Lower bounds to second-order corrections to eigenvalues observables of stationary quantum systems

1968 J. Phys. A: Gen. Phys. 2 140

(http://iopscience.iop.org/0022-3689/2/1/020)

J. PHYS. A (GEN. PHYS.), 1969, SER. 2, VOL. 2. PRINTED IN GREAT BRITAIN

Lower bounds to second-order corrections to eigenvalues of observables of stationary quantum systems

Abstract. This letter finds lower bounds to the second-order correction to the eigenvalue of an observable for the ith excited state of a stationary quantum system.

It was shown in an earlier paper (Sharma 1967, to be referred to as I) how upper bounds to the second-order correction to the ith excited eigenvalue of a Hermitian operator perturbed by another Hermitian operator can be obtained by a modification of the Hylleraas functional. This letter finds the corresponding lower bounds using the same formalism.

We use notations defined in the paragraph preceding theorem 1 of I. Any further notation will be defined as and when needed.

We recall that $E_i^{(2)}(|\Psi\rangle)$ in our notation denotes the Hylleraas functional for the ith excited state. We know from theorem 1 of I that its value, which is stationary for an arbitrary variation in the trial ket, is the exact second-order correction to the eigenvalue and the corresponding ket is the exact first-order correction ket. In other words, as

$$|\Psi\rangle \to |\Phi_i^{(1)}\rangle, \qquad (E_i^{(2)} - \epsilon_i^{(2)}) \to 0. \tag{1}$$

We define a ket $|\gamma(|\Psi\rangle)\rangle$ depending on the trial ket $|\Psi\rangle$ as follows:

$$|\gamma(|\Psi\rangle)\rangle = (\hat{H}_0 - \epsilon_i^{(0)})|\Psi\rangle + (\hat{H}_1 - \epsilon_i^{(1)})|\Phi_i^{(0)}\rangle. \tag{2}$$

It is obvious that the norm of $|\gamma(|\Psi\rangle)\rangle$, which we shall denote by $\|\gamma(|\Psi\rangle)\|$, is another functional whose absolute minimum corresponds to the exact first-order correction ket; in other words, as

$$|\Psi\rangle \to |\Phi_i^{(1)}\rangle, \qquad \|\gamma(\Psi\rangle)\| \to 0. \tag{3}$$

The Hylleraas functional for the ith excited state (provided that i is finite) was shown in I to be related to a convenient upper bound to the second-order correction to the eigenvalue. Since the norm is necessarily non-negative, by subtracting a suitable multiple of $\|\gamma(|\Psi\rangle)\|$ from the upper bound one can always get a lower bound. Relations (1) and (3) indicate that the deviation of the Hylleraas functional from the second-order correction could be related to the square of the norm of $|\gamma(|\Psi\rangle)\rangle$. If this is so, it should be possible to find the lowest value of α for which we can say with certainty that

$$B_i^{(2)}(|\Psi\rangle) = E_i^{(2)}(|\Psi\rangle) - \alpha\|\gamma(|\Psi\rangle)\|^2 \leqslant \epsilon_i^{(2)}. \tag{4}$$

Using the expansion defined in equation (3) of I for $|\Psi\rangle$ it is easy to derive that

$$\|\gamma(|\Psi\rangle)\|^2 = \mathop{\mathrm{S}}' (\epsilon_n^{(0)} - \epsilon_i^{(0)})^2 \left(\left|a_n + \frac{\langle\Phi_n^{(0)}|\hat{H}_1|\Phi_i^{(0)}\rangle}{\epsilon_n^{(0)} - \epsilon_i^{(0)}}\right|^2\right). \tag{5}$$

We recall from I that

$$E_i^{(2)}(|\Psi\rangle) - \epsilon_i^{(2)} = \mathop{\mathrm{S}}'(\epsilon_n^{(0)} - \epsilon_i^{(0)}) \left(\left|a_n + \frac{\langle\Phi_n^{(0)}|\hat{H}_1|\Phi_i^{(0)}\rangle}{\epsilon_n^{(0)} - \epsilon_i^{(0)}}\right|^2\right). \tag{6}$$

