Commentary

Rediscovering Eckart

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We show that an upper bound derived in a recent paper is identical to an inequality obtained more than ninety years ago. The early paper is not cited in spite of the fact that it has been discussed, reformulated, and generalized by many authors over several decades.

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1. Introduction

Many years ago, Eckart[1] developed a lower bound for the overlap between the ground-state eigenfunction and an arbitrary state. This formula became quite popular and many authors proposed all kinds of improvements to it[2][3][4][5][6][7][8][9][10][11]. In a recent paper, Shilling et al.[12] derived a universal relation based on an upper an a lower bound to the overlap but they did not mention Eckart at all. The purpose of this short note is to investigate whether one of these bounds is related to Eckart's one.

The derivation of Eckart's upper bound is quite easy. We simply focus on the Schrödinger equation

$$H\psi_j = E_j\psi_j, j = 0, 1, \ldots, E_0 < E_1 \leq E_2 \leq \ldots, \tag{1}$$

and assume that $\langle\psi_i|\psi_j\rangle = \delta_{ij}$.

Consider a normalized trial function φ that can be expanded in terms of the eigenfunctions of H

$$\varphi = \sum_{j=0}^{\infty} c_j\psi_j, c_j = \langle\psi_j|\varphi\rangle. \tag{2}$$

Taking into account that

$$\langle\varphi|H|\varphi\rangle - E_0 = \sum_{j=0}^{\infty} |c_j|^2 (E_j - E_0) \geq (E_1 - E_0) \sum_{j=1}^{\infty} |c_j|^2 = (E_1 - E_0) \left(1 - |c_0|^2\right), \tag{3}$$

we obtain Eckart's upper bound

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$$\frac{\langle H\rangle - E_0}{E_1 - E_0} \geq 1 - |c_0|^2, \tag{4}$$

by just setting $E = -\langle H\rangle$, $E_0 = -W_1$, $E_1 = -W_2$ and $|c_0|^2 = a_1^2$. This equation is exactly one of the inequalities derived by Shilling et al.[12]. Note that $|c_0|^2 = \langle \hat{\pi}_{E_0}\rangle = \|\hat{\pi}_{E_0}\varphi\|^2$, where $\hat{\pi}_{E_0} = |\psi_0\rangle\langle\psi_0|$ is the projector onto the ground-state. This equation is also valid when the ground state is degenerate if we assume that $\hat{\pi}_{E_0}$ is the projection operator onto the subspace of degenerate states that share the eigenvalue E_0.

In fact, in the case that the ground state is degenerate we can repeat the proof given above in terms of the spectral resolutions of H and the identity operator I, namely,

$$H = \sum_{J=0}^{\infty} E_j P_j, I = \sum_{J=0}^{\infty} P_j, \tag{5}$$

where P_j is the projection operator onto the subspace spanned by the degenerate states that share the same eigenvalue E_j. One can repeat the proof above by simply noting that $1 \geq \langle\varphi|P_j|\varphi\rangle = \langle P_j\varphi|P_j\varphi\rangle \geq 0$. The proof remains valid if we generalize equation (5) by the addition of the contribution of the continuum spectrum.

Conclusion: Equation (4) is mathematically identical to the inequality derived by Eckart[1] more than ninety years ago. This result, which provides a lower bound to the overlap between a trial state and the ground state in terms of the energy expectation value, has been discussed, reformulated, and generalized by many authors over several decades[2][3][4][5][6][7][8][9][10][11]. Surprisingly, neither Eckart's original work nor this substantial body of subsequent literature is cited in Ref.[12], where the same inequality is presented as part of a set of universal relations.

Shilling et al.[12] derived also a lower bound because they considered a finite Hilbert space. In addition to be rather unrealistic such a case may be treated in a somewhat trivial way as shown elsewhere[13].

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