

A new method for disagonalization
of the nuclear shell model Hamiltonian
with large dimensions

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Congratulations on your 70th Birthday
and

Thank you very much for your warm friendship
with me for many years.

Outline

- Introduction
- Linear correlation between diagonal matrix elements and the eigenvalues
- A new approach of approximations based on perturbation in diagonalization
- Summary

I. Introduction

The motivation of this work

These days, because of the rapid development of supercomputers, consideration of models and development of approximation methods do not attract attention of researchers. However, still we cannot diagonalize the nuclear shell model Hamiltonian for heavy nuclei in the foreseeable future.

Truncation and approximations for example are still necessary. Here we report our recent study of the approximation in diagonalization of the shell model Hamiltonian.

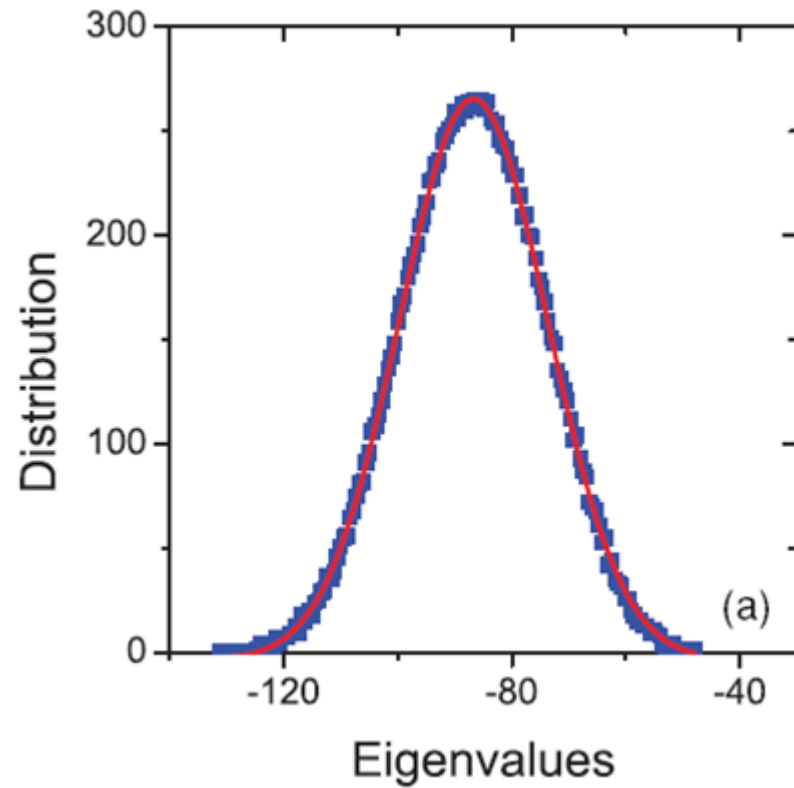
II. Linear correlation between eigenvalues and diagonal matrix elements

Let us consider a shell model Hamiltonian $H^{(I)}$ with dimension D and total spin I .

We assume that the Hamiltonian consists of two-body effective interactions.

The distribution of eigenvalues of shell model Hamiltonians with two-body interactions has been known to be Gaussian (normal).

J.B.French and S.S.M.Wong, Phys. Lett. B33, 449(1970) etc.



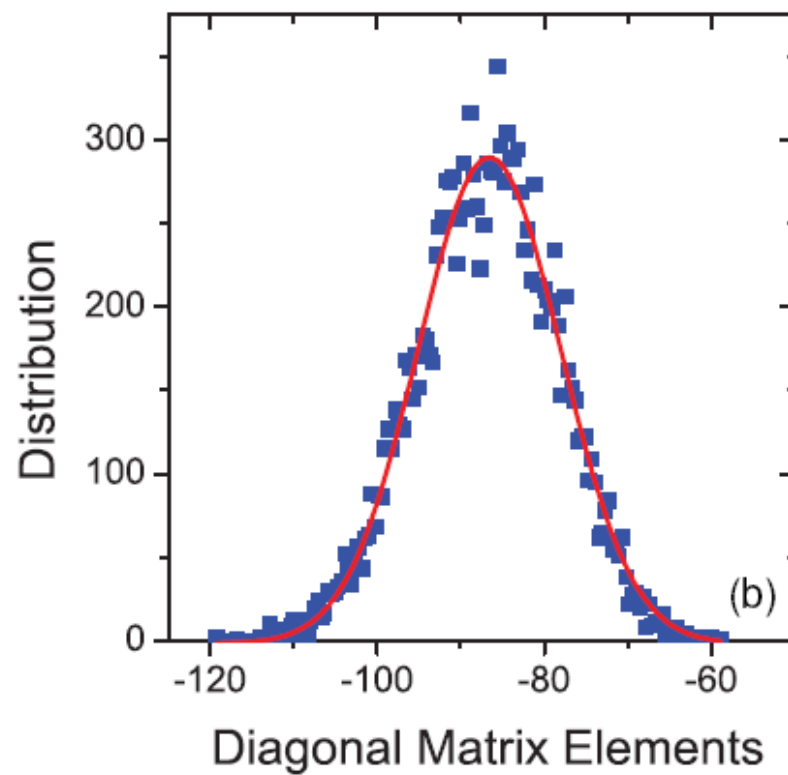
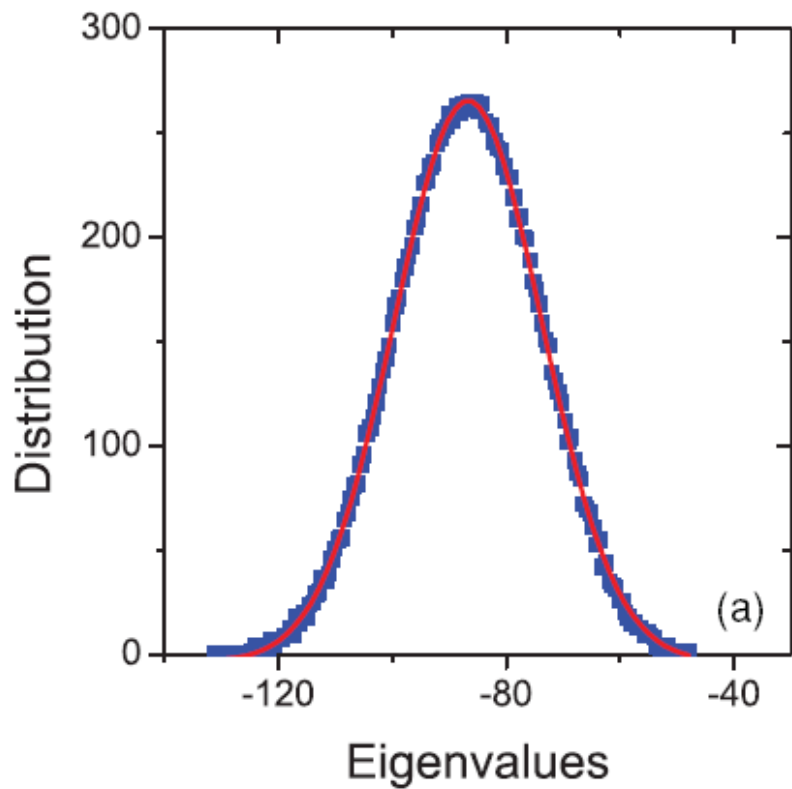
Distribution of eigenvalues $E_i^{(I=4)}$
of the Wildenthal USD interactions for ^{28}Si .

First we sort the matrix elements $H_{ij}^{(I)}$ in such a way that the diagonal elements are sorted from smaller values to larger ones

$$H_{ii}^{(I)} \left(H_{11}^{(I)} \leq H_{22}^{(I)} \leq \dots \leq H_{dd}^{(I)} \right)$$

The eigenvalues $E_j^{(I)}$ ($i = 1, \dots, d$) of the original matrix are not changed by this operation.

We find that the distribution of the diagonal elements is almost Gaussian.

