Research Article

# On the Application of the Rayleigh-Ritz Method to a Projected Hamiltonian

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**We apply the well known Rayleigh-Ritz method (RRM) to the projection of a Hamiltonian operator chosen recently for the extension of the variational principle to ensemble states. By means of a toy model we show that the RRM eigenvalues approach to those of the projected Hamiltonian from below in most cases but a few ones. We also discuss the effect of an energy shift and the projection of the identity operator.**

## 1. Introduction

The Rayleigh-Ritz method (RRM) is one of the most widely used approaches for the study of the electronic structure of atoms and molecules[1][2]. One of its main advantages is that the RRM eigenvalues converge from above towards the exact energies of the physical system[3] (see also[4] and references therein).

In their introduction to the Rayleigh-Ritz variational principle Ding et al[5] resorted to a most curious Hamiltonian operator on a $D$-dimensional Hilbert space. Although such an operator is quite unrealistic for the treatment of actual physical problems, it seems to be worth further investigation.

## 2. The Rayleigh-Ritz method

The RRM applies to any Hermitian operator $H$ with eigenvalues $E_k$ and eigenvectors $|\psi_k\rangle$

$$H|\psi_k\rangle = E_k|\psi_k\rangle, k = 0, 1, \ldots. \tag{1}$$

If we have a complete set of non-orthogonal vectors $|u_i\rangle$, $i = 0, 1, \ldots$, then the approximate RRM eigenvalues $W_n$ are roots of the secular determinant[1][2][6]

$$|\mathbf{H} - W\mathbf{S}| = 0, \tag{2}$$


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where $\mathbf{H}$ and $\mathbf{S}$ are $N \times N$ matrices with elements $H_{ij} = \langle u_i|H|u_j\rangle$ and $S_{ij} = \langle u_i|u_j\rangle$, $i, j = 0, 1, \ldots N-1$, respectively. It is well known that $W_k \geq E_k$ for all $k = 0, 1, \ldots, N-1$[1][2][3][4][6].

## 2.1. Projected Hamiltonian

In their introduction to the Rayleigh-Ritz variational principle, Ding et al[5] considered the projection

$$H_D = \sum_{k=0}^{D-1} E_k \left|\psi_k\right\rangle \left\langle\psi_k\right|, \tag{3}$$

of $H$ on a subspace $\mathcal{H}_D$ of dimension $D$ spanned by the set of eigenvectors $\mathcal{S}_D = \{\left|\psi_k\right\rangle, k = 0, 1, \ldots, D-1\}$. They correctly stated that

$$\frac{\langle\psi|H_D|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0 \forall \psi \in \mathcal{H}_D. \tag{4}$$

This introduction of the variational principle is far from what we commonly face in ordinary applications of nonrelativistic quantum mechanics where we do not know $\mathcal{H}_D$. If we already know $\mathcal{H}_D$ then we can choose a complete basis set $\mathcal{B} = \{\left|i\right\rangle, i = 0, 1, \ldots, D-1\}$ of orthonormal vectors and, consequently, the diagonalization of the matrix of $H_D$ in such a basis is a trivial problem. For this reason, in what follows we assume that $\mathcal{H}_D$ is unknown. Typically, we have to deal with a Hamiltonian operator $H$ defined on an infinite-dimensional Hilbert space $\mathcal{H}$ and we do not know its eigenvalues and eigenvectors. However, we can try and do something interesting with the projected Hamiltonian of Ding et al by simply assuming that $\mathcal{H} \subset \mathcal{H}_D$.

If we assume that $H_D$ is also defined on $\mathcal{H}$ we can apply the RRM to this projected Hamiltonian. In such a case, the matrix elements are given by

$$(H_D)_{ij} = \sum_{k=0}^{D-1} E_k \left\langle u_i|\psi_k\right\rangle \left\langle\psi_k|u_j\right\rangle, \tag{5}$$

where $\{\left|u_j\right\rangle, j = 0, 1, \ldots\}$ spans the Hilbert space $\mathcal{H}$. We do not assume the vectors $\left|u_j\right\rangle$ to be orthonormal.

