Comment on "Criterion for a good variational wave function"

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In a recent paper C. Gros reported the empirical observation that the variance of the energy can be taken as a measure of the quality of a variational trial wave function. Exact quality criteria based on the variance are well established and we give a short review of some of those criteria.

In a recent paper[1] Gros reported the empirical observation, that the variance of the energy is a measure of the quality of the variational trial wave function for the antiferromagnetic Heisenberg model and suggested that this criterion should be valid for all quantum systems. Exact relations of this kind which give bounds on the error in energy as a function of the variance have been known for a long time. Such a criterion was proposed by Weinstein in 1934.[2] Even though those criteria are very useful, they cannot be found in most textbooks on quantum mechanics, one exception being the textbook by Pauling and Wilson.[3] This perhaps explains why those criteria were not used in the field of Monte Carlo simulations of highly correlated systems prior to the paper by Gros. We therefore give a short review over the most useful of these criteria.

THE WEINSTEIN CRITERION

Let us consider a Hamiltonian H with eigenvalues E_i and normalized eigenfunctions ψ_i, where E_1, ψ_1 denote the ground state, and the eigenvalues are assumed to be in increasing order. Let Φ be a normalized trial wave function and E_Φ its energy expectation value:

$$E_\Phi = \langle \Phi | H | \Phi \rangle \ , \quad \langle \Phi | \Phi \rangle = 1 \ .$$

The residue vector $|r_\Phi\rangle$ for the state $|\Phi\rangle$ is then defined as

$$|r_\Phi\rangle = (H - E_\Phi)|\Phi\rangle \ .$$

The length of the residue vector equals the variance of the energy expectation E_Φ

$$\begin{aligned}\langle r_\Phi | r_\Phi \rangle &= \langle \Phi | (H-E_\Phi)^2 | \Phi \rangle \\ &= \langle \Phi | H^2 | \Phi \rangle - \langle \Phi | H | \Phi \rangle^2 = \sigma_\Phi^2 \ .\end{aligned}$$

The Weinstein criterion now states that at least one eigenvalue can be found in the interval

$$[E_\Phi - \sigma_\Phi, E_\Phi + \sigma_\Phi] \ .$$

Therefore if σ_Φ tends to zero, Φ becomes arbitrary close to the exact eigenfunction and σ_Φ is indeed a measure of how good the trial wave function is.

Since the proof of this criterion is so easy we will just reproduce it from the above-mentioned book by Pauling and Wilson.[3]

Expanding Φ in its orthonormal eigenfunctions ψ_i, $\Phi = \sum_i \alpha_i \psi_i$, we obtain for $\langle r_\Phi | r_\Phi \rangle$

$$\begin{aligned}\langle r_\Phi | r_\Phi \rangle &= \langle \Phi | (H-E_\Phi)^2 | \Phi \rangle \\ &= \sum_i |\alpha_i|^2 (E_i - E_\Phi)^2 \ .\end{aligned}$$

Now we take the eigenvalue E_k which is closest to E_Φ; $|E_k - E_\Phi| \le |E_i - E_\Phi|$, $i \ne k$:

$$\sum |\alpha_i|^2 (E_i - E_\Phi)^2 \ge \sum_i |\alpha_i|^2 (E_k - E_\Phi)^2 = (E_k - E_\Phi)^2 \ .$$

This gives the Weinstein criterion

$$|E_\Phi - E_k| \le \sqrt{\langle r_\Phi | r_\Phi \rangle} = \sigma_\Phi \ .$$

The Weinstein criterion guarantees that one has found an eigenstate, but unfortunately it does point out which one. This is however no serious drawback in practice since one usually knows which eigenstate is approximated. In the case where E_Φ is sufficiently close to the ground state (i.e., $|E_1 - E_\Phi| \le |E_i - E_\Phi| i = 2, \ldots$), the upper bound can of course be replaced by the expectation value of the energy and the criterion reads

$$E_\Phi - \sigma_\Phi \le E_1 \le E_\Phi \ .$$

Since these criteria give a lower bound they are also frequently called lower bound criteria.

THE TEMPLE CRITERION FOR THE GROUND STATE

Another criterion which often gives better lower bounds is the Temple criterion

$$E_\Phi - \frac{\sigma_\Phi^2}{E_2 - E_\Phi} \le E_1 \le E_\Phi \ ,$$

where E_2 is the second exact eigenvalue or a lower bound to it. As in the case of the Weinstein criterium for the ground state, it is only valid if E_Φ is sufficiently close to the ground-state energy. For the proof of the above criterion as well as for its extensions we refer the reader to a review article by Abdel-Raouf,[4] where other criteria are also given.

GENERAL REMARKS

Finally we would like to point out, that it is not possible for any Hamiltonian bounded from below to find a trial wave function Φ which has the energy of the ground state and a nonvanishing variance. This is easily seen by expanding Φ in its eigenfunctions

$$\langle \Phi|H|\Phi\rangle=\sum_i |\alpha_i|^2 E_i \ .$$

Since Φ is in Hilbert space the sum $\sum_i |\alpha_i|^2$ must be finite. In our case it is normalized to 1 for convenience. If the energy expectation value equals E_1, it follows that all α_i are zero except α_1 (assuming a nondegenerate ground state). But then Φ is an eigenvector and its variance vanishes. The counterexample constructed by Gros is not valid since his trial wave function at $\omega_0=0$ is outside the allowed space.

Nevertheless, as was stated by Gros, it is possible to find a trial wave function whose energy is arbitrarily close to the ground state but whose variance may be arbitrarily large. To illustrate this let us consider the wave function $\Phi=\alpha_1\psi_1+\alpha_m\psi_m$. We now chose α_1 and α_m such that Φ is normalized and has energy $E_1+\varepsilon$. Then it is easy to show that its variance is given by

$$\sigma_\Phi^2=\left[1-\frac{\varepsilon}{E_m-E_1}\right]\varepsilon^2+\frac{\varepsilon}{E_m-E_1}(E_m-E_1-\varepsilon)^2 \ .$$

If now E_m tends to infinity while ε being fixed, σ_Φ tends to infinity, too. In practice however, one deals with Hamiltonians which are bounded from above. In this case the variance becomes arbitrarily small whenever the error in the eigenvalue becomes arbitrarily small. The proof of this for the ground state goes as follows. Let us consider a sufficiently good approximation such that $\varepsilon=E-E_1\le E_2-E_\Phi\le\dots\le E_n-E_\Phi$. Then we have

$$\begin{aligned}\sigma_\Phi^2&=\sum_{i=1}^{n}|\alpha_i|^2(E_i-E_\Phi)^2=|\alpha_1|^2(E_1-E_\Phi)^2+\sum_{i=2}^{n}|\alpha_i|^2(E_i-E_\Phi)^2\\&\le|\alpha_1|^2(E_1-E_\Phi)^2+(E_n-E_\Phi)\sum_{i=2}^{n}|\alpha_i|^2(E_i-E_\Phi)\\&=|\alpha_1|^2(E_1-E_\Phi)^2+(E_n-E_\Phi)|\alpha_1|^2(E_\Phi-E_1)\\&\le\varepsilon^2+(E_n-E_\Phi)\varepsilon=(E_n-E_1)\varepsilon \ .\end{aligned}$$

[1]C. Gros, Phys. Rev. B **42**, 6835 (1990).
[2]D. H. Weinstein, Proc. Natl. Acad. Sci. U.S.A. **20**, 529 (1934).
[3]L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics* (McGraw-Hill, New York, 1935).
[4]M. A. Abdel-Raouf, Phys. Rep. **84**, 216 (1982).