A comparison of equations (5) and (6) and a moment's reflection makes it evident that the desired value of α is given by

$$\alpha = \frac{1}{\epsilon_{i+1}^{(0)} - \epsilon_i^{(0)}}. \tag{7}$$

For this value of α, $B_i^{(2)}(|\Psi\rangle)$ is a lower bound to $\epsilon_i^{(2)}$, even though it is not possible to assert that $E_i^{(2)}(|\Psi\rangle)$ is an upper bound. Derivation of a rigorous upper bound from

$E_i^{(2)}(|\Psi\rangle)$ requires the addition of some further terms (see I). The calculation of the very same extra terms makes it possible to find a better lower bound. It is easy to derive that

$$\epsilon_i^{(2)} \geqslant B_i^{(2)}(|\Psi\rangle) + \sum_{n<i} (\epsilon_i^{(0)} - \epsilon_n^{(0)}) \left(\frac{\epsilon_{i+1}^{(0)} - \epsilon_n^{(0)}}{\epsilon_{i+1}^{(0)} - \epsilon_i^{(0)}}\right) \times \left(\left|\frac{\langle\Phi_n^{(0)}|\hat{H}_1|\Phi_i^{(0)}\rangle}{\epsilon_n^{(0)} - \epsilon_i^{(0)}} + \langle\Phi_n^{(0)}|\Psi\rangle\right|^2\right) \geqslant B_i^{(2)}(|\Psi\rangle) \tag{8}$$

which is the desired final result. It is plainly obvious that if $|\Psi\rangle$ has the form prescribed by any of the corollaries of I, $B_i^{(2)}(|\Psi\rangle)$ itself becomes the better lower bound, for, under these prescribed restrictions, the terms under the summation sign in relation (8) all vanish identically.

It is interesting to note that for $i = 0$ we revert to the ground state and in the configuration space the two lower bounds of relation (8) both become identical with the lower bound derived by Robinson (1969) for the ground state and the configuration space using an entirely different approach and formalism. Our result is completely general and is valid for the ground state as well as the excited states and for any complete inner-product space.

Department of Mathematics,
Birkbeck College,
University of London

C. S. Sharma
3rd October 1968

Robinson, P. D., 1969, *J. Phys.* A (*Gen. Phys.*), [2], **2**, in the press.
Sharma, C. S., 1967, *Proc. Phys. Soc.*, **91**, 50–3.

J. PHYS. A (GEN. PHYS.), 1969, SER. 2, VOL. 2. PRINTED IN GREAT BRITAIN

Internal energy and gravitation

Abstract. A previous theory of the interaction of an ideal fluid with the gravitational field, as given by Rastall in 1968, is modified. It is now assumed that the natural internal energy per unit mass of the fluid is a function of the natural pressure and density.

In a recent paper (Rastall 1968, to be referred to as II) the interaction of an ideal fluid and a gravitational field was discussed. It was assumed in II, § 6, that $U_E(x)$, the proper internal energy per unit proper mass of the fluid at the point with coordinates x, is a function of the proper pressure $p(x)$ and the proper mass per unit proper volume $\rho(x)$, but is independent of the gravitational potential Φ. (The suffix E in U_E indicates that this quantity is measured in natural units, while the absence of a suffix on p and ρ means that they are measured in Φ_0 units, i.e. the units corresponding to one of the preferred charts of the theory.) We now think that this is not the most natural assumption. We still suppose that U_E is independent of Φ. This follows from the fundamental hypothesis that physical quantities measured in natural units are the same in the potential Φ as in the potential $\Phi + k$ for any constant k, and from the more special assumption† that $U_E(x)$ depends on Φ

† We exclude the possibility that U_E depends on the derivatives of Φ, which it may in strong gravitational fields.