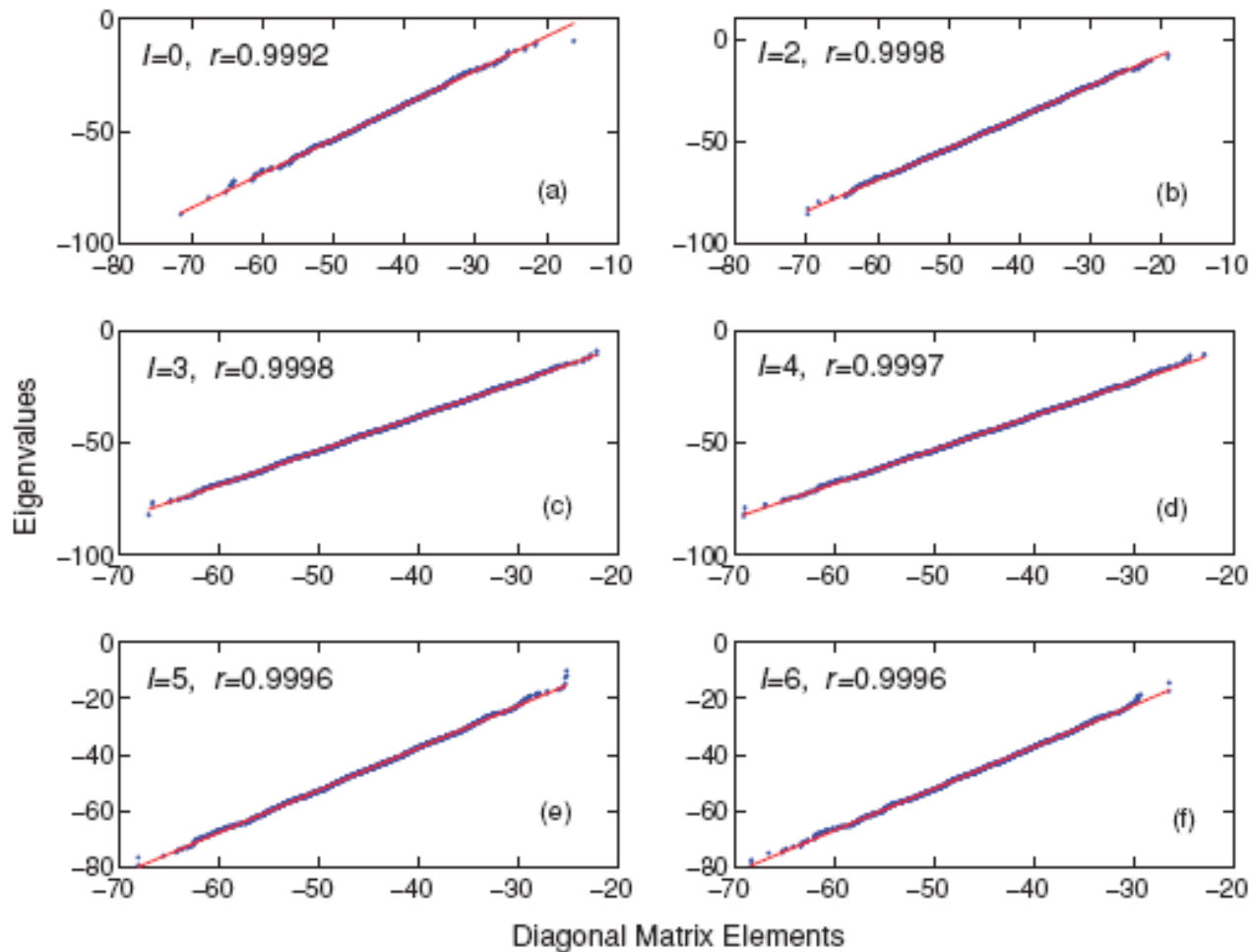


Distribution of eigenvalues $E_i^{(I=4)}$ and diagonal elements $H_{ii}^{(I=4)}$ of the Wildenthal USD interactions for ^{28}Si .

Linear correlation

Because the distributions of both the eigenvalues and diagonal matrix elements are Gaussian.

With precisely the same average, they are expected to exhibit the linear correlation. Indeed the correlation is remarkably good. We found that this correlation is well applicable not only to realistic systems, but also to any two-body random ensemble. Below we give a few examples.



Linear correlation between eigenvalues and sorted diagonal matrix elements for ^{24}Mg , r is the linear correlation coefficients.

Correlation between eigenvalues and diagonal matrix elements after sorting for ^{24}Mg -Panels (a) – (f) correspond to $l=0,2,3,4,5,6$ states. The USD interaction is used. (B.A.Brown and B.H.Wildenthal, Ann. Rev. Nucl. Part 38, 29(1988))

Agreement between predicted values by a straight line indicated by red color and exact eigenvalues is good.

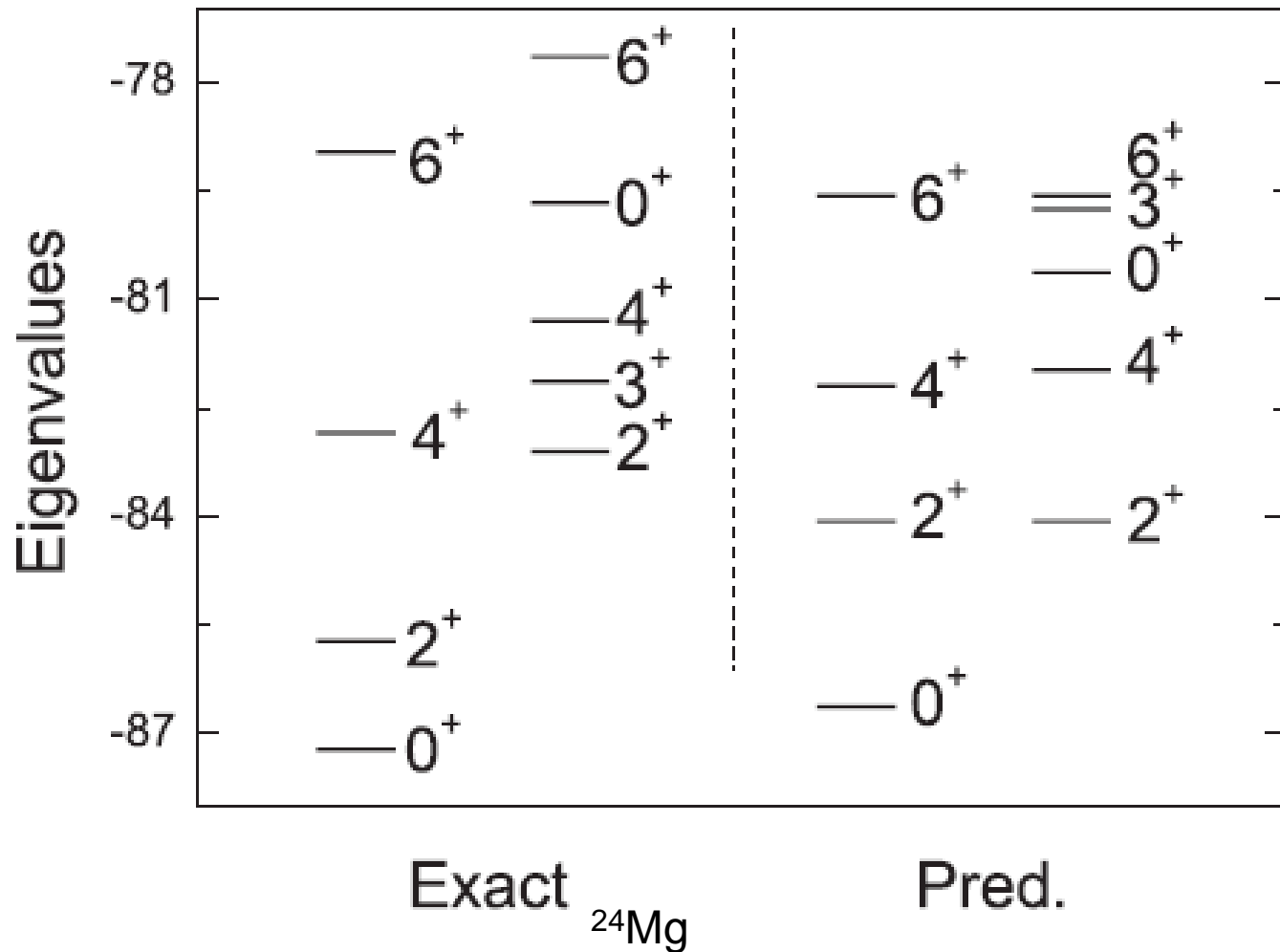
Agreement is especially very good in medium energy.

If we assume the linear correlation, we easily have the following equations.

$$E_i^{(I)} = \alpha H_{ii}^{(I)} + \beta,$$

$$\alpha = \frac{\overline{(H^{(I)})^2} - \overline{(H^{(I)})}^2}{\sum_i (H_{ii}^{(I)})^2 / D - \overline{(H^{(I)})}^2}, \beta = (1 - \alpha) \overline{(H^{(I)})}$$

If the above formula is accurate, we can predict all eigenvalues easily without diagonalization.

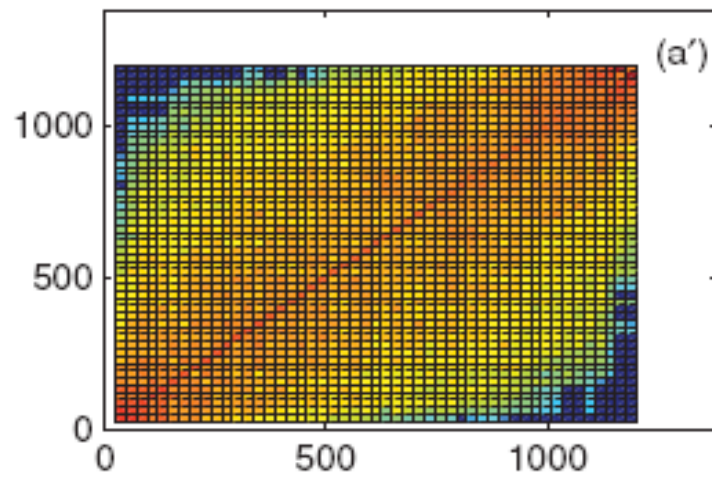
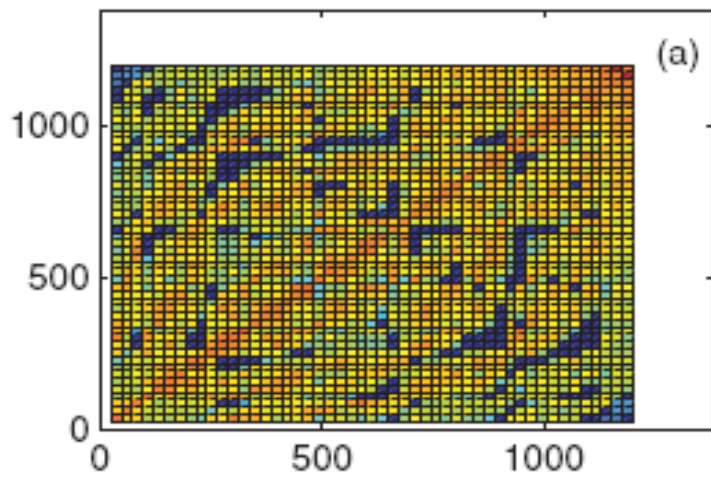


This is an example how this simple correlation works for low-lying states. As already indicated in the figures, they are very good for medium energies, and reasonable but not good enough (not bad, either!) for low-lying states.

