Comment

Comment on "Full quantum eigensolvers based on variance" by Li et al.

P. D. Stevenson
University of Surrey, Guildford, Surrey, GU2 7XH

Abstract. A recent paper uses a variance minimization method to find eigenstates of three different Hamiltonians. The first of these – a Hamiltonian for the deuteron – is presented in a misleading way with trivial solutions mixed up with intersting solutions on the same footing. We clarify the physical meaning of the eigenstates and point out a confusion between a molecular and nuclear system, and between units.

In a recent paper, Li *et al.* [1] (from now on, the paper will be referred to as just "Li" for brevity) present a quantum algorithm which minimizes Hamiltonian variance in order to target ground and excited states. In this comment, we wish to specifically address Li's use of the deuteron as an example, as their presentation of the model is problematic.

The deuteron model they use is taken from the paper of Dumitrescu *et al.* [2] (from now on referred to as just "Dumitrescu"). We briefly restate some key points of that model.

The model is based on a pionless effective field theory that describes the interaction between nucleons to give the nucleus with one proton and one neutron, known as the deuteron, being the nucleus of the heavy hydrogen isotope deuterium. The model represents the deuteron wave function in a harmonic oscillator basis such that the deuteron is taken as a single particle, and the neutron and proton are not formally dealt with separately at the level of the effective Hamiltonian, which is (as given in Dumitrescu),

$$H_N = \sum_{n,n=0} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n, \tag{1}$$

with given matrix elements.

The Hamiltonian is thus a single particle one and a state $|n\rangle$ means that a deuteron exists in the oscillator state $|n\rangle$. In (1), N corresponds to the total number of oscillator levels included in the basis. Li specialise to the case $N = 2$ meaning that there are two oscillator levels, each of which can be occupied by a single deuteron (N.B. despite the deuteron having integer spin, the operators in (1) are fermionic operators since the model seeks to formalize the expansion of a single deuteron in oscillator states).

With $N = 2$ there are four possible states formally. Dumitresu denotes these as : $|n_1 n_0\rangle = \{|\uparrow\uparrow\rangle\,|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. Here the up arrow denotes zero deuterons in state

$|n_i\rangle$ while the down arrow indicates one deuteron in that state. Thus, the $|\uparrow\uparrow\rangle$ state describes the vacuum, with no deuterons, and $|\downarrow\downarrow\rangle$ represents a two deuteron state, and indeed the only two deutron state expressible in the basis.

Given this discussion, it is clear that to describe *a single* deuteron, only the $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ subspace is needed. Indeed, Dumitrescu makes this clear, and restricts their calculation to this subspace.

Both Dumitrescu and Li present the Hamiltonian (1) in the Pauli spin basis, which we write here as

$$H_2 = 5.906709 I_0 I_1 + 0.218291 Z_0 I_1 - 6.125 I_0 Z_1 - 2.143304 (X_0 X_1 + Y_0 Y_1), \quad (2)$$

where the subscripts on the Pauli operators indicate on which qubit they act and the operators spanning the space of qubits 0 and 1 are understood to be taken as Kronecker products. We have been explicit with identity matrices where they were left implied in both Dumitrescu and Li in different ways. We have also included the full precision of coefficients given by Dumitrescu while Li rounded them somewhat.

Equivalently we can write the Pauli operators in (2) explicitly in matrix form and find

$$H_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 12.15 & -4.28661 & 0 \\ 0 & -4.28661 & -0.436582 & 0 \\ 0 & 0 & 0 & 11.8134 \end{pmatrix}. \quad (3)$$

The matrix form makes it particularly clear that the problem as stated is already decoupled into the zero, one, and two deuteron sectors, through the block-diagonal matrix structure. The zero deuteron solution has eigenvalue 0 and there is no "computation" to be done to find it. Similarly, the single two deuteron basis state has no other states to mix with and has a trivial solution with energy $E = 11.8134$ MeV.

The interesting problem, for which some computation *is* required is in the 2x2 matrix in the centre of the 4x4 matrix.

The presentation by Li includes the following aspects, which are deserving of comment here:

- The deuteron is referred to as a "molecule". However, the Hamilonian presented is not for molecular deuterium, but for the deuteron nucleus.
- The energies, as shown in Figure 4 of Li, are given in units of Hartree, but these numbers should be MeV. I.e. the stated energies in Li are around five orders of magnitude too small.
- The authors present the four eigenvalues on an equal basis, while the model they present is already diagonal in the E_2 and E_3 (their notation) eigenstates, and these moreover do not represent single deuteron solutions as claimed. They are the zero and two deuteron "solutions" for which no computation is required. There is no

acknowledgement that the two trivial solutions are indeed trivial and that they do not realistically test the method presented.

- The unnecessary rounding in Li of the coefficients of the Hamiltonian as presented in Dumitrescu results in the energy of the zero deuteron state not being exactly zero.

We note in searching the literature, that although Li cites Dumetrescu in which a correct description may be found, some of the same problems (e.g. identification as a molecule) already appear in another paper [3] cited by Li. We believe it is worthwhile to stop the further misuse of the model in the literature, and in this spirit submit the present comment. This comment does not affect any other part of the Li paper beyond the deuteron example.

Acknowledgments

The author gratefully acknowledges support from the UK Science and Technology Facilities Council (STFC) via award ST/W006472/1.

References

[1] Li R N, Tao Y H, Liang J M, Wu S H and Fei S M 2024 *Physica Scripta* **99** 095207 ISSN 1402-4896 URL https://dx.doi.org/10.1088/1402-4896/ad664c

[2] Dumitrescu E F, McCaskey A J, Hagen G, Jansen G R, Morris T D, Papenbrock T, Pooser R C, Dean D J and Lougovski P 2018 *Physical Review Letters* **120** 210501 ISSN 0031-9007 URL http://dx.doi.org/10.1103/PhysRevLett.120.210501

[3] Liang J M, Lv Q Q, Shen S Q, Li M, Wang Z X and Fei S M 2022 *Advanced Quantum Technologies* **5** 2200090 ISSN 2511-9044 URL https://dx.doi.org/10.1002/qute.202200090