Under the conditions given above the results may be unexpected. For example, if $\psi \in \mathcal{H} \subset \mathcal{H}_D$ and $\langle\psi_k|\psi\rangle = 0$, $k = 0, 1, \ldots, n-1, n+1, \ldots, D-1$, then

$$\frac{\langle\psi|H_D|\psi\rangle}{\langle\psi|\psi\rangle} = E_n \frac{\left|\langle\psi_n|\psi\rangle\right|^2}{\langle\psi|\psi\rangle} \leq E_n \frac{\langle\psi_n|\psi_n\rangle \langle\psi|\psi\rangle}{\langle\psi|\psi\rangle} = E_n, \tag{6}$$


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where we have used the Cauchy-Schwartz inequality[7]. We appreciate that it is possible to obtain lower bounds instead of upper ones.

### 2.2. *Simple example*

A suitable toy model is given by

$$H = -\frac{1}{2}\frac{d^2}{dx^2}, \tag{7}$$

with the boundary conditions $\psi(0) = \psi(1) = 0$. This example was chosen in recent discussions of the RRM[4][6]. The exact eigenvalues and eigenfunctions are

$$E_k = \frac{k^2\pi^2}{2}, \psi_k(x) = \sqrt{2}\sin(k\pi x), k = 1, 2, \ldots. \tag{8}$$

For simplicity, we choose the non-orthogonal basis set

$$u_i(x) = x^i(1-x), i = 1, 2, \ldots, \tag{9}$$

already used earlier[6]. Table 1 shows that the RRM eigenvalues $W_k$ converge from above towards the exact eigenvalues $E_k$ as expected[1][2][3][4][6].

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| $N$ | $W_1$ | $W_2$ | $W_3$ | $W_4$ |
|---|---|---|---|---|
| 1 | 5 | | | |
| 3 | 4.934874810 | 21 | 51.06512518 | |
| 5 | 4.934802217 | 19.75077640 | 44.58681182 | 100.2492235 |
| 7 | 4.934802200 | 19.73923669 | 44.41473408 | 79.99595777 |
| 9 | 4.934802200 | 19.73920882 | 44.41322468 | 78.97848206 |
| 11 | 4.934802200 | 19.73920880 | 44.41321981 | 78.95700917 |
| 13 | 4.934802200 | 19.73920880 | 44.41321980 | 78.95683586 |
| 15 | 4.934802200 | 19.73920880 | 44.41321980 | 78.95683521 |
| 17 | 4.934802200 | 19.73920880 | 44.41321980 | 78.95683520 |
| 19 | 4.934802200 | 19.73920880 | 44.41321980 | 78.95683520 |

**Table 1.** Lowest RRM eigenvalues for the Hamiltonian (7)

Tables 2 and 3 show the RRM results for the projected Hamiltonian $H_D$ with $D=1$ and $D=2$, respectively (note that $k=1,2,\ldots,D$ in this example). We appreciate that there are $D$ meaningful eigenvalues $W_k\neq 0,\ k=1,2,\ldots,D$, and the remaining roots vanish $W_k=0,\ D<k\leq N$. It is interesting that the RRM yields the eigenvalues $E=0$ exactly while the others are approximate (though, they converge towards the exact ones as $N$ increases). A most curious fact is that the RRM eigenvalues $W_k$ converge towards the exact ones $E_k$ from below. However, this result is not general. In table 4 we show RRM eigenvalues for $D=3$. We see that this approach yields an upper bound to $E_1$ for $N=1$ and lower bounds to all the eigenvalues for $N>1$. The well known proofs for the upper bounds mentioned above [3][4] (and references therein) do not apply here because the functions $u_i(x)$ cannot be expressed in terms of the finite set $\{\psi_k(x),k=1,2,\ldots,D\}$.


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| $N$ | $W_1$ | $W_k, 1 < k \leq N$ |
|---|---|---|
| 1 | 4.927671482 | |
| 3 | 4.934799721 | 0 |
| 5 | 4.934802200 | 0 |
| 7 | 4.934802200 | 0 |

**Table 2.** RRM for the projected Hamiltonian with $D = 1$

| $N$ | $W_1$ | $W_2$ | $W_k, 2 < k \leq N$ |
|---|---|---|---|
| 1 | 4.927671482 | | |
| 3 | 4.934799721 | 19.40270646 | 0 |
| 5 | 4.934802200 | 19.73799899 | 0 |
| 7 | 4.934802200 | 19.73920734 | 0 |
| 9 | 4.934802200 | 19.73920880 | 0 |
| 11 | 4.934802200 | 19.73920880 | 0 |