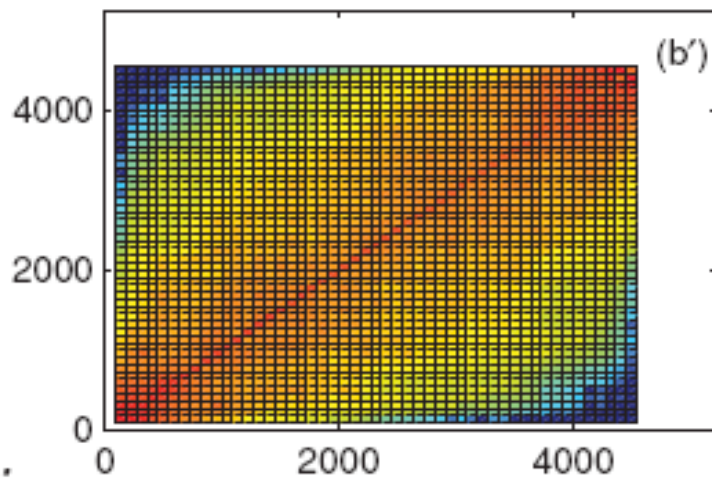
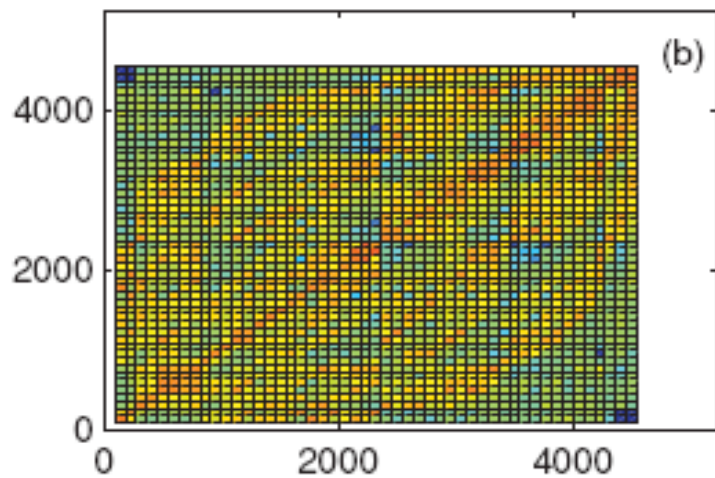
The influence of sorting the diagonal elements can be seen in the change of distribution of non diagonal elements.

As example ^{24}Mg $0+$ (a) and $2+$ (b) are taken.

The USD interactions are used.



i



j

Without sorting

With sorting

Relative magnitudes of matrix elements with and without sorting the diagonal matrix elements are seen in these figures.

The sorting procedure of diagonal elements redistributes non-diagonal elements more systematically. Large non-diagonal elements are found in a narrow band near the diagonal elements.

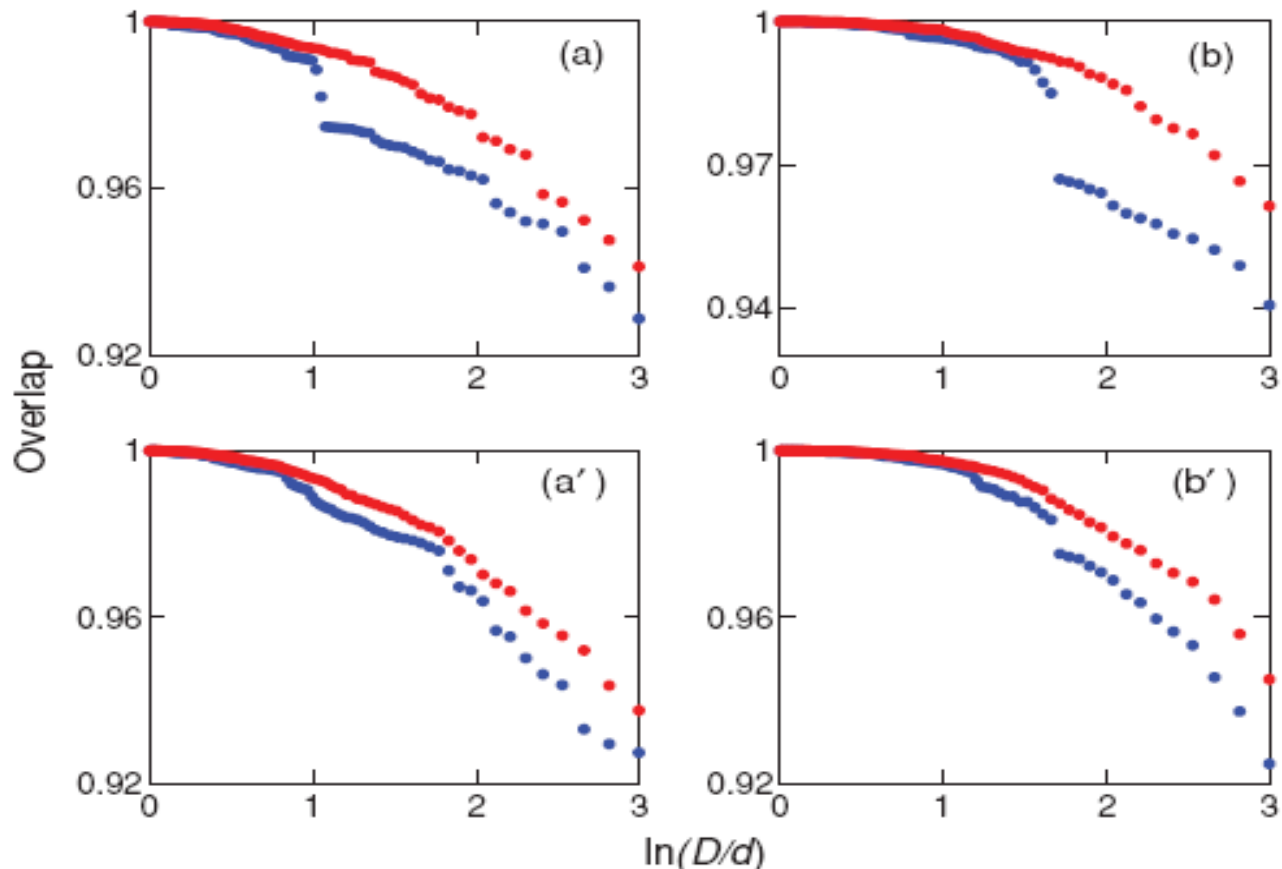
Now we compare two truncation schemes: one is the conventional truncation based on the single-particle occupation.

The other is the truncation based on the sorting the diagonal matrix elements.

Questions: Are they more or less close to each other ? If not, which is better ?

In the following, D means the total dimension of the original Hamiltonian and d is the dimension of a truncated Hamiltonian.

Overlaps of exact wave functions and those obtained by truncation



Results in red are obtained by sorting the diagonal matrix elements; Results in blue correspond to those obtained by following the single-particle energies. One sees that the truncation based on the sorting diagonal matrix elements is better. D , the total number of spin l states, d : dimension of the truncated space. Here we take $l=0$ and 2 for Si-28 and Ti-46 as examples.

Also it is easier to introduce an extrapolation method to predict exact eigenvalues, because the red curves are more smoothly connected.

III. Extrapolation approach

- As observed above, we had better truncate our basis by sorting the diagonal matrix elements from the smaller to the larger. The dimension of the original Hamiltonian H is denoted by D .
- Then we diagonalize the sub-matrix h with small dimension d . We predict the lowest eigenvalue by extrapolations [*Shen, Zhao, Arima, Phys. Rev. C82, 014309*].

$$H = \begin{pmatrix} \overset{\leftarrow d \rightarrow}{h} & G_1 \\ G_1 & G_2 \end{pmatrix} \begin{matrix} \uparrow \\ D \\ \downarrow \end{matrix}$$

The diagram illustrates a block matrix H with a vertical dashed line separating the columns. The top-left element is h , and the top-right and bottom-left elements are G_1 . The bottom-right element is G_2 . A horizontal dashed line is also present, intersecting the vertical one. A double-headed arrow above h is labeled d . A vertical double-headed arrow on the right is labeled D .

$$V^T h V = V^T \begin{pmatrix} H_{1,1} & \cdots & H_{1,d} \\ \vdots & \ddots & \vdots \\ H_{d,1} & \cdots & H_{d,d} \end{pmatrix} V = \begin{pmatrix} \varepsilon_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \varepsilon_d \end{pmatrix}$$

$$\begin{pmatrix} V^T & 0 \\ 0 & I_{D-d} \end{pmatrix} H \begin{pmatrix} V & 0 \\ 0 & I_{D-d} \end{pmatrix} = H_0 + H_1$$

$$H_0 = \begin{pmatrix} \varepsilon_1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & \varepsilon_d & 0 & \cdots & 0 \\ 0 & \cdots & 0 & H_{d+1,d+1} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & H_{D,D} \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & V^T G_1 \\ G_1 V^T & G_2 \end{pmatrix}$$

$$G_1 = \begin{pmatrix} H_{1,d+1} & \dots & H_{1,D} \\ \vdots & \ddots & \vdots \\ H_{d,d+1} & \dots & H_{d,D} \end{pmatrix},$$

$$G_2 = \begin{pmatrix} 0 & H_{d+1,d+2} & \dots & H_{d+1,D} \\ H_{d+2,d+1} & 0 & \ddots & H_{d+2,D} \\ \vdots & \ddots & \ddots & \vdots \\ H_{D,d+1} & H_{D,d+2} & \dots & 0 \end{pmatrix}.$$

$$H_0|\gamma\rangle = \varepsilon_\gamma|\gamma\rangle, \quad (\gamma = 1, 2, \dots, d),$$

$$H_0|d+i\rangle = H_{d+i,d+i}|d+i\rangle. \quad (i = 1, 2, \dots, D-d).$$

$$H = H_0 + H_1$$

$$H|\Psi_\omega\rangle = \lambda_\omega|\Psi_\omega\rangle$$

$$\begin{aligned}\langle\gamma|(H_0 + H_1)|\Psi_\omega\rangle &= \varepsilon_\gamma\langle\gamma|\Psi_\omega\rangle + \langle\gamma|H_1|\Psi_\omega\rangle \\ &= \lambda_\omega\langle\gamma|\Psi_\omega\rangle\end{aligned}$$

$$(\varepsilon_\gamma - \lambda_\omega)\langle\gamma|\Psi_\omega\rangle + \langle\gamma|H_1|\Psi_\omega\rangle = 0$$

$$\begin{aligned}\langle d+i|(H_0 + H_1)|\Psi_\omega\rangle &= H_{d+i,d+i}\langle d+i|\Psi_\omega\rangle + \langle d+i|H_1|\Psi_\omega\rangle \\ &= \lambda_\omega\langle d+i|\Psi_\omega\rangle\end{aligned}$$

$$(H_{d+i,d+i} - \lambda_\omega)\langle d+i|\Psi_\omega\rangle + \langle d+i|H_1|\Psi_\omega\rangle = 0$$

If we define the w -th lowest eigenvalue of H to be λ_w , and its wave function to be Ψ_w , we obtain

$$(\varepsilon_\gamma - \lambda_w)\langle \gamma | \Psi_w \rangle + \langle \gamma | H_1 | \Psi_w \rangle = 0,$$

$$(H_{d+i,d+i} - \lambda_w)\langle d+i | \Psi_w \rangle + \langle d+i | H_1 | \Psi_w \rangle = 0.$$

Let us rewrite them and obtain formulas which can be used recursively.

$$(\varepsilon_\gamma - \lambda_w)\langle \gamma | \Psi_w \rangle + \sum_{\gamma'} \tilde{H}_{\gamma,d+i} \langle \gamma' | \Psi_w \rangle = 0,$$

$$\langle d+i | \Psi_w \rangle = \frac{1}{\lambda_w - H_{d+i,d+i}} \left[\sum_{\gamma'} \tilde{H}_{d+i,\gamma'} \langle \gamma' | \Psi_w \rangle + \sum_{j \neq i} H_{d+i,d+j} \langle d+j | \Psi_w \rangle \right]$$

Where $\tilde{H}_{i,j+d} \equiv \sum_{k=1}^d V_{k,i} H_{k,j+d}$.

