

## Peer Review

# Review of: "On the Application of the Rayleigh–Ritz Method to a Projected Hamiltonian"

Andreas Savin<sup>1</sup><sup>1</sup>. Laboratoire de Chimie Theorique, Sorbonne University, Paris, France

The paper applies the Rayleigh–Ritz method (RRM) to the Hamiltonian  $H_D$ , eq. (3). It concludes that the “RRM eigenvalues approach to those of the projected Hamiltonian from below.” If I understand the statement correctly, it means that the expression of the l.h.s. of the inequality (4) is less than or equal to the eigenvalues  $E_k$  showing up in eq.1 and the construction of  $H_D$ . A simple example is given to prove this statement.

I think that the numerical example is correct, but not the conclusions. In my understanding,  $H_D$  has eigenvalues  $E_k$  for all  $D$  eigenstates showing up in the definition of  $H_D$ . However, it has a 0 eigenvalue for all states orthogonal to the eigenstates present in  $H_D$ , as can be seen from the definition of  $H_D$ . Let  $E_0$  be the lowest eigenvalue of  $H$ . If  $0 < E_0 < \dots$  an admixture of the states orthogonal to those present in the definition of  $H_D$  lowers the energy. In fact, a sufficiently flexible ansatz for the wave function should obtain any of the eigenstates of the space orthogonal to the  $D$  eigenstates present in  $H_D$  because the lowest eigenvalue of  $H_D$  is 0. When  $E_0 < 0$ , one approaches  $E_0$  from above, in contrast to the statement made by the author.

In order to substantiate my statement with a numerical example, let me slightly change the example used in the paper and shift the potential by a constant,  $c$ . To recover the results of the paper, we can set  $c=0$ . We have:  $E_0 = \pi^2/2 + c$  and  $W_0 = (480/\pi^4)(1 + 2c/\pi^2)$ . As in the paper,  $W_0 - E_0$  is negative for  $c=0$ , but becomes positive when  $c < -\pi^2/2$ .

Of course, one could easily produce more counter-examples, e.g., the H atom.

In conclusion, in my opinion, the paper should not be published in its present form. Even if corrected (in the spirit described above), I abstain from giving a recommendation for or against its publication for the following reason. The paper looks to me more like an exercise to give to students than a scientific paper. However, I cannot draw a sharp limit between these.

## Declarations

**Potential competing interests:** No potential competing interests to declare.