**Table 3.** RRM for the projected Hamiltonian with $D = 2$

| $N$ | $W_1$ | $W_2$ | $W_3$ | $W_k, 3 < k \leq N$ |
|---|---|---|---|---|
| 1 | 4.988506932 | | | |
| 3 | 4.934799541 | 19.40270646 | 41.72191568 | 0 |
| 5 | 4.934802200 | 19.73799899 | 44.37877225 | 0 |
| 7 | 4.934802200 | 19.73920734 | 44.41306667 | 0 |
| 9 | 4.934802200 | 19.73920880 | 44.41321950 | 0 |
| 11 | 4.934802200 | 19.73920880 | 44.41321980 | 0 |
| 13 | 4.934802200 | 19.73920880 | 44.41321980 | 0 |

**Table 4.** RRM for the projected Hamiltonian with $D = 3$

For every RRM eigenvalue $W_k$ we obtain an approximate solution[1][2][6]

$$|\varphi_k\rangle = \sum_{j=1}^{N} c_{jk} |u_j\rangle, \tag{10}$$

and we choose such solutions to be orthonormal $\langle\varphi_k|\varphi_n\rangle = \delta_{kn}$. The results of tables 2, 3 and 4 suggest that

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \langle\varphi_i|H_D|\varphi_j\rangle |\varphi_i\rangle \langle\varphi_j| = \sum_{i=1}^{D} W_i |\varphi_i\rangle \langle\varphi_i|, \tag{11}$$

because $\langle\varphi_i|H_D|\varphi_j\rangle = W_i\delta_{ij}$[1][2][6].

In order to investigate the particular case $N = 1$ in more detail we calculated the expectation value $\langle H_D\rangle$ with the function $u_1(x)$. The results in table 6 clearly show that $\langle H_1\rangle < E_1 < \langle H\rangle = 5$ and $E_1 < \langle H_D\rangle < \langle H\rangle$ for $D > 1$. The table suggests the obvious conclusion that $\lim\limits_{D\to\infty} \langle H_D\rangle = \langle H\rangle$ that can be proved analytically:

$$\sum_{k=1}^{\infty} \frac{k^2\pi^2}{2} \frac{\langle u_1|\psi_k\rangle \langle\psi_k|u_1\rangle}{\langle u_1|u_1\rangle} = \frac{240}{\pi^4} \sum_{k=1}^{\infty} \frac{1-(-1)^k}{k^4} = 5. \tag{12}$$

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It is worth adding that for $D=4$ we have $W_1>E_1$ for $N=1$ as aready discussed and also $W_2>E_2$ for $N=3$.

We also carried out some numerical experiments with $E_k=k^2\pi^2/2+c$, where $c$ is a real constant. Table 5 shows that for $c=-5$ $W_1$ becomes an upper bound while $W_2$ and $W_3$ remain lower bounds.

| $N$ | $W_1$ | $W_2$ | $W_3$ | $W_k, 3<k\leq N$ |
|---|---|---|---|---|
| 1 | $-0.01111693899$ | | | |
| 3 | $-0.06519776461$ | 14.48794350 | 37.02490009 | 0 |
| 5 | $-0.06519779945$ | 14.73830544 | 39.38265032 | 0 |
| 7 | $-0.06519779945$ | 14.73920771 | 39.41308391 | 0 |
| 9 | $-0.06519779945$ | 14.73920880 | 39.41321953 | 0 |
| 11 | $-0.06519779945$ | 14.73920880 | 39.41321980 | 0 |
| 13 | $-0.06519779945$ | 14.73920880 | 39.41321980 | 0 |

**Table 5.** RRM for the projected Hamiltonian with $D=3$ and $E_k=k^2\pi^2/2-5$


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| $D$ | $\langle H_D \rangle$ |
|---|---|
| 1 | 4.927671482 |
| 3 | 4.988506932 |
| 5 | 4.996391207 |
| 7 | 4.998443548 |
| 9 | 4.999194603 |
| 11 | 4.999531169 |
| 13 | 4.999703701 |
| 15 | 4.999801038 |
| 17 | 4.999860037 |
| 19 | 4.999897849 |
| 21 | 4.999923186 |
| 23 | 4.999940795 |
| 25 | 4.999953410 |
| 27 | 4.999962682 |
| 29 | 4.999969649 |
| 31 | 4.999974985 |
| 33 | 4.999979140 |
| 35 | 4.999982424 |
| 37 | 4.999985053 |
| 39 | 4.999987183 |
| 41 | 4.999988927 |
| 43 | 4.999990368 |
| 45 | 4.999991570 |