We obtain readily the effective Hamiltonian

$$H'(\lambda_w)|\Psi_w\rangle = \lambda_w|\Psi_w\rangle,$$

$$H'(\lambda_w) = H_0 + \sum_{n=2}^{\infty} V^T A(B^{n-2})CV$$

$$A_{i,j} = H_{i,d+j}, \quad B_{i,j} = (1 - \delta_{ij}) \frac{H_{d+i,d+j}}{\lambda_w - H_{d+i,d+i}},$$

$$C_{i,j} = \frac{H_{d+i,j}}{\lambda_w - H_{d+i,d+i}}.$$

$$\langle \gamma | H'(\lambda_\omega) | \Psi_\omega \rangle = \lambda_\omega \langle \gamma | \Psi_\omega \rangle$$

$$\left\langle \gamma \left| H_0 + \sum_n V^T A(B^{n-2}) CV \right| \Psi_\omega \right\rangle = \lambda_\omega \langle \gamma | \Psi_\omega \rangle$$

$$(\varepsilon_\gamma - \lambda_\omega) \langle \gamma | \Psi_\omega \rangle + \langle \gamma | V^T A C V | \Psi_\omega \rangle + \dots = 0$$

$$(\varepsilon_\gamma - \lambda_\omega) \langle \gamma | \Psi_\omega \rangle + \sum V_{k\gamma} A_{ki} C_{ij} V_{j\gamma'} \langle \gamma' | \Psi_\omega \rangle + \dots = 0$$

$$(\varepsilon_\gamma - \lambda_\omega) \langle \gamma | \Psi_\omega \rangle + \sum V_{k\gamma} H_{k,d+i} \frac{H_{d+i,j}}{\lambda_\omega - H_{d+i,d+i}} V_{j\gamma'} \langle \gamma' | \Psi_\omega \rangle + \dots = 0$$

$$(\varepsilon_\gamma - \lambda_\omega) \langle \gamma | \Psi_\omega \rangle + \sum \tilde{H}_{k,d+i} \frac{1}{\lambda_\omega - H_{d+i,d+i}} \tilde{H}_{d+i,\gamma'} \langle \gamma' | \Psi_\omega \rangle + \dots = 0$$

Now we simplify our calculations by requiring that

(1) summation index n is a finite number instead of infinity.

If we keep only $n=2$, we obtain

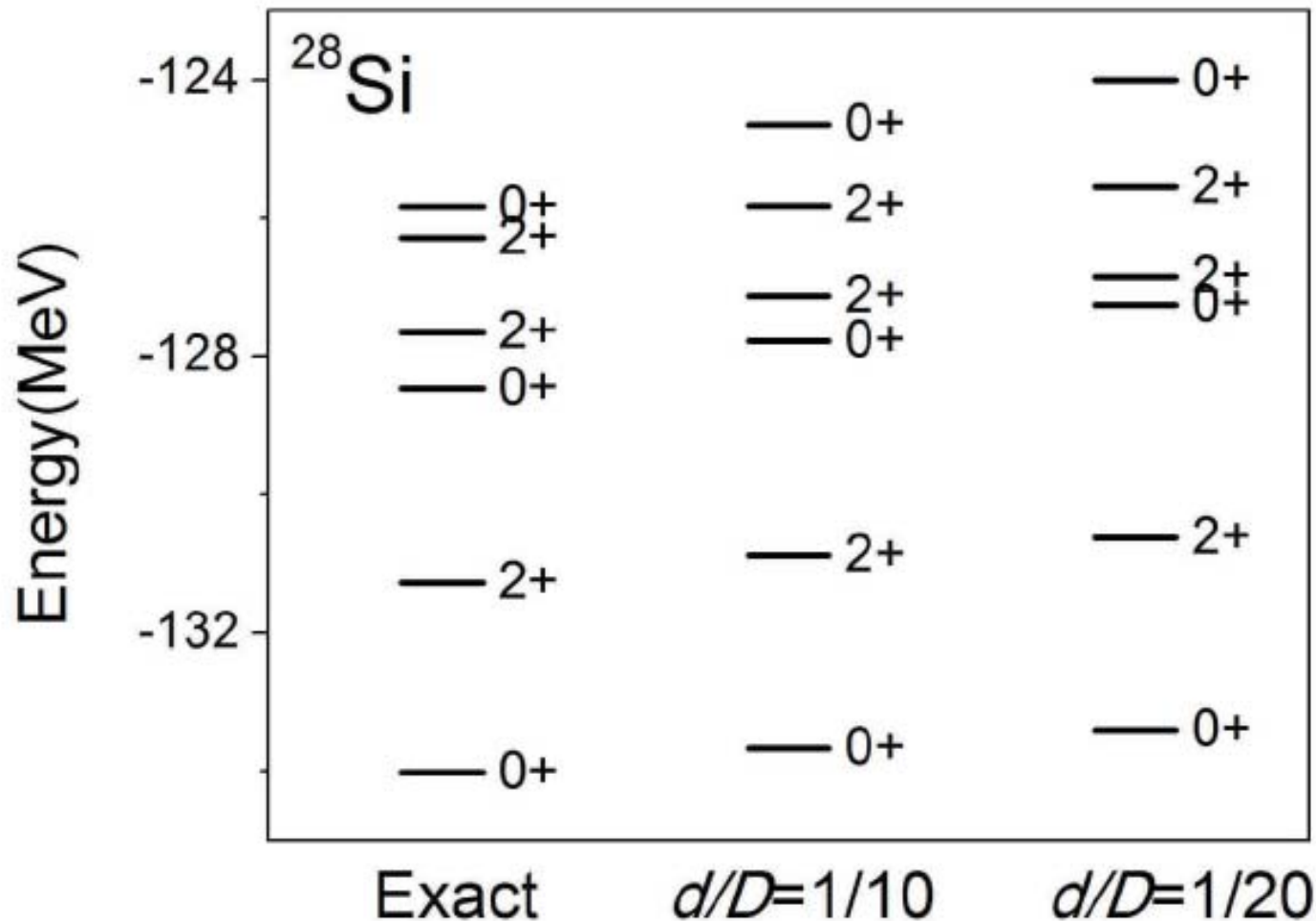
$$H'_{1,1} = \varepsilon_1 + \sum_i^{D-d} \frac{\left(\sum_{k=1}^d V_{k,1} H_{k,d+i} \right)^2}{\varepsilon_1 - H_{d+i,d+i}}.$$

This is the eigenvalue with the second order perturbation.

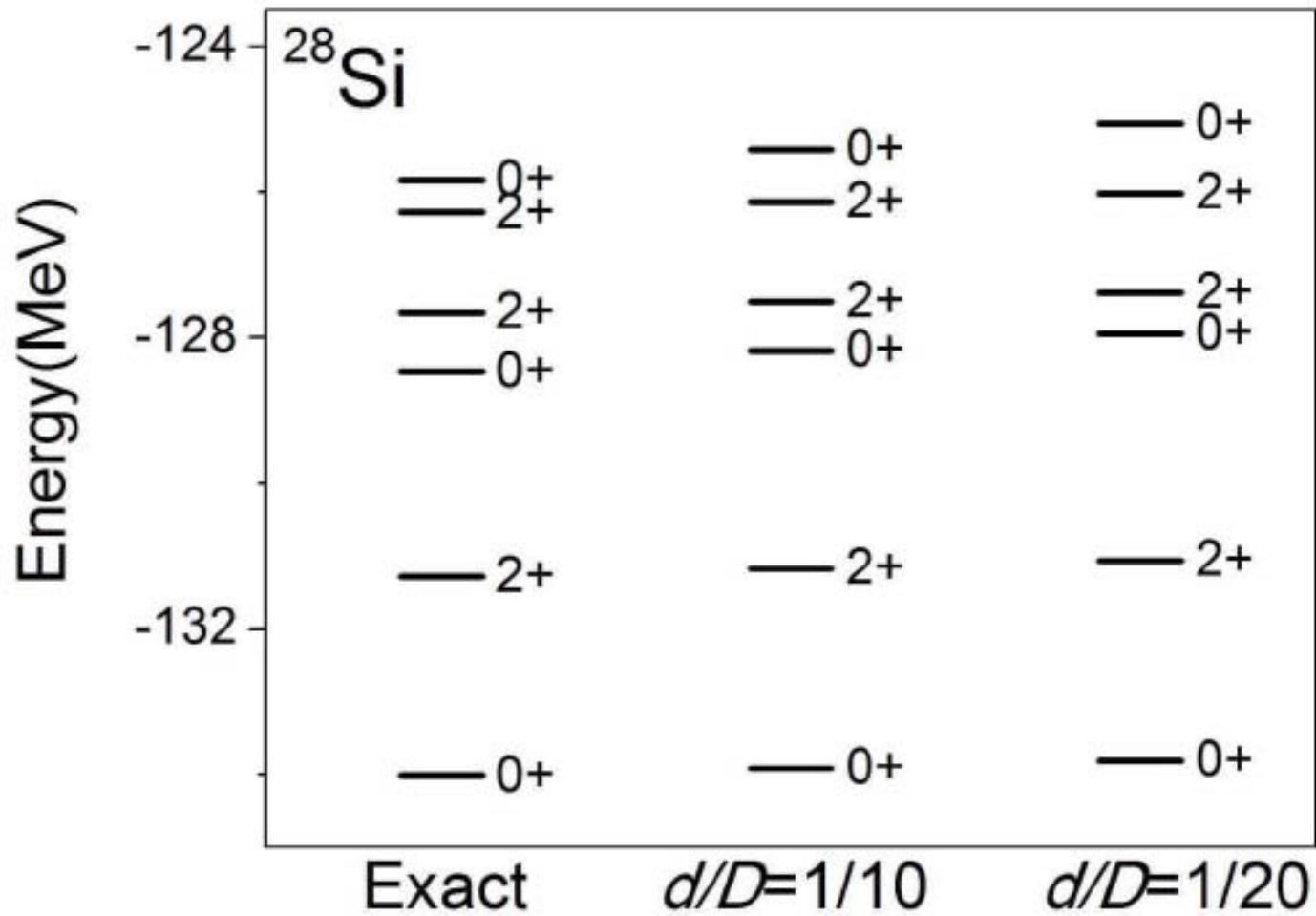
Now let me give a few examples how our method works. In these examples We consider the three lowest 0^+ and 2^+ states, as examples. The left column corresponds to exact solution, and the middle and the left columns correspond to those obtained by diagonalizing the effective hamiltonian, with $d/D= 1/10, 1/20$, respectively.

