that one needs $\sum_{i=1}^{D} H_{ii}$, $\overline{H}$, and $\overline{H^2}$ to obtain coefficients A and B. Once A and B are fixed, one needs diagonal matrix elements in evaluation of eigenvalues successively.

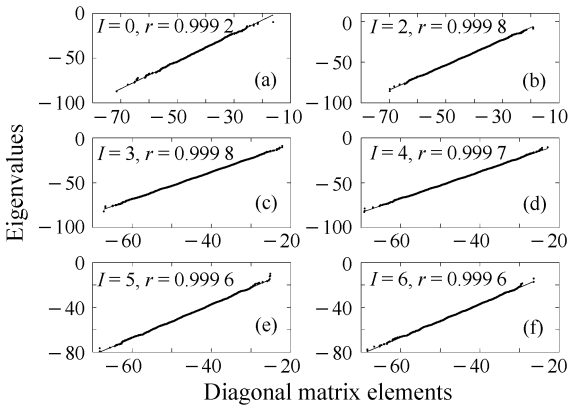

Fig. 1 Correlation between eigenvalues and diagonal matrix elements for ^{24}Mg. Dimension for these I states are: $D_{I=0}=1\ 161$, $D_{I=2}=4\ 518$, $D_{I=3}=4\ 968$, $D_{I=4}=4\ 734$, $D_{I=5}=3\ 843$, $D_{I=6}=2\ 799$. We define $r=\frac{\sum_i (H_{ii}-\overline{H})(E_i^{\text{exact}}-\overline{H})}{\sqrt{\sum_i (E_i^{\text{exact}}-\overline{H})^2 \sum_i (H_{ii}-\overline{H})^2}}$. If there exists a strong linear correlation between E_i^{exact} and H_{ii} ($i=1$, 2, $\cdots$ D), $|r| \to 1$. One sees that $1-r<10^{-3}$ here, suggesting the strong linear correlation.

We note without details that such correlation holds well for two-body random systems and matrices with all matrix elements are uniformly distributed random numbers.

4 Summary

In this paper we present a very brief review of our recent works on eigenvalues of two-body interacting systems. First, we present an improved formula to evaluate the lowest eigenvalue of given Hamiltonian. We are able to consider the third moment without introducing any new parameters.

We also present our recent discovery of strong correlation between eigenvalues and diagonal matrix elements. Although there are large deviations for low-lying states obtained by using the linear correlation, our predicted eigenvalues are very good for high excited states. Improvement on eigenvalues of low-lying states is in progress.

Details of these efforts can be found in Ref. [7].

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