**Table 6.** Expectation value of $H_D$ with $u_1(x)$

### *2.3. Arbitrary example*

We can extend the results of the preceding subsection to a more general case based on the same toy model. Suppose that we have a set of orthonormal vectors $|\psi_k\rangle$, $k = 1, 2, \ldots, D$ and construct the projected Hamiltonian operator

$$H_D = \sum_{k=1}^{D} \alpha_k |\psi_k\rangle \langle\psi_k|, \tag{13}$$

where $\alpha_k$ are arbitrary real numbers. We can obviously apply the RRM as in the preceding example. Table 7 shows RRM eigenvalues for the case $D = 3$ and $\alpha_k = k$. In this case we appreciate that $W_1 > 1$ for $N = 1$ and $W_1 < 1$ for all $N > 1$. Also $W_2 > 2$ for $N = 3$ and $W_2 < 2$ for all $N > 3$. We conclude that the RRM yields upper and lower bounds for this kind of projected Hamiltonian operators.

| $N$ | $W_1$ | $W_2$ | $W_3$ | $W_k, 3 < k \leq N$ |
|---|---|---|---|---|
| 1 | 1.002664294 | | | |
| 3 | 0.9999994479 | 2.027339721 | 2.818209291 | |
| 5 | 0.9999999999 | 1.999877421 | 2.997673155 | 0 |
| 7 | 0.9999999999 | 1.999999852 | 2.999989656 | 0 |
| 9 | 0.9999999999 | 1.999999999 | 2.999999979 | 0 |
| 11 | 0.9999999999 | 1.999999999 | 2.999999999 | 0 |
| 13 | 1.0000000000 | 1.999999999 | 2.999999999 | 0 |

**Table 7.** RRM for the arbitrary Hamiltonian (13) with $D = 3$ and $\alpha_k = k$

## 3. What about the identity operator?

In the calculations discussed above we have considered the identity operator on $\mathcal{H}$

$$I=\sum_{k=1}^{\infty}\left|\psi_k\right\rangle\left\langle\psi_k\right|, \tag{14}$$

so that the overlap matrix is given by $S_{ij}=\langle u_i|I|u_j\rangle$, $i,j=1,2,\ldots,N$. We obtain completely different results if we consider the projection of $I$ on $\mathcal{H}_D$

$$I_D=\sum_{k=1}^{D}\left|\psi_k\right\rangle\left\langle\psi_k\right|, \tag{15}$$

and the overlap matrix $S_{i,j}^D=\langle u_i|I_D|u_j\rangle$, $i,j=1,2,\ldots,N$. In this case, we obtain upper bounds for $1\leq N<D$ and the exact eigenvalues when $N=D$. For example, for $D=N=5$ we have

$$\left|\mathbf{H}_D-W\mathbf{S}^D\right|=\frac{67108864\left(\pi^2-2W\right)\left(2\pi^2-W\right)\left(8\pi^2-W\right)\left(9\pi^2-2W\right)\left(25\pi^2-2W\right)}{9765625\pi^{46}}, \tag{16}$$

that yields the fifth lowest eigenvalues exactly.

# 4. Conclusions

It is not clear to us why Ding et al[5] introduced the variational principle by means of a projected Hamiltonian operator because this principle as well as the properties of the RRM have already been proved for the kind of operators commonly found in actual physical problems[3][4]. However, when the RRM is applied to the projected Hamiltonian in the usual way, one obtains lower bounds in most cases as shown above. It is interesting that the null $N-D$ eigenvalues are given exactly for all $N>D$ although the linear combinations of the approximate basis vectors $|u_i\rangle$ only yield the exact ones $|\psi_k\rangle$ in the limit $N\rightarrow\infty$. We have also shown that the RRM yields upper bounds for $1\leq N<D$ and exact eigenvalues for $N=D$ when we consider the identity operator (15) instead of (14).

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## Declarations

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