In the following six pages the only approximation we have made is the restriction on values of k . For exact solutions, k is infinite. However, in practice a very small number of k is actually good enough.

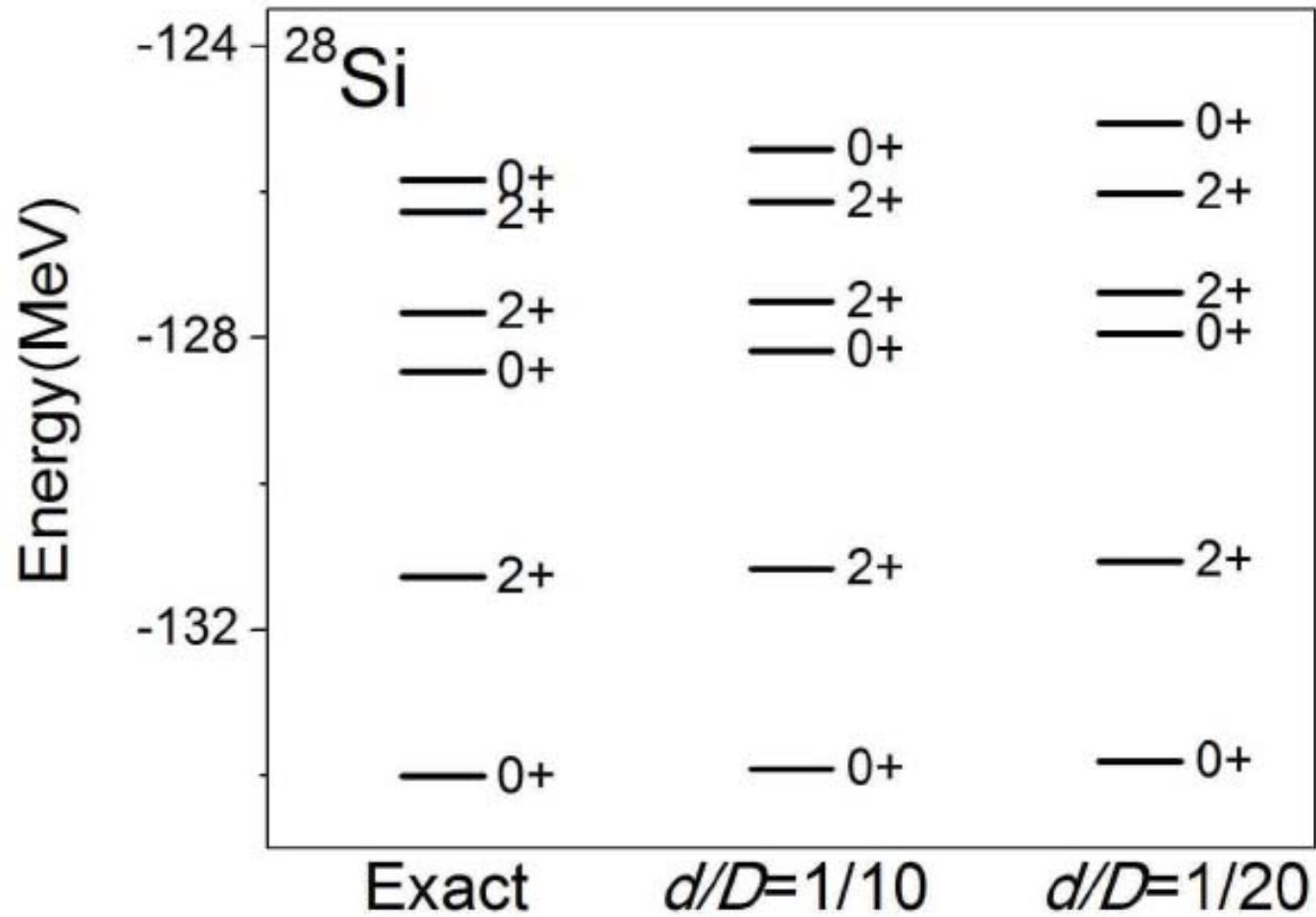
The level



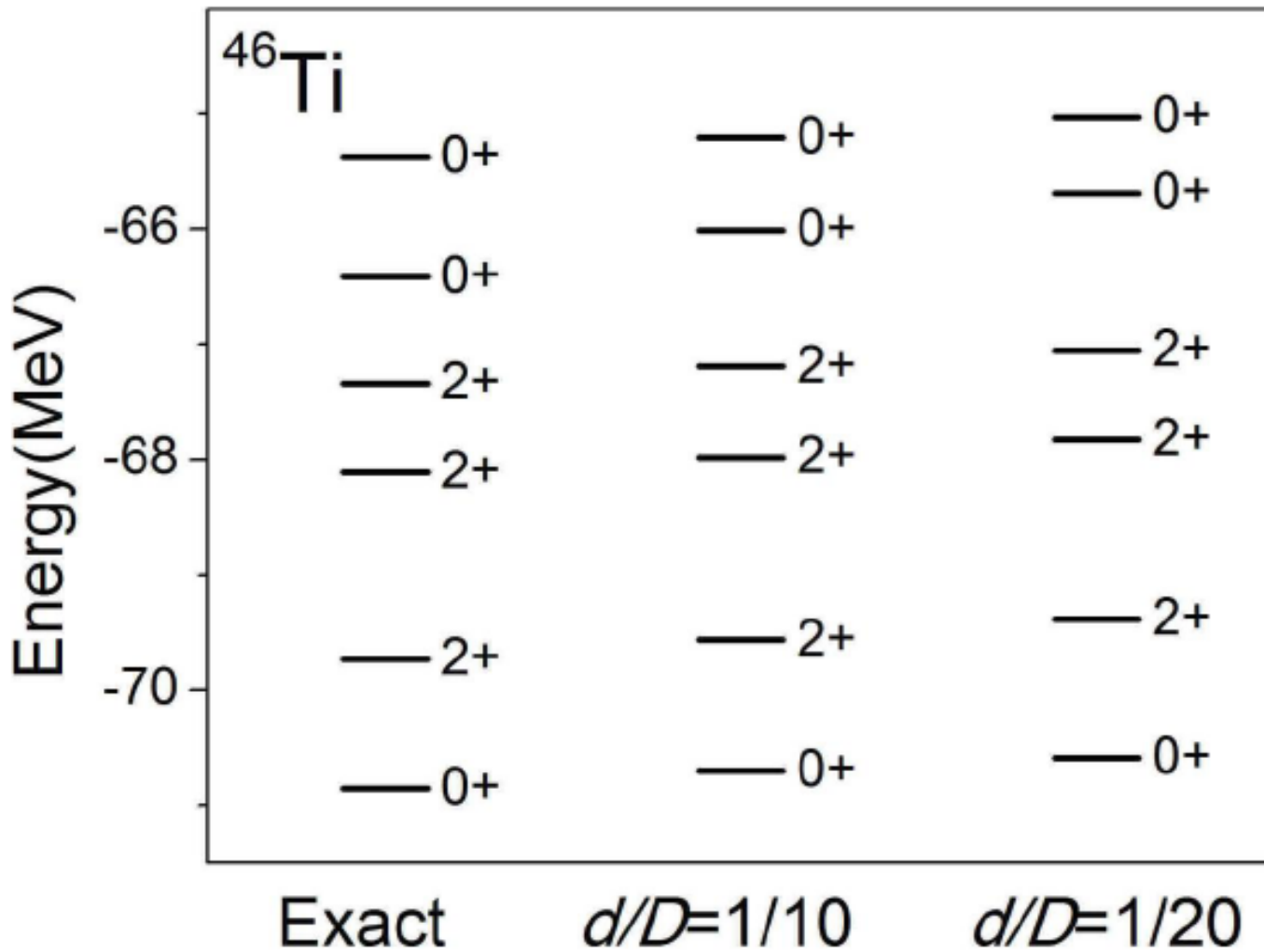
Now let me give a few examples how our method works. In this Figure we take the USDB interaction for Si-28 and concentrate on the three lowest 0+ and 2+ states. The left corresponds to exact solution, and the middle and the left column correspond to those obtained by diagonalizing the effective hamiltonian with $k=2$, with $d/D= 1/10, 1/20$, respectively.



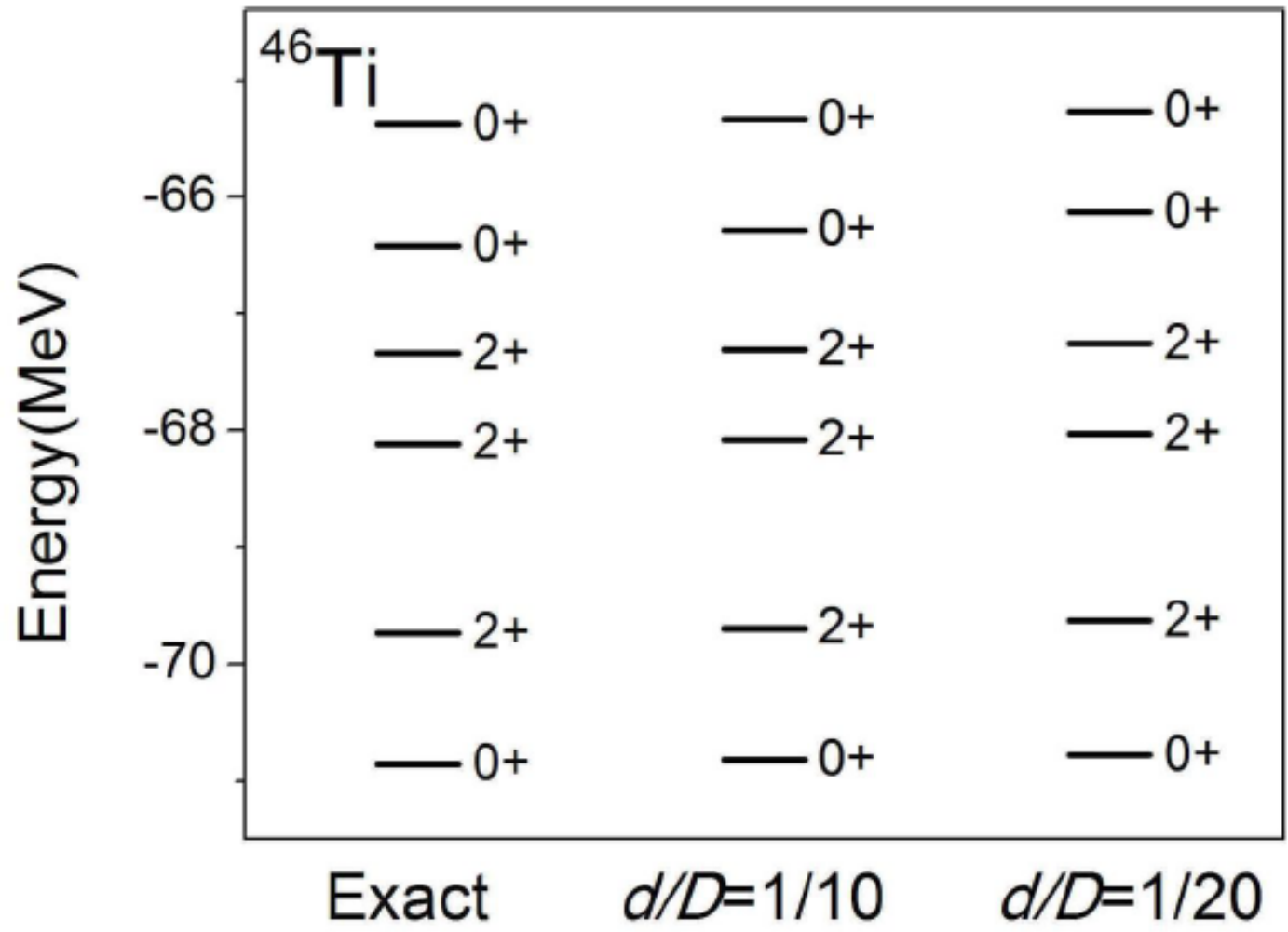
This figure is the same as the last one, except $k=4$.



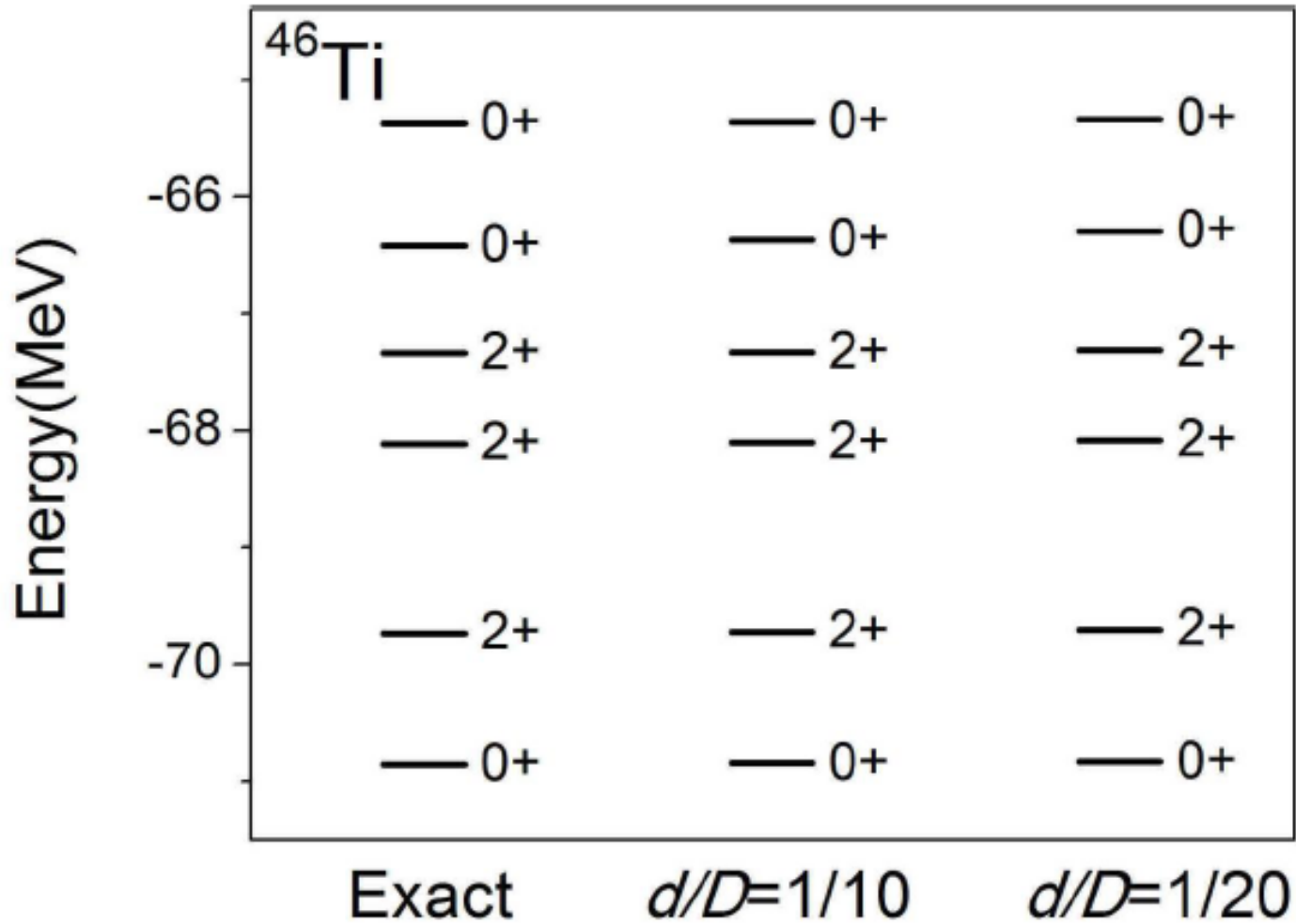
Here $k=6$



The same as the last page, except that here we investigate Ti-46 by using the GXPF1 with $k=2$.



Ti-46, GXPF1 interaction, $k=4$



Ti-46, GXPF1 interaction, $k=6$

The second approximation is enlightened by the fact that the magnitude of matrix elements close to the diagonal ones is much larger than the magnitude of matrix elements far from the diagonal ones.

Therefore our second approximation is straightforward. One neglect the contribution of matrix elements far from the diagonal ones. To expedite this process, we divide the matrix H into m^2 sub-matrices with dimension d' .

Let us denote

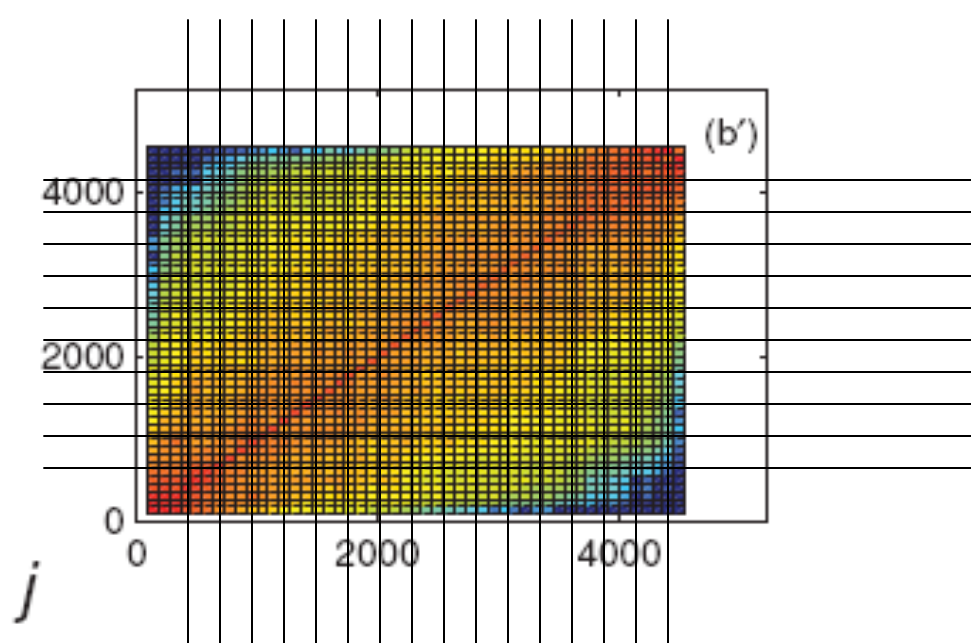
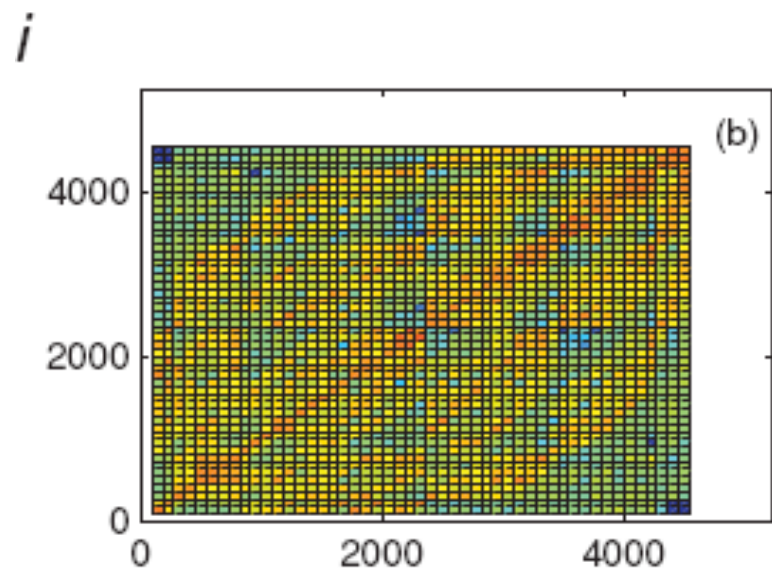
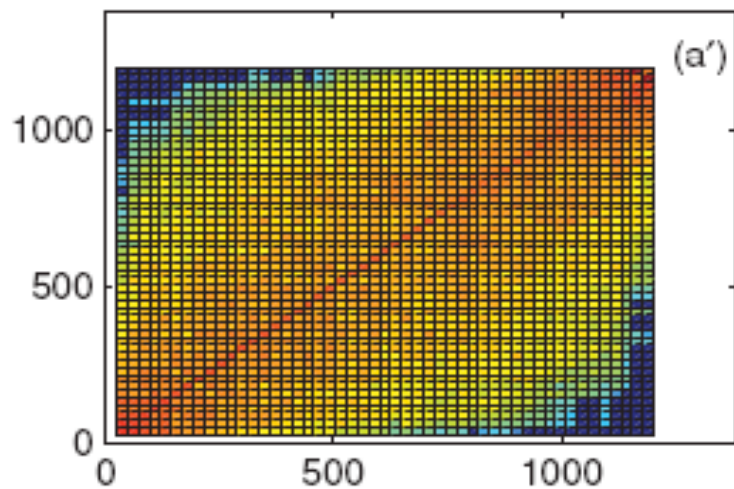
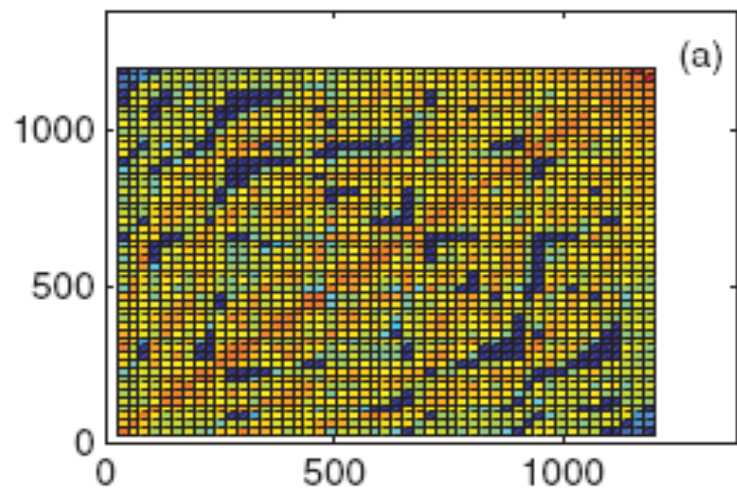
$$a(i)_{p,q} = A_{p,(i-1)d'+q},$$

$$b(ij)_{q,q'} = B_{(i-1)d'+(j-1)d'+q'},$$

$$c(i)_{q,p} = C_{(i-1)d'+q,p},$$

$$p = 1, 2, \dots, d; q, q' = 1, 2, \dots, d'.$$

$$\begin{array}{c}
 \leftarrow d \quad \rightarrow \quad \leftarrow D-d \quad \rightarrow \\
 \\
 \left(\begin{array}{cccc}
 & & & \\
 & & & A \\
 & b_{11} & b_{12} & \dots & b_{1m} \\
 & b_{21} & b_{22} & & \\
 C & & & G & \\
 & & & & \cdot \\
 & & & & b_{mm}
 \end{array} \right) \\
 \leftarrow D \quad \rightarrow
 \end{array}$$



$$H'(\lambda_w) = H_0$$

$$+ \sum_{n=2}^{\infty} V^T A(B^{n-2})CV$$

$$H'(\lambda_w)V'_w = \lambda_w V'_w$$

$$\Psi_w = \begin{pmatrix} I_d \\ \sum_{n=1}^k (b_{11}^{n-1})c_1 \\ \sum_{n=1}^k (b_{22}^{n-1})c_2 \\ \vdots \\ \sum_{n=1}^k (b_{mm}^{n-1})c_m \end{pmatrix} VV'_w.$$

k-th order
Perturbation

$$\approx \sum_{n=2}^k V^T A(B^{n-2})CV$$

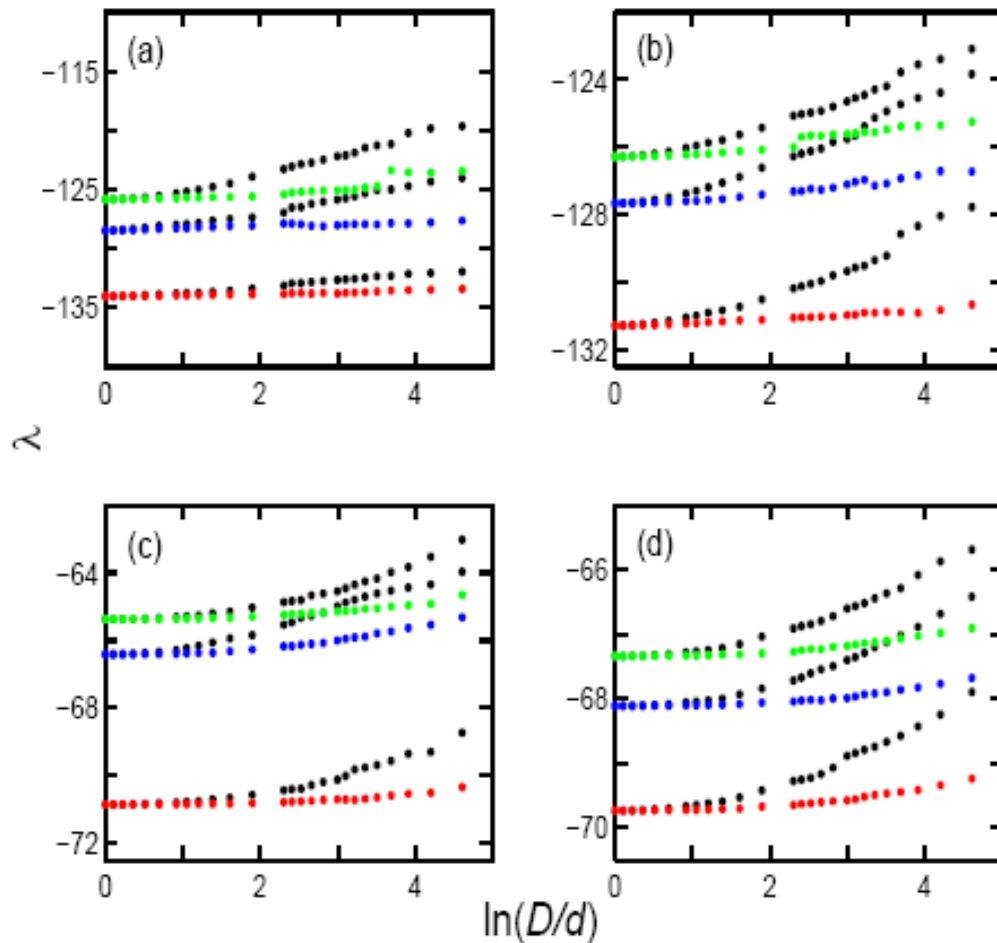
$$= \sum_{n=2}^k \sum_{i=1}^m V^T a_{i1} (b_{i_1 i_2} b_{i_2 i_3} \cdots b_{i_{n-1} i_n}) c_{i_n} V$$

$$\approx \sum_{n=2}^k \sum_{i=1}^m V^T a_i (b_{ii}^{n-2}) c_i V.$$

After sorting, large matrix elements of the shell model Hamiltonian are distributed along the diagonal line.

Therefore matrix elements of b_{ii} are much larger than those of $b_{i, j \neq i}$.

Wave functions thus obtained are neither orthogonal with each other and normalized.

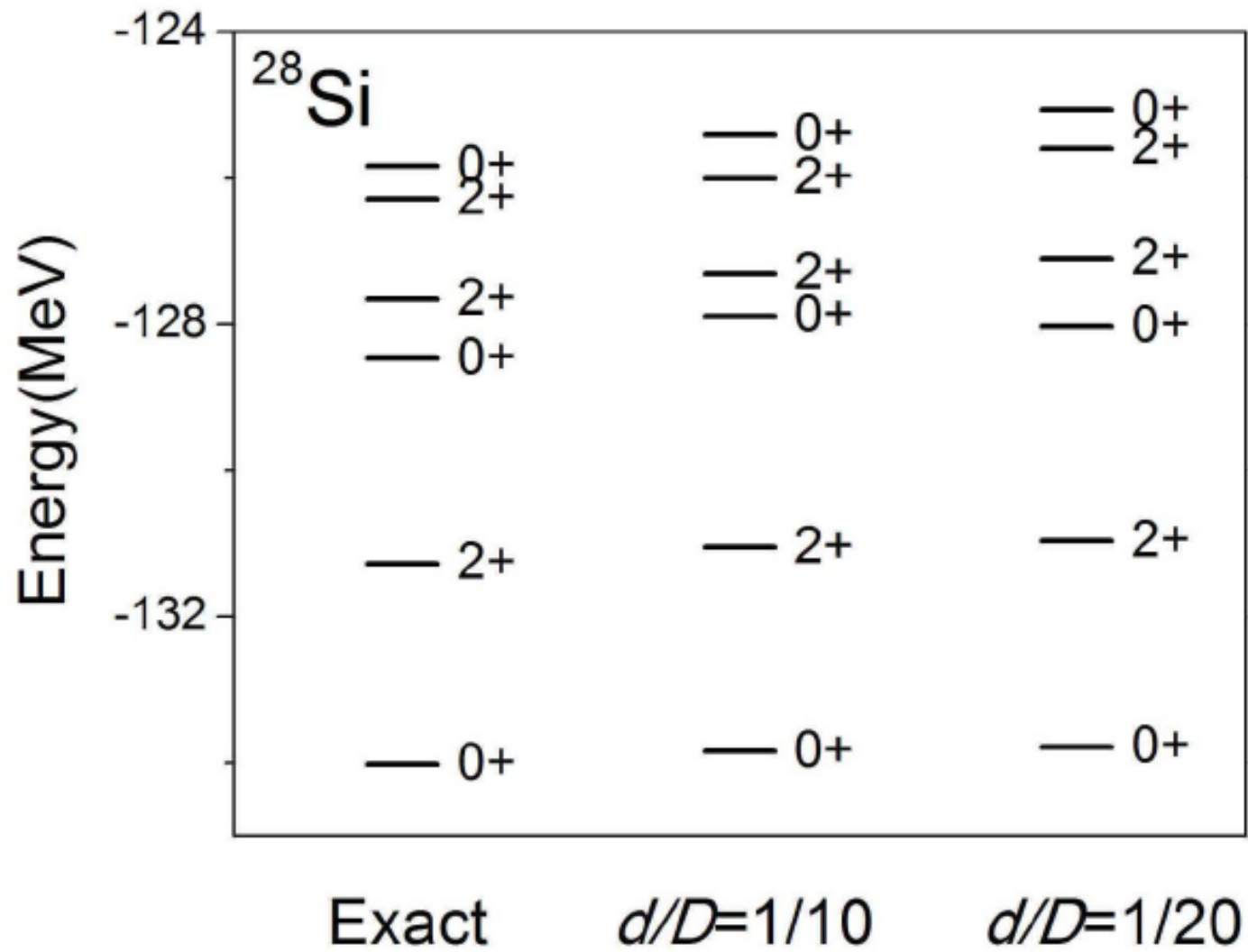


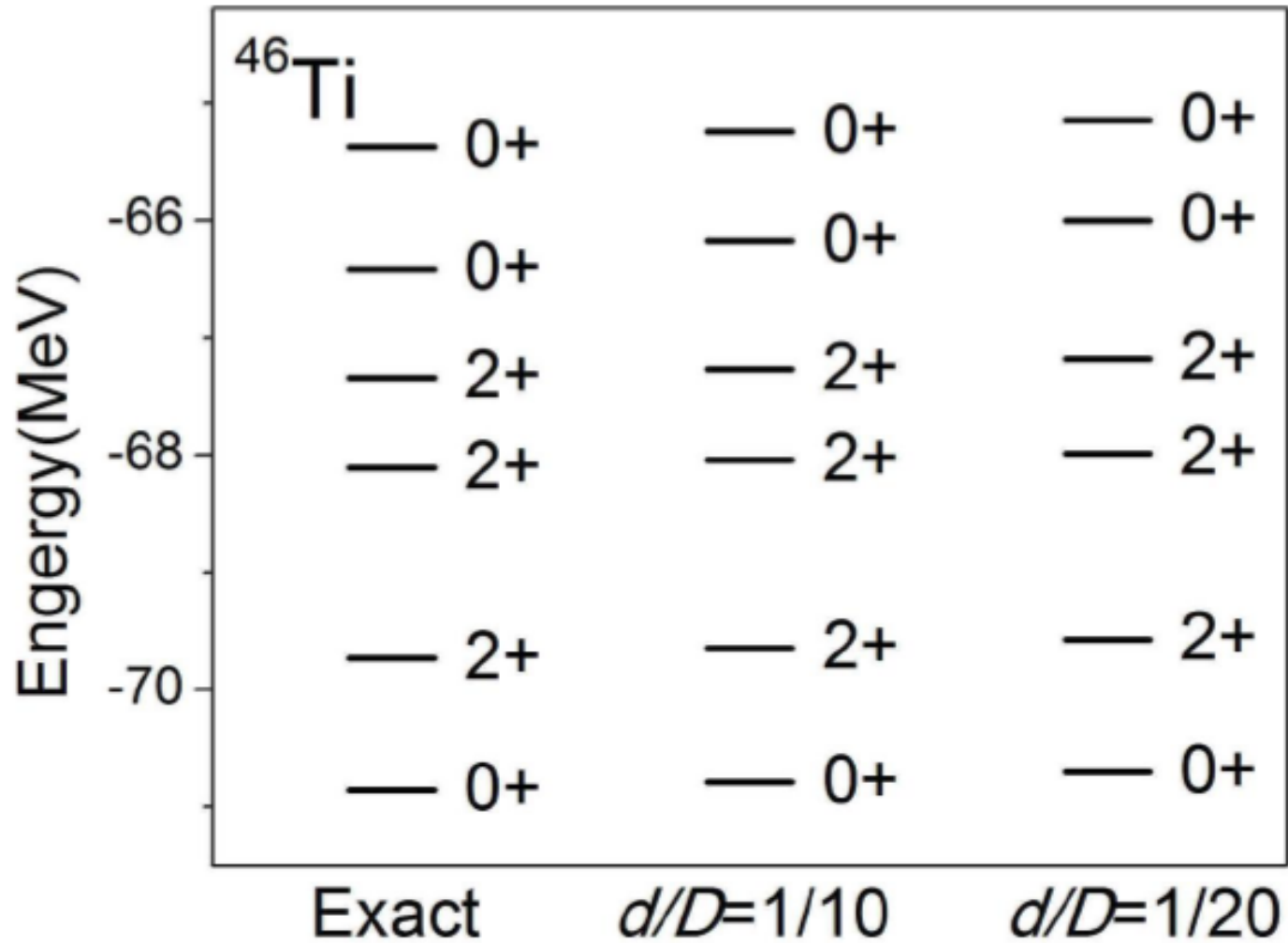
Eigenvalues of three lowest states versus $\ln[D/d]$,

(a) $l=0$ of Si28, (b) $l=2$ of Si-28, (c) $l=0$ of Ti-46, (d) $l=2$ of Ti-46.

Calculated results of three lowest energies versus $\ln D/d$.

Dots in black are obtained by exact diagonalizations, and dots in other colors are our predictions by using our new perturbation method of 4th order.





Ti-46, GXPF1 interaction, $k=4$

Now we discuss how good (or not good) of our effective Hamiltonian in terms of d/D . We take $I=0$ states ($D=41335$) Cr-48 as an example.

d/D	$k=2$	$k=4$	$k=6$
0.01	-99.0903	-99.5185	-99.7076
0.02	-99.3342	-99.6542	-99.7865
0.03	-99.4359	-99.7052	-99.8145
0.04	-99.4946	-99.7343	-99.83
0.05	-99.5519	-99.7631	-99.8451

Exact=-99.9126

Here we make only one approximation: we restrict the value of k .

d/D	$k=4$
0.01	-99.3141
0.02	-99.5065
0.03	-99.5881
0.04	-99.6394
0.05	-99.6834
0.1	-99.7732
0.2	-99.8567
0.3	-99.8825
0.4	-99.8988
0.6	-99.909
0.8	-99.9121
1	-99.9126

Here we made all three approximations, i.e., (1) restriction on values of $k=4$ (as above); (2) the diagonalization of h is limited to the three lowest states; (3) we consider only the diagonal submatrices with dimension much smaller than D .

d/D	$k=0$	$k=1$	$k=2$	$k=3$	$k=4$
0.01	0.895357	0.964923	0.980063	0.987542	0.991673
0.02	0.92916	0.979124	0.988903	0.99343	0.99578
0.03	0.943724	0.984173	0.991901	0.995368	0.997107
0.04	0.95187	0.986828	0.993417	0.996316	0.997739
0.05	0.959264	0.989359	0.994842	0.997191	0.998312
0.1	0.977186	0.995328	0.998055	0.999068	0.99949

Here we list the overlaps between the wave functions of exact shell model calculations and the wave functions of our effective shell model Hamiltonian. Here we have restriction on k only.

It takes large computational time to diagonalize large matrixes with dimension D .

This time is approximately proportional to D^3 . However, by our new approximation method, we can reduce this time to $D d'^2$.

This means we can save very much computational time.

Part IV

Summary and conclusions

We have shown that

- Diagonal matrix elements, if sorted from the smaller to the larger, display linear correlation with eigenvalues.
- We derived formulas for higher order perturbations in the way as the effective interaction theory.
- Sorting the diagonal matrix elements provides us with a new method of truncating the huge shell model space.
- The new approach by using perturbation presents nice agreement with exact solutions.

I hope that this method will be useful in future study of nuclear structure theory and wish to use them to study for example intruder states such as in ^{12}C and ^{16}O and heavier nuclear mysteries.

References

J.J.Shen, A.Arima, Y.M.Zhao and N.Yoshinaga

Strong correlation between eigenvalues and diagonal Matrix elements

Phys. Rev.C 78, 044305 (2008)

J.J.Shen, Y.M.Zhao and A.Arima

Lowest eigenvalues of random Hamiltonian

Phys. Rev.C82, 014309(2010)

J.J.Shen, Y.M.Zhao and A.Arima

New perturbation method of diagonalizing the nuclear shell model Hamiltonian, to be published

Collaborators

Y.M.Zhao, J.J.Shen and N.Yoshinaga

Franco; Congratulations on your 70th Birthday!

Be active and healthy for many more years!

Thank you for your attention !